

JA*F LEOBEN 2023

May 11-12, 2023

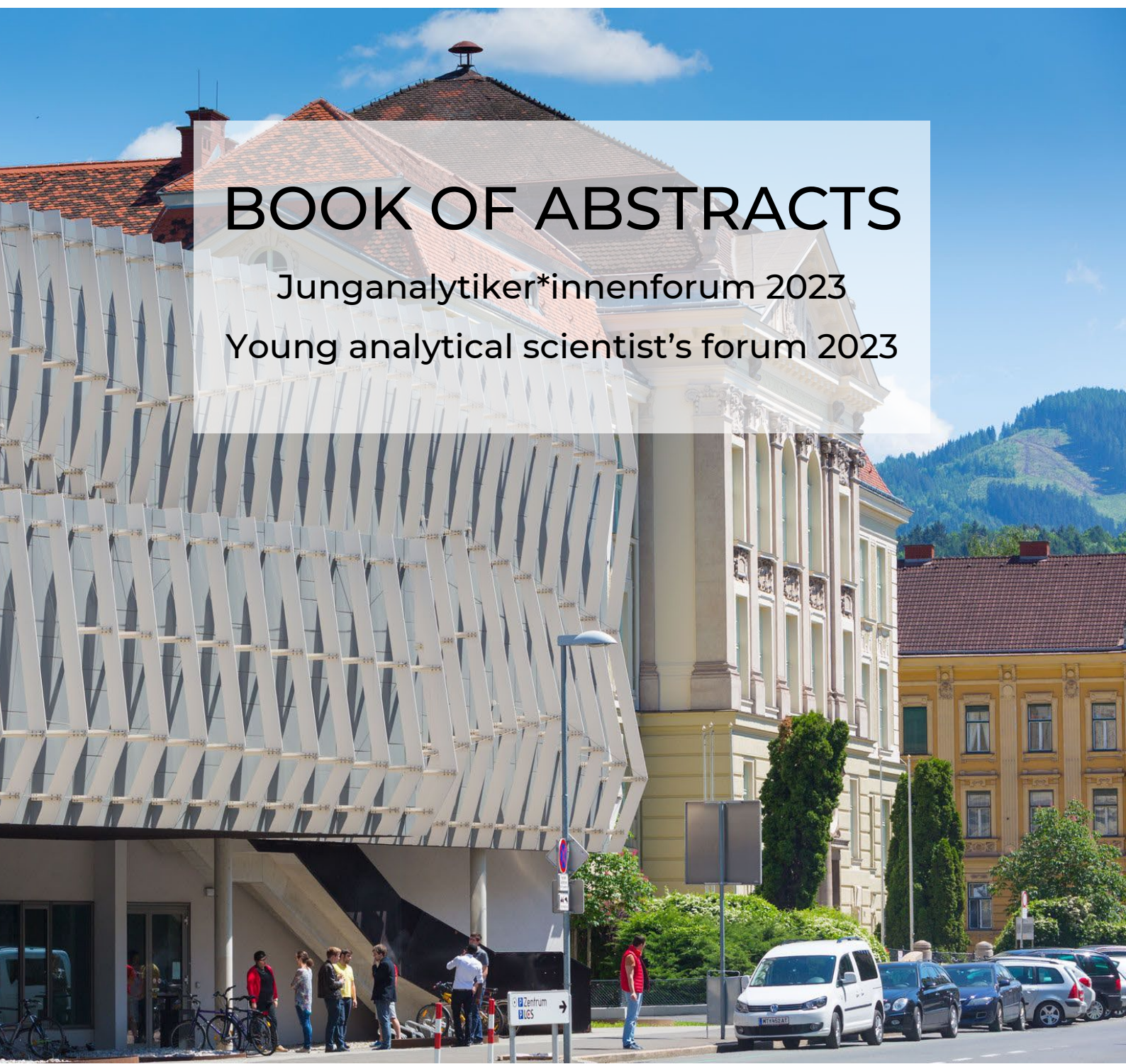
Montanuniversität Leoben, Austria



BOOK OF ABSTRACTS

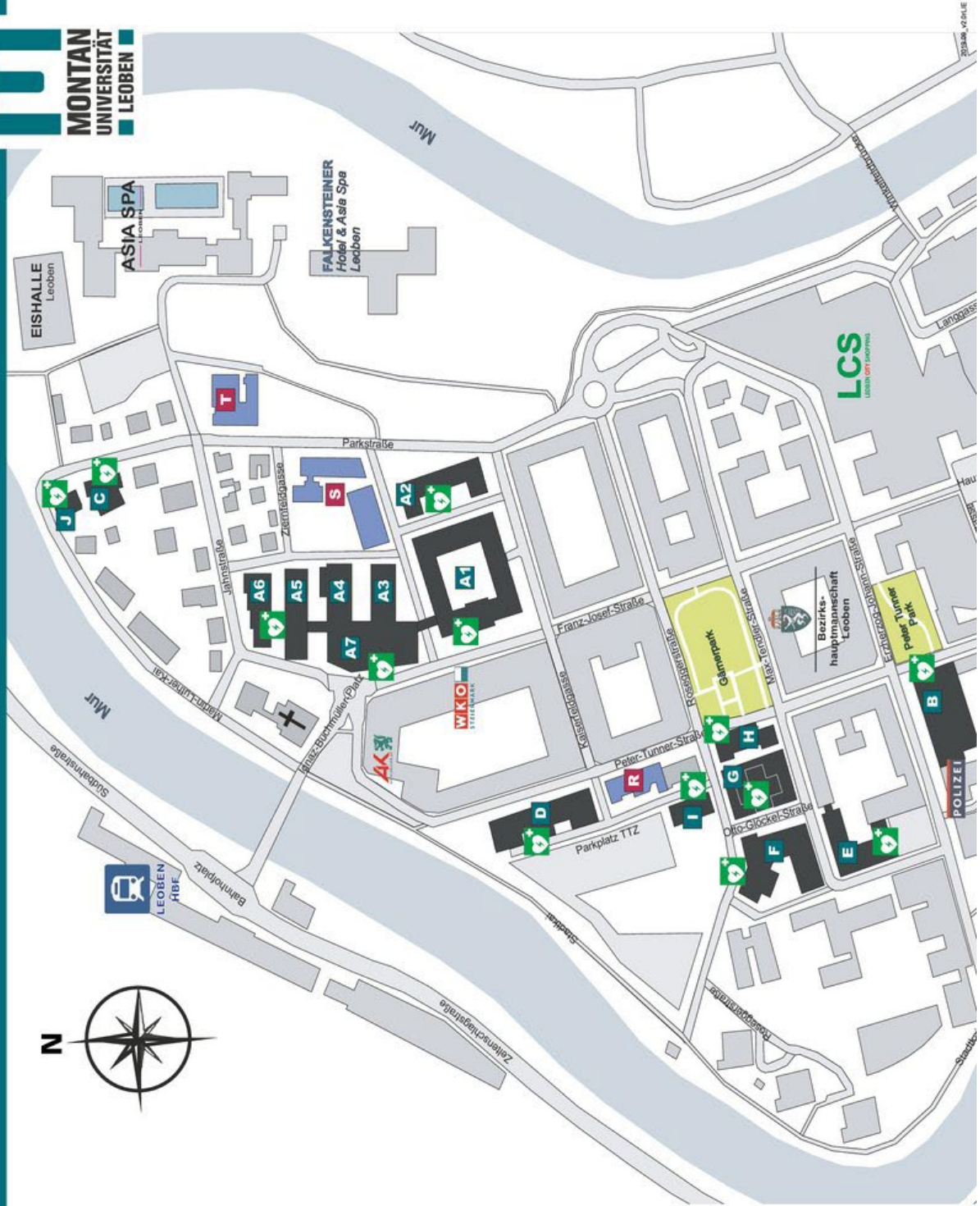
Junganalytiker*innenforum 2023

Young analytical scientist's forum 2023



Venue

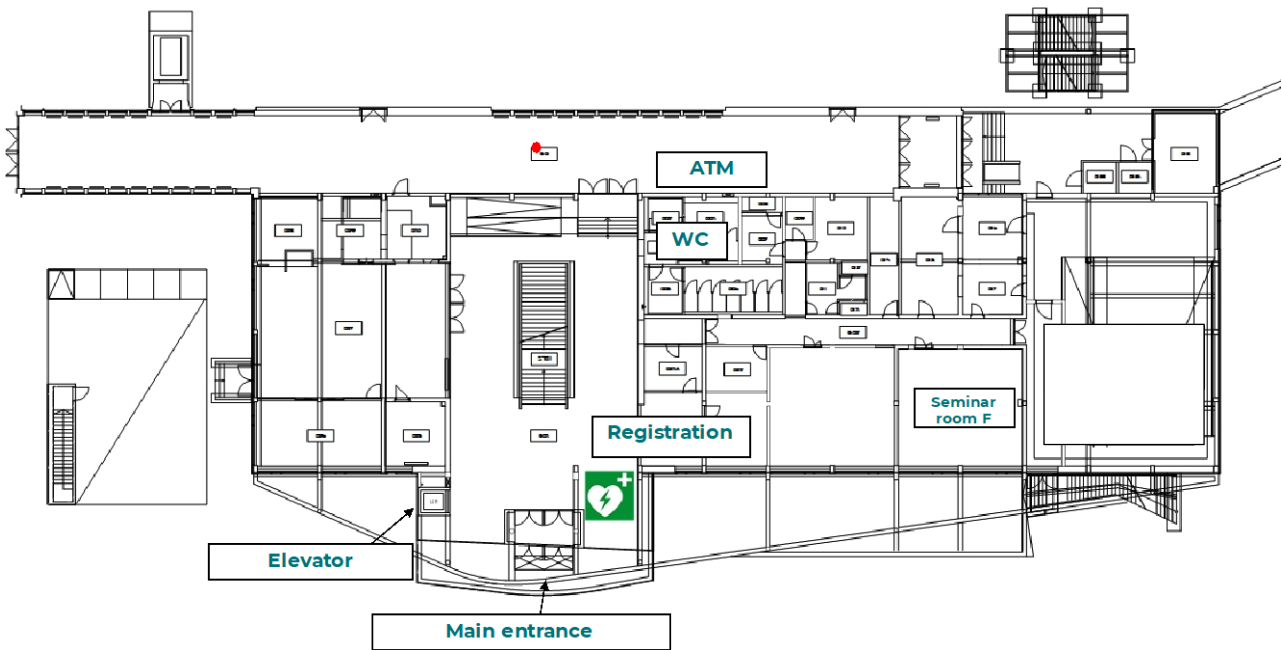
CAMPUS – Montanuniversität LEOBEN



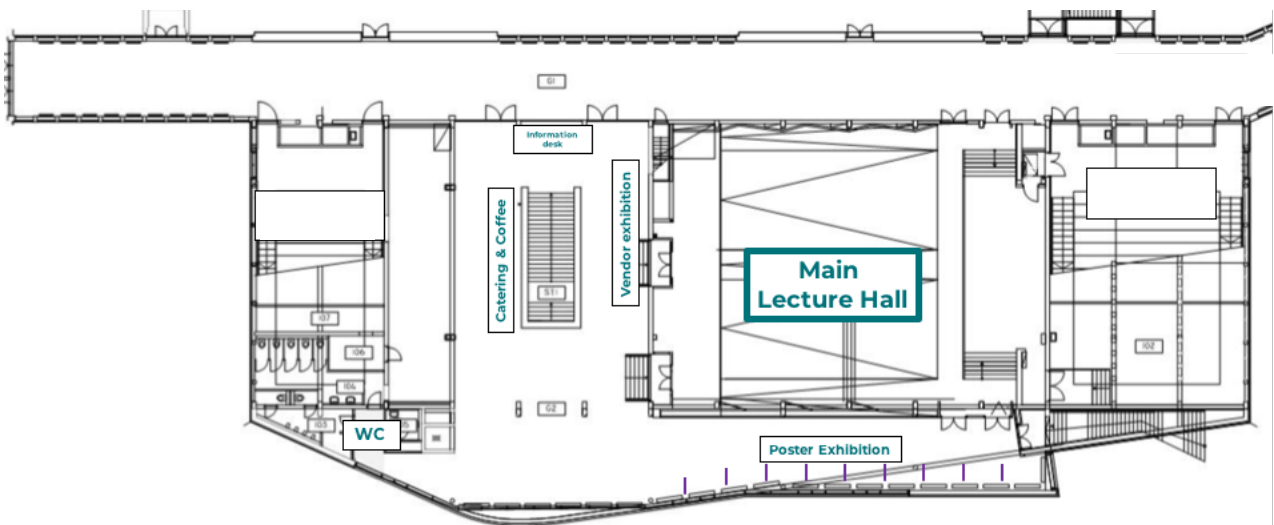
- A1** Hauptgebäude
- HG** - Franz-Josef-Straße 18
- A2** Rittingergebäude (RI)
- A3** Chemiegebäude (CH)
- A4** Umweltschutzgebäude (UM)
- A5** Metallurgebäude (ME)
- A6** Werkhallen (WH)
- A7** Erzherzog-Johann-Trakt (EJT - Hörsaalgebäude)
- B** Peter-Tunner-Gebäude
- 50** PTG - Peter-Tunner-Straße 5
- C** Petroleum Engineering
- 21** PE - Parkstraße 27
- D** Technologie-Transfer-Zentrum
- 30** TTZ - Peter-Tunner-Straße 25
- E** Rohstoff- und Werkstoffzentrum
- 40** RIZ - Erzherzog-Johann-Straße 3
- F** Impulszentrum für Rohstoffe
- 80** IZRW - Roseggerstraße 12
- G** Zentrum für Kunststofftechnik
- 71** KT - Otto-Glockel-Straße 2
- H** Akademie Montanuniversität Leoben
- 70** AMU - Peter-Tunner-Straße 15
- I** Impulszentrum für Rohstoffe
- 85** IZR - Roseggerstraße 11a
- J** Parkstraße 31
- 22** PS - Parkstraße 31
- R** Zentrum für angewandte Technologie Leoben GmbH
- ZAT** - Peter-Tunner-Straße 19
- S** Österreichisches Gießerei-Institut
- OGI** - Parkstraße 21
- T** Österreichische Akademie der Wissenschaften
- 10** AK - Jährlestraße 72
- Defibrillator Standorte**

Venue

Ground floor



First floor



General Information

Conference venue

Montanuniversität Leoben

Franz-Josef-Straße 18

8700 Leoben

Austria



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Conference webpage: <https://aach.unileoben.ac.at/veranstaltungen/tagung>

Registration hours

Thursday, 11.5., 8.30 am – 9.30 am

The registration desk can be found at the entrance of the university building.

If you arrive outside of opening hours, contact the conference team before the start of the conference and we will be happy to help.

Recordings

Photographs will be taken at this event. If you do not wish to be photographed or filmed, you can contact the photographer directly. The recording of lectures during the conference is not permitted.

Acknowledgements

Sponsors



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der Stadt



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Nascu**

Scientific Programme

Thursday, 11th of May

08:30-09:30	REGISTRATION & COFFEE Montanuniversität Leoben Franz-Josef-Strasse 18 8700 Leoben
09:30-9:45	WELCOME
9:45-10:15	AWARD LECTURE 1: Proteolytic Profiling of Streptococcal Pyrogenic Exotoxin B (SpeB) by Complementary HPLC-MS Approaches <i>Constantin Blöchl</i>
10:15-11:15	SESSION A: MATERIAL AND SURFACE SCIENCE
10:15-10:30	A.01 X-ray Photoelectron spectroscopy (XPS) – A powerful surface characterization technique <i>Christine Bandl</i>
10:30-10:45	A.02 Polyoleomics: Degradation products as quality markers for polyolefin recycling <i>Alexander Felgel-Farnholz</i>
10:45-11:00	A.03 Simultaneous Thermogravimetric Analysis and Near-infrared Reflection Spectroscopy for In Situ Monitoring of a Phenolic Resin Curing Reaction <i>Sebastian Friedl</i>
11:00-11:15	A.04 Development of diffusive gradients in thin films (DGT) combined with LA-ICP-MS for the in situ localization of aluminium corrosion <i>Gulnaz Mukhametzianova</i>
11:15-11:45	COFFEE BREAK
11:45-13:00	SESSION B: ENVIRONMENTAL AND FOOD ANALYSIS
11:45-12:00	B.01 Evaluation of the application potential of carbon produced by methane plasmalysis in agriculture <i>Nadine Abu Zahra</i>
12:00-12:15	B.02 Development of MC-ICP-MS based methods for Ni isotope analysis to study plant hyperaccumulation <i>Alexander Epov</i>
12:15-12:30	B.03 MURmap – Assessing the natural and anthropogenic impact in a historically contaminated river from (mining) industry <i>Ulrike Moser</i>
12:30-12:45	B.04 Spectroscopy and mass spectrometry for improving vinification and predictive modelling of wine quality <i>Pegah Mousazadehfazeli</i>
12:45-13:00	B.05 Identification of a novel arsenic compound in macrofungi as a potential step in the arsenic biotransformation pathways in the mycosphere <i>Martin Walenta</i>
13:00-14:00	LUNCH BREAK <i>Buffet (Mensa MU Leoben)</i>
14:00-14:30	AWARD LECTURE 2: Accurate Lipid Quantification- Challenges and Solutions <i>Harald Schöny</i>

Scientific Programme

14:30-15:00	PITCH SESSION <i>Company presentations, 5 min each</i>
15:00-15:30	COFFEE BREAK
15:30-16:15	SESSION C: LIQUID CHROMATOGRAPHY
15:30-15:45	C.01 Polyphenol Biomonitoring in Human Biofluids by LC-(HR)MS(/MS) <i>Ian Oesterle</i>
15:45-16:00	C.02 MetInclude: A User-Configurable Method for Constructing Optimized Inclusion Lists for Untargeted LC-HRMS/MS Measurements <i>Jonathan Matthew Samson</i>
16:00-16:15	C.03 Sweat of the Dead: Subcutaneous Extraction of Residual Biofluids for the Forensic Analysis of Deceased Individuals <i>Daniel Wasinger</i>
16:15-16:45	<u>INVITED LECTURE:</u> Hugo Bondy (1900-1985): His life and contribution to the development of mass spectrometry in the 20th century <i>Michael Schober</i>
16:45-18:15	POSTER SESSION
18:30-21:30	CONFERENCE DINNER <i>Weinlaube Schwarzer Hund, Hauptplatz 10, 8700 Leoben</i> <i>Sponsored by ESI</i>

Scientific Programme

Friday, 12 th of May	
08:15-09:15	GUIDED LAB TOURS <i>Chair of General and Analytical Chemistry Montanuniversität Leoben</i>
9:30-10:00	AWARD LECTURE 3: Determination of 48 elements in environmental samples by ICP-MS/MS with a focus on technology-critical elements <i>Simone Trimmel</i>
10:00-10:30	SESSION D: INFRARED SPECTROSCOPY
10:00-10:15	D.01 Unlocking New Insights: The Power of Optical Photothermal Infrared Spectroscopy in Chemical Analysis and Materials Research <i>Kristina Duswald</i>
10:15-10:30	D.02 Online Monitoring of Chemically-induced Unfolding and Refolding of β-Lactoglobulin by Laser-based Mid-Infrared Spectroscopy <i>Shilpa Vijayakumar</i>
10:30-11:00	COFFEE BREAK
11:00-12:00	SESSION E: METABOLOMICS/PROTEOMICS
11:00-11:15	E.01 Proteomics, metabolomics and molecular networking as tools for the identification of fungal RiPPs <i>Isabella Burger</i>
11:15-11:30	E.02 Metronidazole resistance in <i>Trichomonas vaginalis</i> <i>Anna-Lena Mayr</i>
11:30-11:45	E.03 Multilevel Omics-Readouts of in vitro Perturbation Studies are Determined by Memory Effects from Subculture <i>Lukas Skos</i>
11:45-12:00	E.04 Establishment of a Non-invasive Biomonitoring Assay Suitable for Children <i>Michael Wolf</i>
12:00-13:00	LUNCH BREAK <i>Buffet (GenussStube Leoben)</i>
13:00-14:00	SESSION F: METHODOLOGICAL ADVANCEMENTS
13:00-13:15	F.01 Optimization of A High-throughput SPE Clean-up for Urine and Plasma Exposomics <i>Yunyun Gu</i>
13:15-13:30	F.02 Quantum cascade laser based vibrational circular dichroism and its potential for chiral monitoring <i>Daniel-Ralph Hermann</i>
13:30-13:45	F.03 Development of a negative-thermal gradient GC for fast gas chromatography and its application for the study of volatile products formed in lithium-ion batteries <i>Bernhard Klampfl</i>
13:45-14:00	F.04 Optimizing high-throughput sample preparation of volumetric absorptive microsampling (VAMS) for targeted LC-MS metabolomics <i>Bruno Stelzer</i>

Scientific Programme

14:00-14:30	BREAK
14:30-15:00	AWARD CEREMONY
15:00-15:15	CLOSING & FAREWELL
15:15-16:45	EXCURSION WITH "SOPHIE THE GUIDE" <i>Guided sightseeing tour through Leoben</i>

Abstracts

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11:00-11:15	A.04 Development of diffusive gradients in thin films (DGT) combined with LA-ICP-MS for the in situ localization of aluminium corrosion <i>Gulnaz Mukhametzianova</i>

Abstracts

AWARD LECTURE 1

Proteolytic Profiling of Streptococcal Pyrogenic Exotoxin B (SpeB) by Complementary HPLC-MS Approaches

Constantin Blöchl* (1), Christoph Holzner (1), Michela Luciano (1, 2), Renate Bauer (1), Jutta Horejs-Hoeck (1, 2), Ulrich Eckhard (1, 3), Hans Brandstetter (1, 2) and Christian G. Huber (1, 2)

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(2) Cancer Cluster Salzburg, Department of Biosciences, University of Salzburg, Hellbrunner Strasse 34, 5020 Salzburg, Austria

(3) Department of Structural Biology, Molecular Biology Institute of Barcelona, CSIC, Barcelona Science Park, Baldiri Reixac, 15-21, 08028 Barcelona, Spain

Streptococcal pyrogenic exotoxin B (SpeB) is a cysteine protease expressed during group A streptococcal infection in humans and represents a major virulence factor. Although subject to several studies, its role during infection is still under debate, and its proteolytic properties remain insufficiently characterized. Here, we investigated this intriguing protease through a set of complementary approaches relying on state-of-the-art HPLC-MS methods.

To characterize SpeB's amino acid specificity, proteome-derived peptide libraries in combination with stable isotope-labeling were employed. Potential *in vivo* substrates were identified in relevant biological matrices, i.e., human plasma and monocytic secretomes, by N-terminomics followed by verification of selected targets. Investigated peptide libraries revealed a strong preference for hydrophobic and aromatic residues at the P2 site of the cleavage alongside negatively charged amino acids at the P3' to P6' sites. N-terminomics corroborated this specificity, besides identifying more than 200 substrates including proteins of the extracellular matrix, proteins of the immune system, and proteins involved in inflammation. As IgG antibodies were suggested as a potential substrate, we investigated proteolysis of purified IgG in detail by subunit analysis revealing several cleavage sites in the unstructured inter-domain regions.

This study portrays the proteolytic properties of SpeB and provides a library of potential host substrates as a valuable source for further research to unravel the role of SpeB during streptococcal infection.

Abstracts

TALK A.01

X-ray Photoelectron spectroscopy (XPS) – A powerful surface characterization technique

Christine Bandl* (1)

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Surfaces and interfaces gain increasing importance in the field of applied sciences and industrial applications. Surface properties differ distinctly from those of the bulk and can be tailored by physical or chemical surface modification. Some examples include the control of wettability and adhesive properties as well as the generation of binding sites or reactive groups and the immobilization of proteins at surfaces.

In order to understand surface chemistry and investigate the efficacy of surface engineering, surface analysis techniques are indispensable. X-ray Photoelectron spectroscopy (XPS) is a powerful and surface sensitive characterization method, which allows for the qualitative as well as the quantitative analysis of the chemical composition within the top 1-10 nm of the investigated surface. More precisely, with this technique information about elemental composition as well as the chemical and electronic state of the atoms at the surface of a material can be obtained. Therefore, solid samples are irradiated with an x-ray beam, which causes the ejection of core level electrons originating from the first few nanometers of the investigated material. The kinetic energy E_k of the emitted electrons is analyzed by the electron spectrometer. Since E_k is directly related to the binding energy E_B , the obtained data are presented as the intensity over a range of binding energies in the resulting XPS spectrum. Peak position and intensities allow for identification (via E_B) and quantification (integrals) of the elements present at the sample surface. Besides simple point analysis, also line and area scans can be measured. Moreover, depth profiles allow to investigate the cross-sectional composition of layered samples by repeated cycles of surface analysis and ion sputtering. [1,2]

In addition to a short overview about the functional principle of XPS, this contribution presents selected examples of surface analysis to provide a practical understanding of this technique. These examples include the XPS analysis of an anti-adhesive coating based on perfluorinated organosilanes, the proof for the immobilization of new Ge-based photoinitiators as well as the investigation of the oxidation of inorganic substrates along surface activation with plasma-based pretreatment techniques.

[1] J. F. Watts, J. Wolstenholme, An Introduction to Surface Analysis by XPS and AES, Wiley, 2. Edition, 2020, ISBN 9781119417583

[2] <https://www.thermofisher.com/at/en/home/materials-science/xps-technology.html>, date of access 12th of April 2023

Abstracts

TALK A.02

Polyoleomics: Degradation products as quality markers for polyolefin recycling

Alexander Felgel-Farnholz: alexander.felgel-farnholz@jku.at (1), Christian Klampfl (1), Jörg Fischer (2)

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(2) Institute of Polymeric Materials and Testing, JKU, 4040, Linz, Austria

Polymer recycling became more and more important, partially due to more rigid regulations by the European Union, enforcing higher recycling contingents. Mechanical recycling is one of the most common technologies and relies on sorting, pretreatment and remelting of plastics waste. The addition of virgin material as well as polymer stabilizers is beneficial for the material properties of the recyclate and for protection from further degradation. Polymer degradation is a rather complex process depending on various factors including mechanical stress, type of polymer, oxygen content, etc.. The source of the recyclate (i.e. the “former life” of the material) may also be a factor influencing the degree of polymer degradation. So, food-packaging material is less affected than plastic sheets from agriculture with extended outdoor use under direct UV light. Both the degree of degradation and the content of (remaining) stabilizers are of vital interest. Repeated processing/recycling steps require further addition of stabilizers, which are also consumed during production processes. This leads to the presence of increasing amounts of various degradation products from both, the polymer and the stabilizers, throughout the recyclates lifetime. Polyoleomics proposes the use of degradation products as quality markers throughout the lifecycle of polyolefins. This could allow a proper estimation of the degree of degradation of the recyclate, the amount of virgin material added as well as the addition of stabilizers during the different processing steps. In our study, different types of commercially available recyclates were extracted (via dissolution followed by precipitation) and analyzed by HPLC-qTOF-MS. Degradation of both the polymer and two of the most common antioxidants (Irgafos168 and Irganox1010) were investigated by reprocessing polyolefins via extrusion and injection molding under laboratory conditions. Degradation products were searched via analysis-of-variance (ANOVA) and tentative identification was done with MS/MS to build up a database for targeted analysis. This approach was successfully tested on various recyclates mixed with increasing amounts of virgin material under lab conditions. The final step were virgin-recyclate-mixtures (with differing ratios) directly obtained from local manufacturers. Several quality markers were repeatedly found within the different samples and allowed proper differentiation via principal component analysis (PCA) of mixtures with a different content of virgin material added.

Abstracts

TALK A.03

Simultaneous Thermogravimetric Analysis and Near-infrared Reflection Spectroscopy for In-Situ Monitoring of a Phenolic Resin Curing Reaction.

Sebastian Friedl* (1), Robert Zimmerleiter (1), Jovana Kovacevic (2), Daniel Lager (2), Tilman Barz (2), Gerhard Leitner (3), Eduard Pleschutzgig (3), Moritz Mitterbauer (3), Markus Brandstetter (1)

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(1) Research Center for Non-Destructive Testing GmbH / IR and Raman Spectroscopy, 4040 Linz, Austria

(2) Austrian Institute of Technology GmbH, Center For Energy, 1210 Vienna, Austria

(3) Fundermax GmbH, 2355 Wiener Neudorf, Austria

Phenolic resins are essential to produce high-quality laminated panels which are used as facade elements, furniture surfaces, flooring and worktops. To achieve such panels, several layers of resin-impregnated paper are pressed together at high temperature and pressure in a complex manufacturing process. Modern plants use natural gas-driven convection dryers in which the removal of free water and solvent and the curing takes place, causing significant energy consumption and CO₂ emissions. Driven by the increasing cost pressure and complexity of operations, it is important to be able to monitor the curing and drying process in-line and in real-time to ensure both product quality and energy efficiency.

Since the curing is a condensation reaction, the process can be monitored using thermogravimetric analysis (TGA). Normally TGA is combined with infrared spectroscopy to analyze the volatile materials evolving from the resin during processing. In this contribution, we present a novel approach using near-infrared (NIR) reflection measurements to acquire chemical information *directly* from the sample. For that purpose, a special NIR reflection probe was combined with a miniature NIR-spectrometer and halogen light source and inserted directly into the TGA-oven. Critical areas in the absorption spectra, which correspond to the absorption bands of water, methylol-groups, and aromatic C-H bonds were identified and further analyzed using Principal Component Analysis (PCA), revealing the change of the contribution of these absorption bands to the overall NIR spectral response in the sample as a function of time. The analysis of the NIR spectral data shows nice agreement with the simultaneously acquired TGA measurements, thus enabling deeper insights into the ongoing process in real-time, e.g., the degree of crosslinking of phenolic resins.

Abstracts

TALK A.04

Development of diffusive gradients in thin films (DGT) combined with LA-ICP-MS for the *in situ* localization of aluminium corrosion

Gulnaz Mukhametzianova (1)*, Stefan Wagner (1), Masoud Moshtaghi (1), Magdalena Eskinja (1), Gregor Mori (1), Thomas Prohaska (1)

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(1) Montanuniversität Leoben, Department of General, Analytical and Physical Chemistry, Chair of General and Analytical Chemistry, 8700 Leoben, Austria

Diffusive gradients in thin films (DGT) is a passive, non-destructive sampling technique that, in combination with LA-ICP-MS, has become a versatile tool for the two-dimensional (2D) visualization and quantification of chemical processes in aqueous systems. Yet, the extensive majority (>99 %) of DGT publications present environmental applications and, until now, there has been only one publication describing its application in materials and life sciences [1]. In this talk, the development of DGT LA-ICP-MS for the *in situ* localization of corrosion processes will be presented, focusing on pitting corrosion on the example of pure Aluminium (Al99.5) and AlCu alloy 2219 specimens. Studying of pitting corrosion is important since it initiates the formation of micro holes and cavities, which can damage structures by leakage or even can act as a starter for fatigue crack. Polyacrylamide- and polyurethane-based DGT binding gels with homogeneously distributed iminodiacetate (Chelex 100), TiO₂ (Metsorb), or ZrOH binding phases were applied to Al specimens exposed to NaCl solution ($w = 1.5 \%$, $\text{pH} = 4.5$, $T = 22 \text{ }^\circ\text{C}$). The DGT-Al99.5 setups were immersed for 24 h and 72 h, whereas DGT-Al2219 setups were immersed for 15 min and 80 min given their higher pitting corrosion susceptibility already after 15 min. The sampled element distribution on the DGT gels was visualized by LA-ICP-MS. Quantification was achieved by using matrix-matched DGT calibration standards with known analyte mass loadings. Chemical imaging was complemented by SEM/EDX of the metal surface. Results showed that the DGT LA-ICP-MS technique enabled the precise microscale (250 μm – 800 μm) localization of Al³⁺ and Zn²⁺ co-solubilization patterns, likely indicating pitting corrosion processes with Al³⁺ and Zn²⁺ flux maxima up to 50 $\text{pg cm}^{-2} \text{ s}^{-1}$ and 7 $\text{pg cm}^{-2} \text{ s}^{-1}$, respectively, following 15 min of Al2219 immersion in NaCl medium.

[1] S. Wagner et al., "In situ spatiotemporal solute imaging of metal corrosion on the example of magnesium," *Analytica Chimica Acta*, vol. 1212, p. 339910, 2022, doi: 10.1016/j.aca.2022.339910.

Abstracts

Thursday, 11th of May

11:45-13:00	SESSION B: ENVIRONMENTAL AND FOOD ANALYSIS
11:45-12:00	B.01 Evaluation of the application potential of carbon produced by methane plasmalysis in agriculture <i>Nadine Abu Zahra</i>
12:00-12:15	B.02 Development of MC-ICP-MS based methods for Ni isotope analysis to study plant hyperaccumulation <i>Alexander Epov</i>
12:15-12:30	B.03 MURmap – Assessing the natural and anthropogenic impact in a historically contaminated river from (mining) industry <i>Ulrike Moser</i>
12:30-12:45	B.04 Spectroscopy and mass spectrometry for improving vinification and predictive modelling of wine quality <i>Pegah Mousazadehfazeli</i>
12:45-13:00	B.05 Identification of a novel arsenic compound in macrofungi as a potential step in the arsenic biotransformation pathways in the mycosphere <i>Martin Walenta</i>

Abstracts

TALK B.01

Evaluation of the application potential of carbon produced by methane plasmalysis in agriculture

Nadine Abu-Zahra (1)*, Donata Bandoniene (1), Celia Fernández Balado (2), Veronika Kanzler (1), Rebecca Hood-Nowotny (2), Gerhard Soja (3), Robert Obenaus-Emler (4), Stefan Wagner (1), Markus Puschenreiter (2, 5), Thomas Prohaska (1)

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Hydrogen has become a major player in industry and energy transition. A recent approach to hydrogen production is methane pyrolysis e.g., by low temperature plasmas (plasmalysis). The thermal decomposition of methane splits CH_4 into gaseous hydrogen H_2 and solid carbon C. Thereby, the process generates carbon (carbon produced by methane plasmalysis, CMP), becoming an abundant side stream material. As the application of biochar to soils has been known for long time to improve soil properties, agriculture offers a promising application area for CMP. This study aims to characterize the chemical properties of CMP and evaluate its potential for agricultural applications using different experimental setups (i.e., greenhouse and field trials) and analytical techniques (e.g., ICP-MS, colorimetry). Maize (*Zea mays* L.) was used as a model crop in plant experiments. The effect of CMP on soil properties was assessed by analyzing plant-available nutrient fractions in soil using different chemical extraction methods [i.e., $\text{NH}_4\text{-N}$ and $\text{NO}_3\text{-N}$ by K_2SO_4 ($c = 0.5 \text{ mol L}^{-1}$), P and K by calcium acetate lactate (CAL), micronutrients by NH_4NO_3 ($c = 1 \text{ mol L}^{-1}$)]. Macro- and micronutrients in above-ground tissues of maize were analyzed by ICP-MS after microwave-based acid digestion. Finally, the effects of the treatment on physical and biological properties were assessed by determining water holding capacity and microbial activity. Results of the greenhouse trial showed that, depending on the soil type, maize dry biomass increased significantly ($p < 0.01$) from 1.2 g pot^{-1} in controls to 2.2 g pot^{-1} in soils amended with CMP at 25 g kg^{-1} . In the field trial, elevated CAL-extractable P levels in CMP-treated plots (90.4 mg kg^{-1}) as compared to controls (73.2 mg kg^{-1}) were observed ($p < 0.08$), likely indicating mobilization of plant-available P due to CMP addition to soil. These results demonstrate the potential of CMP for agricultural applications, potentially improving soil properties and plant growth, especially in soils with low nutrient availability.

Abstracts

TALK B.02

Development of MC-ICP-MS based methods for Ni isotope analysis to study plant hyperaccumulation

Alexander V. Epov* (1), Stepan M. Chernonozhkin (1), Markus Puschenreiter (2), Thomas Prohaska (1) and Johanna Irrgeher (1)

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(2) University of Natural Resources and Life Sciences, Institute of Soil Research, 3430 Tulln an der Donau, Austria

Hyperaccumulating plants accumulate trace metals often exceeding background levels of regular plants by factors of 10^3 . Ni hyperaccumulating plants were observed to be enriched in heavier Ni isotopes compared to underlying soil with $\Delta^{60}\text{Ni}/^{58}\text{Ni}_{\text{plant-soil}}$ up to +0.40 ‰. Studying Ni isotope fractionation between bedrock, soil and plant material may provide a powerful tool to further understand metal mobilisation processes in the rhizosphere. In this contribution, an analytical protocol consisting of sample digestion, Ni isolation and multi collector inductively coupled plasma mass spectrometry (MC-ICP-MS) was developed and evaluated to measure Ni isotope patterns in plant and soil digests, and soil extracts (representing total and bioavailable Ni in soil).

Soil and plant matrix digestion based on microwave-assisted decomposition using nitric, hydrochloric, and tetrafluoroboric acids was evaluated. An adapted two-step chromatographic separation protocol isolating Fe and Ni using Bio-Rad AG MP-1 and AG 1-X8 anion exchange resins was demonstrated to have quantitative recoveries as prerequisite to avoid isotope fractionation during sample preparation. We present a novel protocol for Ni isotopic measurement using a hexapole collision/reaction cell (CRC) MC-ICP-MS instrument (Nu Sapphire), which reduces spectral interferences by means of ion-molecule reactions. The use of CRC pressurised with H_2 and He removes the $^{40}\text{Ar}^{18}\text{O}^+$ interference on $m/z = 58$ (^{58}Fe and ^{58}Ni) as well as other matrix element based interfering species. However, challenges still arise to fully remove the $^{40}\text{Ar}^{16}\text{O}^1\text{H}^+$ interference on ^{57}Fe . $^{65}\text{Cu}/^{63}\text{Cu}$ was used to account for instrumental isotopic fractionation using the regression model. $\delta^{60}\text{Ni}/^{58}\text{Ni}$ values with an uncertainty down to 0.027 ‰ (1SD, $n = 8$) could be obtained. The validated method was further applied to a set of reference materials to demonstrate its applicability for the Ni hyperaccumulation studies.

Abstracts

TALK B.03

MURmap – Assessing the natural and anthropogenic impact in a historically contaminated river from (mining) industry

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The project MURmap combines multiple analytical methods based on Inductively Coupled Plasma Mass Spectrometry (ICP-MS) in all its facets to comprehensively characterize the Mur/Mura River catchment area and its impacts. Spatial element and isotope ratio distribution in water, suspended particulate matter and stream sediments were investigated on basis of three sampling campaigns along the river carried out in May 2022, August 2022 and February 2023. First results of multi-element (ICP-MS/MS, Perkin Elmer NexION 5000), single particle (ICP-MS, Agilent 8900, Agilent Technologies) and $^{87}\text{Sr}/^{86}\text{Sr}$ isotope ratio (MC-ICP-MS, Nu Plasma HR, Nu Instruments) analysis on filtered ($< 0.45 \mu\text{m}$) water samples provide insight into the geochemical background and on a possible anthropogenic impact. $^{87}\text{Sr}/^{86}\text{Sr}$ isotope ratios revealed e.g., metamorphic ($^{87}\text{Sr}/^{86}\text{Sr} = 0.70978\text{-}0.71101$) and carbonate ($^{87}\text{Sr}/^{86}\text{Sr} = 0.71018\text{-}0.71136$) host rock, respectively, in the upper part of the Mur valley. When entering the Neogene sedimentary basin of the Graz Paleozoic, a stable $^{87}\text{Sr}/^{86}\text{Sr}$ isotope ratio of 0.71066 to 0.71090 was observed towards the Slovenian-Croatian border. Ancient and recent mining activities are evident by single element hot spots. For example, in Rotgüldenbach in the upper part of the Mur River catchment, where As was mined from the 14th to the 19th century, mass fraction of As reaches $w(\text{As}) = 32 \text{ ng g}^{-1}$ compared to a baseline mass fraction range of $w(\text{As}) = 1.12 \text{ to } 1.56 \text{ ng g}^{-1}$ along the Mur River. Another hotspot, likely caused by the use of Gd as a contrast agent in medical treatments, has resulted in a significant positive Gd anomaly nearby larger cities of up to 91% contribution of anthropogenic Gd to total Gd.

Abstracts

TALK B.04

Spectroscopy and mass spectrometry for improving vinification and predictive modelling of wine quality

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Wine is a popular alcoholic beverage that has been consumed for thousands of years. The quality of wine is determined by a wide range of factors, such as grape variety, soil type, climate, winemaking techniques, and aging processes. These factors contribute in varying degrees to the unique flavor, aroma, and texture of each wine, giving it a distinct character and identity. Wine quality evaluation is a complex process that involves sensory and chemical analysis. Sensory analysis directly assesses the organoleptic properties of wine, such as appearance, aroma, flavor, and mouthfeel. In contrast, chemical analysis provides objective data for various chemical components including primary metabolites (e.g., sugars, and organic acids) and secondary metabolites (e.g., phenolic compounds, terpenes, and volatile organic compounds) present in wine.

In our study, we are evaluating the chemical composition of Viennese Grüner Veltliner wine from different winemaking processes by applying microbial, sensory, non-targeted, and targeted metabolomic approaches using liquid- and gas chromatography-mass spectrometry (LC-MS & GC-MS). Moreover, multivariate statistical data analysis such as principal component analysis (PCA) and partial least squares regression (PLS) are used to correlate the metabolomic profiles with the sensory and microbiological attributes of the wine. Finally, the newly developed micro-electromechanical system (MEMS)-based NIR and Raman for rapid analysis of specific physicochemical parameters (e.g., alcohol, density, sugars) in wine are also under evaluation. White wine samples were analyzed using both reference and spectrometric methods and several PLS calibration models were developed. Both techniques presented similar results for the assessment of alcohol strength and relative density ($R_p^2 > 0.80$, RMSEP < 0.18). Raman showed better performance for the measurement of volatile acidity ($R_p^2 = 0.95$, RMSEP = 0.04), malic acid ($R_p^2 = 0.90$, RMSEP = 0.31), and glycerol ($R_p^2 = 0.96$, RMSEP = 0.27).

Abstracts

TALK B.05

Identification of a novel arsenic compound in macrofungi as a potential step in the arsenic biotransformation pathways in the mycosphere

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Many of different arsenic species can be found in the environment and usually it is very clear which arsenic species will presumably be detected in a terrestrial or a marine sample. But it is still unpredictable which arsenic compound is contained in a macrofungal species which had not been investigated for As species before. Some of them mainly contain arsenobetaine (AB), dimethylarsinic acid or inorganic arsenic, while others have a fairly even distribution over many arsenic species and even several unidentified ones. [1] In the presented work we aim to identify a new arsenic species, which can be found in traces in the edible *Boletus edulis* (porcini), the edible *Macrolepiota procera* (parasol), the famous *Amanita muscaria* (fly agaric) [2] and also in *Ramaria sanguinea* (a coral mushroom). The *R. sanguinea* sample analyzed had a total arsenic concentration of around 17 mg As/kg dry mass, and ~80% of the arsenic could be extracted with water. With a cation exchange column and a HPLC-ICPMS setup the unknown species was separated from other arsenic species and was found to make up ~10 % of the total arsenic of the sample. In the *B. edulis* and *A. muscaria* it only accounted for around 1 % (10 and 15 µg As/kg dm) of the total arsenic. From the *R. sanguinea* sample, HPLC fractions containing the unknown species were pooled and enriched by lyophilization. When analyzing the enriched fraction with HPLC-ESI-TOF-MS, a peak with a m/z of 178.021, which would match with a sum formula of $C_5H_{13}AsNO^+$ was detected. Since it has a similar fragmentation pattern to the well-known AB, we hypothesize that the compound's structure is an analogue of AB with a primary amide group. For verification, we are currently working on the synthesis of the pure compound, which will then be characterized and spiked to crude mushroom extracts.

[1] S. Braeuer, W. Goessler (2019) Arsenic species in mushrooms, with a focus on analytical methods for their determination - A critical review. *Analytica Chimica Acta* **1073**, 1-21.

[1] D. Kuehnelt, W. Goessler, K. J. Irgolic (1997) Arsenic Compounds in Terrestrial Organisms II: Arsenocholine in the Mushroom *Amanita muscaria*. *Applied Organometallic Chemistry* **11(6)**, 459-470.

Abstracts

Thursday, 11th of May

14:00-14:30	AWARD LECTURE 2: Accurate Lipid Quantification- Challenges and Solutions <i>Harald Schöny</i>
15:30-16:15	SESSION C: LIQUID CHROMATOGRAPHY
15:30-15:45	C.01 Polyphenol Biomonitoring in Human Biofluids by LC-(HR)MS(/MS) <i>Ian Oesterle</i>
15:45-16:00	C.02 MetInclude: A User-Configurable Method for Constructing Optimized Inclusion Lists for Untargeted LC-HRMS/MS Measurements <i>Jonathan Matthew Samson</i>
16:00-16:15	C.03 Sweat of the Dead: Subcutaneous Extraction of Residual Biofluids for the Forensic Analysis of Deceased Individuals <i>Daniel Wasinger</i>
16:15-16:45	INVITED LECTURE: Hugo Bondy (1900-1985): His life and contribution to the development of mass spectrometry in the 20th century <i>Michael Schober</i>

Abstracts

AWARD LECTURE 2

Accurate Lipid Quantification- Challenges and Solutions

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Guidelines establish standards for how to perform accurate, absolute quantification by MS (eg. Bioanalytical Method Validation Guidance for Industry, FDA, USA), but in the application of omics-type measurement, these metrologically stringent rules and standards can only be partially fulfilled. The vast number of analytes within one measurement or the fact that an analyte-free matrix cannot be produced when all substances in a sample are also analytes contradict the recommended guidelines. Therefore, at least best practice methods are needed to ensure quality.

The special nature of lipids with structural templates within each lipid class enables the use of single surrogate internal standards (ISTD) for all members of the same lipid class, drastically reducing the amount of needed ISTD. However, differences in extraction-, ionization- and fragmentation efficiency need to be considered especially when MS is combined with chromatographic separation.

With the introduction of lipidome isotope labeling of yeast (LILY) (Analyst, 2017, 142, 1891) a useful tool for internal standardized external calibration is available. The fully ¹³C-labeled yeast lipidome with over 250 labeled lipids has been successfully applied to quantify human plasma via a combined flow injection/reversed-phase chromatography-high resolution mass spectrometry workflow (Analyst 2021, 146, 2591). The workflow in combination with the LILY lipid panel enables simultaneous quantification via (1) external multi-point calibration internally standardized and (2) internal one-point calibration with LILY as a surrogate ISTD, increasing coverage while keeping accuracy and throughput high. Additionally, due to the independence of the quantitative values from common deuterated or non-endogenous ISTDs, the novel workflow offers cross-validation of different organic MS-based lipid methods.

As this is crucial for all workflows, especially as certified reference materials are not yet available for global lipidomics workflows, we have further investigated cross-platform validation for shotgun and LC-MS-based lipidomics approaches (Anal. Chem., 2022, 94, 3, 1618–1625). This increases accuracy and can be applied fully traceably when phospholipids are quantified on a lipid class level with nuclear magnetic resonance (NMR) or inductively coupled plasma (ICP)-MS. Applied on yeast, this enables the production of suitable long-term system quality controls and further paves the way for quantitative lipidomics studies to support standardization and harmonization in the field.

Abstracts

TALK C.01

Polyphenol Biomonitoring in Human Biofluids by LC-(HR)MS(/MS)

Ian Oesterle* (1,2,3), Sabrina Berger (1), Kola Ayeni (1), Annette Rompel (2), and Benedikt Warth (1)

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Phytochemicals, such as polyphenols, exhibit various bioactive properties, e.g. acting as antioxidants or anti-inflammatory agents. Due to their high prevalence in plant-based foods, they have the potential to be used as supplements to influence human health and assist in personalized medicine. However, studying human exposure to polyphenols is not straightforward due to the numerous parent molecules that undergo a variety of biotransformation processes yielding a plethora of metabolites, especially phase II conjugated. Thus, in order to comprehensively study polyphenols exposure in humans, a combination of targeted LC-MS/MS and untargeted LC-HRMS approaches need to be used.

Both of these LC-MS approaches were applied in this work to investigate polyphenol exposure in infant-mother pairs from Nigeria, and observe the influence of supplementing breast-feeding with real food. Firstly, a validated targeted UHPLC-ESI-MS/MS method for 90 polyphenol standards of various classes was adapted and used to quantify these polyphenols in human breast milk. Secondly, a developed non-targeted analysis and suspect screening workflow was applied to human breast milk and corresponding baby samples to see the different polyphenols and their respective metabolites present, as well as the change over time. This will allow to better characterize the transfer of polyphenols from mothers to infants, but also the impact on the development of the gut microbiome.

Abstracts

TALK C.02

MetInclude: A User-Configurable Method for Constructing Optimized Inclusion Lists for Untargeted LC-HRMS/MS Measurements

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Data-dependent acquisition (DDA) methods use intensity values for the selection of LC-HRMS/MS precursor ions. Thus, biochemical sample constituents are often excluded due to the presence of mass peaks that represent high background signals. This can limit the number of biologically relevant samples selected for fragmentation.

We present MetInclude, an XCMS-based data-set dependent acquisition (DsDA) method that generates globally optimized inclusion lists from LC-HRMS chromatograms. Background subtraction is included during the run, and peaks are only kept if they are the monoisotopic form in a feature with ¹³C isotopologues. Adducts and in-source fragments can be removed based on the user's request. Relative signal intensity is used to split the remaining features into separate inclusion lists. Loop count will be determined by the user, and if the number of coeluting features exceeds this count for a sample, additional inclusion lists for the same sample will be created. MassHunter- and Xcalibur-based instruments can immediately use the inclusion lists generated by MetInclude; a generic list is also provided so the user can format it for any other software.

Utilizing peak-picking and the further filtering steps, MetInclude has the ability to cover more than 90% of truly biologically-derived features while minimizing false-positives. It also improves on DDA by allowing for coverage of a feature's entire chromatographic peak instead of one or few scans per peak, providing the user with as much fragmentation information as possible.

Abstracts

TALK C.03

Sweat of the Dead: Subcutaneous Extraction of Residual Biofluids for the Forensic Analysis of Deceased Individuals

D. Wasinger^{1,2}; M. Wolf^{1,2}; E. Deal¹; A. Bileck^{1,3}; K. Stolz⁴; S. M. Meier-Menches^{1,3,5}; F. Kanz⁴; C. Gerner^{1,3}

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In forensic science, investigations through toxicological examination of cadavers to answer questions of potentially criminal context is of great importance. Despite high demand for precise analytical tools to determine evidence of drug abuse or exact time of death, forensic analysis in this area remains challenging, mainly because of the difficulty involved with sample collection. Currently, sampling is costly, requiring trained personnel and specialized equipment.

Here, we present a novel method for simple and quick analysis for drugs of abuse, using subcutaneous extracts of the skin of deceased individuals. The method was adapted from a previously established procedure for metabolic phenotyping. In a pilot study with forensic partners, the hands and feet of a cohort of 94 cadavers, implicated in the use of illicit drugs, were sampled. After sample processing, the samples were analyzed using ultra-high-performance liquid chromatography coupled with high-resolution tandem mass spectrometry.

Data analysis revealed the presence of various drugs of abuse in the extracts of all samples, including cocaine, heroin, methamphetamine, fentanyl, and MDMA. These findings were independently confirmed by classical toxicological screening, revealing an overlap of over 80% for the two approaches. Furthermore, our untargeted assay also succeeded in the identification of various metabolites not covered by classical toxicology, with the potential to further investigate the biochemical status ante-mortem. For example, the endogenous metabolite hypoxanthine, a known marker for oxidative stress and hypoxia.

Remarkably, this assay represents a cheap and fast alternative for initial toxicological screening, open to be certified in the future.

Abstracts

INVITED LECTURE

Hugo Bondy (1900-1985): His life and contribution to the development of mass spectrometry in the 20th century

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The development of mass spectrometry fundamentally revolutionized analytical chemistry in the 20th century. Richard Herzog and Josef Mattauch conducted research in the field of double-focusing sector-field mass spectrometry and developed together a geometry in 1934, which is still used in science to this day. Nevertheless, the first double-focusing mass spectrometer was constructed by Hugo Bondy and his colleagues from the University of Vienna in 1933, after the theoretical considerations of Walter Bartky and Arthur Jeffrey Dempster. This Austrian scientific contribution was forgotten due to the later works of Herzog and Mattauch.

The aim of this talk is to present the origin and development of the first double-focusing mass spectrometer as well as the biography of its constructor in the historical context of the time. To reconstruct the historical events a critical-scientific research was conducted in Austrian archives and libraries as well as an evaluation of scientific literature from the designer was performed. The focus of the presentation was on the functionality and principle of the apparatus, and on the biography of Hugo Bondy with his expulsion from science and prosecution because of his Jewish descend.

The scientific contribution of Bondy and his colleagues gives the opportunity to rediscover and understand an original design of a mass spectrometer. Furthermore, the biography of Hugo Bondy brings insights into the extraordinary situation of a persecuted scientist in Austria during the 20th century. Both aspects together illustrate the mechanisms of scientific discoveries and persecution within a research community in this time period.

Abstracts

Friday, 12 th of May	
9:30-10:00	AWARD LECTURE 3: Determination of 48 elements in environmental samples by ICP-MS/MS with a focus on technology-critical elements <i>Simone Trimmel</i>
10:00-10:30	SESSION D: INFRARED SPECTROSCOPY
10:00-10:15	D.01 Unlocking New Insights: The Power of Optical Photothermal Infrared Spectroscopy in Chemical Analysis and Materials Research <i>Kristina Duswald</i>
10:15-10:30	D.02 Online Monitoring of Chemically-induced Unfolding and Refolding of β-Lactoglobulin by Laser-based Mid-Infrared Spectroscopy <i>Shilpa Vijayakumar</i>

Abstracts

AWARD LECTURE 3

Determination of 48 elements in environmental samples by ICP-MS/MS with a focus on technology-critical elements

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Technology-critical elements (TCEs) are a non-uniformly defined group of elements which are deemed indispensable in the development of high-tech applications across various fields, such as information, telecommunication and energy technology, semiconductors, alloys or catalysts. Their increased use during the last couple of decades is expected to result in elevated levels in the environment. The FWF-funded project TecEUS (P 33099-N; www.teceus.at) investigates the occurrence of TCEs in the environment with a special interest on plant samples from urban greening. However, the low levels of these elements remain an analytical challenge.

Seven plant certified reference materials (NIST SRM1515 Apple Leaves, NIST SRM1547 Peach Leaves, BCR-129 Hay Powder, BCR-670 Aquatic Plant, GBW07603 Bush Twigs and Leaves, GBW10015 Spinach Leaves and NCS ZC73036a Green Tea) were analysed for their mass fractions of 48 elements by inductively coupled plasma tandem-mass spectrometry (ICP-MS/MS) with a particular focus on TCEs. The average bias relative to the certified values is $-1 \% \pm 13 \%$. The detection limits based on the procedural blanks range from 13 fg g^{-1} (Tb) to 52 ng g^{-1} (Ca). This talk presents the optimised measurement procedure and demonstrates its applicability with 292 leaf samples from green facades from Vienna. The data set provides so far unknown insights into the distribution of scarcely investigated elements within an urban environment, which can form a base for future studies on the identification of environmental TCE sources.

Abstracts

TALK D.01

Unlocking New Insights: The Power of Optical Photothermal Infrared Spectroscopy in Chemical Analysis and Materials Research

Kristina Duswald* (1), Alexander Ebner (1), Sebastian Friedl (1), Paul Gattinger (1), Verena Karl (1), Elisabeth Leiss-Holzinger (1), Robert Zimmerleiter (1), Ivan Zorin (1) and Markus Brandstetter (1)

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Infrared (IR) spectroscopy is a powerful analytical technique used to identify and characterize molecules based on their unique vibrational modes. In particular, hyperspectral imaging (HSI) is trending upward as it provides spatial information in addition to chemical information. HSI is widely employed, e.g. in material science, biology, and medicine. The recently developed optical photothermal infrared (O-PTIR) spectroscopy technique circumvents the diffraction limit of traditional IR-vibrational spectroscopy. This enables a spatial resolution of 500 nm, which is an order of magnitude better than in conventional IR spectroscopic imaging. Furthermore, this technique allows to obtain an IR spectrum and a Raman spectrum from each measurement spot simultaneously. This ensures that the measurement position is exactly the same for both IR and Raman spectrum. Since these two methods complement each other, the information content can be improved in addition to the excellent spatial resolution.

The spatial resolution achieved in the submicron regime facilitates new perspectives in materials research [1]. Experimental results of various applications will be presented: starting with biological and medical applications, followed by the investigation of smallest contaminations. O-PTIR spectroscopy enables the detection and characterization of submicron spots and structures that can not be detected with other analytical techniques. This enables more detailed, comprehensive and non-destructive analysis of chemical samples and surfaces, leading to a deeper understanding of their properties and behavior. O-PTIR spectroscopy further has the potential to improve the sensitivity and specificity of chemical analysis, especially for complex mixtures and heterogeneous samples.

[1] Sandt, C., & Borondics, F. (2023). Super-resolution infrared microspectroscopy reveals heterogeneous distribution of photosensitive lipids in human hair medulla. *Talanta*, 254, 124152.

Abstracts

TALK D.02

Online Monitoring of Chemically-induced Unfolding and Refolding of β -Lactoglobulin by Laser-based Mid-Infrared Spectroscopy

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Introduction

Mid-infrared (IR) spectroscopy is a versatile analytical technique that is sensitive to the secondary structure of proteins, which makes it especially suited to protein denaturation and interaction studies. A drawback in the study of proteins using mid-IR spectroscopy, however, is the high absorption of water that overlaps with the protein amide I band between 1600 -1700 cm^{-1} , which imposes a limit on the pathlengths that can be used to avoid total absorption. [4], [5]. Furthermore, this low employable path length poses a significant hindrance to high-throughput and flow-through measurements [6], due to the high propensity of the cell to be clogged by protein aggregates and viscous analytes. This problem can be combated by utilizing high-power light sources such as lasers, that enable the use of longer path lengths. The extended path lengths facilitate continuous flow through measurements without clogging.

Methods

In this work, the folding and unfolding of beta-lactoglobulin (β -LG) by chemical agents was studied using a commercially available laser-based mid-IR spectrometer. To this end, a titration between β -LG and two surfactants, sodium dodecyl sulfate (SDS) and octaethylene glycol monododecyl ether (C12E8) was performed, while continuously flowing the solution through a custom-made, temperature-controlled cell to spectroscopically monitor the reaction. Subsequently, the spectra were subjected to a multivariate curve resolution analysis (MCR) to retrieve pure spectra of both surfactants and folded and unfolded β -LG, along with their respective concentration profiles.

Results

The obtained spectral and concentration profiles closely match the original absorbance spectra of the corresponding reagents, emphasizing the ability of the employed method to handle complex solutions. This study hence demonstrates the potential of online reaction monitoring through mid-IR spectroscopy combined with chemometric techniques as a powerful and adaptable tool in downstream quality control and process automation.

Abstracts

Friday, 12th of May

11:00-12:00	SESSION E: METABOLOMICS/PROTEOMICS
11:00-11:15	E.01 Proteomics, metabolomics and molecular networking as tools for the identification of fungal RiPPs <i>Isabella Burger</i>
11:15-11:30	E.02 Metronidazole resistance in <i>Trichomonas vaginalis</i> <i>Anna-Lena Mayr</i>
11:30-11:45	E.03 Multilevel Omics-Readouts of in vitro Perturbation Studies are Determined by Memory Effects from Subculture <i>Lukas Skos</i>
11:45-12:00	E.04 Establishment of a Non-invasive Biomonitoring Assay Suitable for Children <i>Michael Wolf</i>

Abstracts

TALK E.01

Proteomics, metabolomics and molecular networking as tools for the identification of fungal RiPPs

Isabella Burger* (1), Matthias Schmal (2), Christian Zimmermann (2) Ruth Birner-Gruenberger (3) and Matthias Schittmayer (1)

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Among the known classes of natural products, ribosomally synthesized and post-translationally modified peptides (RiPPs) constitute an attractive compound class for therapeutic developments, due to their bio-active properties. In contrast to bacteria, fungal RiPPs have remained rather understudied so far. Despite the possibility to predict RiPP-precursor peptide sequences by genome mining tools, the numerous and diverse post-translational modifications arising during their maturation make it virtually impossible to predict the final structure.

For working protocol establishment, first experiments were done studying already known fungal RiPPs from the fungus *Aspergillus flavus*. Wildtype, knock-out and overexpression strains for these gene clusters were investigated. Routine proteomics workflows are only sufficient for identification of the precursor and associated tailoring enzymes from the gene cluster, but not for the mature peptide. Instead, quantitative untargeted metabolomics methods are employed to identify features with altered expression, ideally including the mature RiPP of interest. Metabolomics measurements have to be conducted with both reversed-phase (RP) and hydrophilic interaction chromatography (HILIC), in positive and negative ionization mode to cover the vast chemical space occupied by RiPPs.

Instead of identifying single metabolites, we subject extracted features to a feature-based molecular network search, resulting in a molecular metabolite network. Since the amino acid sequence and therefore mass of the RiPP precursor is known, we envision that via analysis of the feature network containing the RiPP precursor the RiPP intermediates can be tracked up to the mature RiPP. This approach will be transferred to novel potential fungal RiPP candidates.

Abstracts

TALK E.02

Metronidazole resistance in *Trichomonas vaginalis*

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Trichomonas vaginalis is a human parasite, causing urogenital tract infections, mainly in women. It is one of the most frequent sexually transmitted pathogens worldwide, causing hundreds of millions of infections annually. [1] Furthermore it can cause adverse pregnancy outcomes [2] and increase the risk of contracting HIV. [3] The pathogen is commonly treated with the antibiotic metronidazole, but resistances are increasingly becoming an issue in the treatment of patients. The mechanisms of resistance are not yet fully understood, however, the TVC1 cell line depleted of iron showed a similar pattern of downregulated proteins, as the resistant cell line. Proteomic analysis was performed to learn more about the differences between these two cell lines, and thus gain more understanding on metronidazole resistance in *Trichomonas vaginalis*. To do so, TVC1 cells were cultured with 2,2-bipyridil to deplete them of iron and a metronidazole resistant cell line was culture alongside them. Protein extraction was performed with TCA/acetone, followed by an enzymatic digestion using Trypsin/ LysC and 3kDa FASP filter units. Peptides were then separated using a nano-HPLC Ultimate 3000 RSLC system (Dionex) with a 25 cm Acclaim PepMap C18 column, directly linked via ESI interface to a high-resolution Q-Exactive HF Orbitrap mass spectrometer. Using a quantitative Proteomics approach, we were able to highlight the differences in similarities between the resistant and non-resistant cell lines, as well as the iron depleted group.

[1] Lamien-Meda, A., Leitsch, D. Identification of the NADH-oxidase gene in *Trichomonas vaginalis*. *Parasitol Res* 119, 683–686 (2020). <https://doi.org/10.1007/s00436-019-06572-8>

[2] Silver BJ, Guy RJ, Kaldor JM, Jamil MS, Rumbold AR (2014 Jun) (2014) *Trichomonas vaginalis* as a cause of perinatal morbidity: a systematic review and meta-analysis. *Sex Transm Dis* 41(6):369–376

[3] Masha SC, Cools P, Sanders EJ, Vaneechoutte M, Crucitti T (2019) *Trichomonas vaginalis* and HIV infection acquisition: a systematic review and meta-analysis. *Sex Transm Infect* 95:36–42

Abstracts

TALK E.03

Multilevel Omics-Readouts of *in vitro* Perturbation Studies are Determined by Memory Effects from Subculture

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Data variance is a critical parameter for a meaningful data interpretation. For method optimization we systematically investigated the role of cell culture conditions on the variance of multi-omics data. For this purpose, the colon carcinoma cell line SW480 was treated with the clinically used arsenic trioxide at sub-cytotoxic concentrations for 24 h. We analyzed treatment-induced changes in the eicosanoid profile from supernatants, as well as in the proteomic profiles from whole cell lysates, including global proteomics and phosphoproteomics. SW480 cells were subcultured in the Lag (1:20 split), Log (1:10 split) and Plateau (1:2 split) phases of cell growth. Subsequently, 250.000 cells were seeded per well in 6-well plates. Two 6-well plates were prepared using cells from the Log phase only (homogeneous) and two 6-well plates were prepared using cells from the three different plate conditions, each in duplicate (heterogeneous). Thus, a total of 12 replicates were prepared per condition and half of them were treated with 5 μ M arsenic trioxide. The growth kinetics and plate conditions of the 6-well plates were continuously monitored with the Cellwatcher M (PHIO scientific GmbH). Then, the cells were processed and analyzed by mass spectrometry according to specified protocols for eicosanoids, proteins and phosphoproteins and the drug effects were evaluated across the different omics-levels. Indeed, omics results from the heterogeneous subculture displayed a lower number of significant changes compared to the homogeneous subculture. This was mainly caused by an increase in experimental variance from 1% to 3% for eicosadomics, 11% to 23% for proteomics, 24% to 53% for phosphoproteomics. In conclusion, the quality of multi-omics data critically depends on memory effects from subculture and their control facilitates discovery efforts.

Abstracts

TALK E.04

Establishment of a Non-invasive Biomonitoring Assay Suitable for Children

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The prevalence of various chronic diseases in children rises at a concerning rate and the lack of sampling compliance in children remains a substantial problem. Thus, non-invasive sampling methods to monitor the health status in children are needed.

We have developed a non-invasive assay, called Metabo-tip, collecting finger sweat and subsequently analyzing the metabolome. For this purpose, untargeted high throughput RP-UHPLC-HRMS/MS using an Orbitrap Exploris 480 mass spectrometer was applied. This approach was carried out in a pilot study with 124 children. Approximately a third was classified as adipose to support the evaluation of individual metabolite profiles, nutritional behavior, specific endogenous factors, and detect medication.

Various xenobiotics, *inter alia* sweeteners and medication, were detected in the finger sweat samples. Furthermore, numerous metabolites of interest including amino acids, peptides, vitamins, hippuric acid (biomarker for fruit and vegetable consumption), methionine sulfoxide (predictive marker for diabetes), and hypoxanthine (predictive marker for hypoxic sequelae and physical performance) were detected.

Clearly, finger sweat analysis represents a promising approach to monitor the health status of children. The possibility to sample children without compliance issues and the additional option to sample repeatedly in time intervals provides numerous possibilities to monitor the lifestyle and health status of children.

Abstracts

Friday, 12th of May

13:00-14:00	
SESSION F: METHODOLOGICAL ADVANCEMENTS	
13:00-13:15	F.01 Optimization of A High-throughput SPE Clean-up for Urine and Plasma Exposomics <i>Yunyun Gu</i>
13:15-13:30	F.02 Quantum cascade laser based vibrational circular dichroism and its potential for chiral monitoring <i>Daniel-Ralph Hermann</i>
13:30-13:45	F.03 Development of a negative-thermal gradient GC for fast gas chromatography and its application for the study of volatile products formed in lithium-ion batteries <i>Bernhard Klampfl</i>
13:45-14:00	F.04 Optimizing high-throughput sample preparation of volumetric absorptive microsampling (VAMS) for targeted LC-MS metabolomics <i>Bruno Stelzer</i>

Abstracts

TALK F.01

Optimization of A High-throughput SPE Clean-up for Urine and Plasma Exposomics

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Objectives/hypotheses: Liquid-liquid extraction and protein precipitation are commonly employed sample preparation techniques in exposome research due to their broad analyte coverage. However, they were frequently reported with strong matrix effects and poor reproducibility. Solid phase extraction (SPE) could potentially solve these issues, but it is difficult to apply SPE for exposome-scale sample pretreatment because of its high specificity.

Methods: In this study, a high-throughput clean-up method for exposome research will be presented. Ninety-five environmental and food-related toxicants were selected, including plastic components, perfluorinated alkylated substances, industrial side-products, pesticides, endogenous estrogens, phytoestrogens, mycoestrogens, personal care product ingredients, pharmaceuticals, phytotoxins, disinfection by-products, food processing by-products, air pollutants as well as some sulfate and glucuronide metabolites. Water was spiked with the analyte mixture in a concentration range of 0.25-250 ng/mL for some initial tests, including comparison of two SPE cartridges, evaluation of sample buffer, and optimization of SPE elution solvents. The optimized conditions were applied in spiked human samples, i.e. urine and plasma, to estimate the extraction recoveries and matrix effects. To increase throughput, 96-well plates were tested with the same sorbent.

Results: Oasis PRiME HLB (Waters Corporation) was selected for further optimization due to its promising extraction recoveries (59% - 89%) for the majority of analytes, methanol was selected as the elution solvent, and most analytes spiked in human samples obtained good results of extraction recoveries (80% - 120%) and signal suppression enhancement ratios (80% - 120%) with both SPE cartridges and 96-well plates.

Conclusions: The developed promising approach will be used in large-scale human biomonitoring and other exposomic applications.

Abstracts

TALK F.02

Quantum cascade laser based vibrational circular dichroism and its potential for chiral monitoring

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Chiral small molecules have been a staple of most medicinal cabinets for decades. Recent progresses in research have shown improved pharmacokinetics and efficacy for enantiopure drugs in contrast to previously used racemic mixtures.^[1] As a consequence, the chiral identity of a chosen analyte have become important analytical questions.^[1] While nuclear magnetic resonance and X-ray crystallography are suitable for this purpose, they require both extensive knowledge and time consuming pretreatment. Vibrational Circular Dichroism (VCD) on the other hand offers chiral information in a pre-treatment free manner and can be performed in solution.^[1] Unfortunately, the low intensity of VCD spectra necessitates long measurements (hours), limiting its application for dynamic processes.

Our recently constructed quantum cascade laser based VCD instrument employs the unique characteristics of this laser source (high intensity and highly polarized light) to significantly reduce the measurement time for low noise VCD measurements.^[2] With the goal of future on-line monitoring in mind, we performed simulated racemization of the enantiomeric pair R/S-1,1'-Bi-2-naphthol in CHCl₃, which was monitored at a time resolution of 6 minutes. The dataset included 3 different concentrations, spanning both enantiomeric and concentration dependent space, enabling valid chemometric evaluation with predictive errors as low as 2.8 % enantiomeric excess. Further instrument design can be performed in a more informed way, as dedicated QCL-arrays based on the significant bands identified by the multivariate statistics can improve time resolution further without sacrificing predictive accuracy.

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[2] Hermann, D. R.; Ramer, G.; Kitzler-Zeiler, M.; Lendl, B. Quantum Cascade Laser-Based Vibrational Circular Dichroism Augmented by a Balanced Detection Scheme. *Anal. Chem.* (2022), 94 (29), 10384–10390.

Abstracts

TALK F.03

Development of a negative-thermal gradient GC for fast gas chromatography and its application for the study of volatile products formed in lithium-ion batteries

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Improving the longevity, energy density and safety of lithium-ion batteries (LIBs) is essential for their viability. To achieve this, research on LIBs is focused on optimizing the composition of their electrolyte and gaining a deeper understanding of the mechanisms that lead to their degradation. To investigate these mechanisms a real-time-(operando) method is required that can analyze the electrolyte's degradation as it occurs. Highly time-resolved analysis of the gas species formed during the use of LIBs is crucial to understanding the process dynamics. To achieve this, a GC/MS system equipped with a fast-measuring system to enable short injection intervals is utilized, as the long cycle times of conventional temperature-programmed gas chromatography were found to be inadequate for this purpose.

In order to achieve rapid heating rates (>20 K/s), directly heated short columns were considered as a viable solution. To improve separation efficiency, the suitability of negative thermal gradients was explored. Various setups were designed and tested to determine their ability to facilitate fast separations.

We report here an experimental setup capable of producing spatially resolved temperature gradients along a GC column. The system achieved rapid changes in the shape of its gradients and enabled fast separations of analytes with high volatility range. It was shown that base-line separated measurements of a C8-C20 n-alkane standard could be realised in less than 30 seconds with this system. The device significantly reduces energy and carrier gas consumption in comparison to conventional gas chromatography.

These aspects make this technology a viable asset for the monitoring of fast changing processes. Negative thermal gradient gas chromatography is thus a powerful tool for the detection and identification of degradation products in LIB electrolytes.

Abstracts

TALK F.04

Optimizing high-throughput sample preparation of volumetric absorptive microsampling (VAMS) for targeted LC-MS metabolomics

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Emerging microsampling techniques ($\leq 50 \mu\text{L}$ volume) such as volumetric absorptive microsampling (VAMS) offer an alternative to classical paper-based dried blood spots (DBS) with the advantage of a constant blood sampling volume (e.g. $10 \mu\text{L}$) regardless of the hematocrit level or the viscosity of blood (HCT-effect) [1]. High-throughput capability is an increasingly important aspect of method development, especially in regard to the technical and economic feasibility of larger cohort studies. An existing workflow for safety reaction vessels [2] was adapted to extract the metabolites simply and fast from VAMS sampling sticks in acetonitrile: water 70:30 (v/v). Extraction times, sonication, shaking, and the use of internal standards were optimized, and the extraction was directly performed in a 96-filter plate. Undesired evaporation and contamination were investigated, and the workflow was adopted accordingly. A comprehensive reversed-phase (RP) and hydrophilic interaction liquid chromatography (HILIC) coupled with high-resolution mass spectrometry (HR-MS) as a metabolomics analysis platform revealed sufficient metabolite extraction after 10 minutes instead of one hour, reducing preparation time drastically. The injection of the filtered extraction solvent without evaporation/ resuspension further reduced the workload. The overall reduction of time and chemicals results in a reduction of costs and enables further automatization via pipette robots in the future.

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- [2] Volani C, Caprioli G, Calderisi G, Sigurdsson BB, Rainer J, Gentilini I, Hicks AA, Pramstaller PP, Weiss G, Smarason SV, Paglia G. Pre-analytic evaluation of volumetric absorptive microsampling and integration in a mass spectrometry-based metabolomics workflow, *Anal Bioanal Chem.* 2017 Oct; 409(26)

POSTER SESSION

Thursday, 11th of May, 16:45-18:15

P.01	Distribution of elements in stream sediments in the Mura River by applying ICP-MS <i>Barbara Čeplak</i>
P.02	Development and validation of an HPLC-MS/MS multi-class method for the analysis of different classes of veterinary drug residues in milk and poultry feed <i>Lidija Kenjeric</i>
P.03	Fostering inclusive access to analytical instrumentation <i>Michael Schober</i>
P.04	Tracing the origin of non-metallic inclusions by elemental and isotopic fingerprints <i>Kathrin Thiele</i>
P.05	Click Chemistry Modification of Metal Nanoparticles for targeted SERS <i>Stefan Seidl</i>
P.06	High-performance liquid chromatography and mass spectrometry of chronic lymphocytic leukaemia cells reveal changes in hexosamine metabolism upon Ibrutinib treatment <i>Maximilian Lebede</i>
P.07	Challenges in analytical process monitoring of biochemical separation of cotton/polyester textiles <i>Philip Pathy</i>
P.08	Detection of inorganic arsenic in rice using a field test kit: a screening method with Cola extraction <i>Marc Preihs</i>
P.09	Analytical evaluation of the chemistry of Ti(Si)N coatings by atom probe tomography <i>Saeideh Naghdali</i>
P.10	Development of a fast GC-MS/MS method for the simultaneous measurement of peroxisomal key metabolites including saturated and polyunsaturated fatty acids and one ether lipid biosynthesis intermediate <i>Karin Preindl</i>
P.11	Assessment of the levels of trace elements and Polycyclic Aromatic Hydrocarbons (PAHs) in ambient air in the city of Kampala <i>Doreen Mirembe</i>
P.12	Green facades as model systems for anthropogenic emissions of technology-critical elements <i>Simone Trimmel</i>
P.13	Electrodeposition as an encapsulation tool for atom probe tomography of Cu nanoparticles <i>Aydan Cicek</i>
P.14	Investigation of iron uptake in the human placenta using LA-ICPMS <i>Elisabeth Foels</i>
P.15	Repurposing an Existing Natural Gas Pipeline for 100% Hydrogen Transport <i>Ahmed Hamed</i>
P.16	Applicability of selected pipe materials for underground hydrogen storage facilities <i>Bernd Loder</i>

POSTER SESSION

Thursday, 11th of May, 16:45-18:15

P.17	On the hydrogen uptake of line pipe steels L80 and P110 under gaseous hydrogen charging up to 1000 bar and 200°C <i>Matthias Eichinger</i>
P.18	Recent progress in a study on the development of hydrogen resistant martensitic steels: influence of Mo carbides addition and surface treatment <i>Magdalena Eskinja</i>
P.19	Characterization of Jet Fuel by Comprehensive Two-Dimensional Gas Chromatography <i>Lim Noemae</i>
P.20	Hydrogen Applicability of Steels in Gas Storage Facilities <i>Saurabh Bhosale</i>

POSTER P.01

Distribution of elements in stream sediments in the Mura River by applying ICP-MS

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The aim of this work, as a part of MURmap project, is to present the chemical composition of stream sediments in the river system of the Mur/Mura. The Mur/Mura River was chosen as the area of interest because of its diverse geological and morphological features as well as past and present anthropogenic activities. In Styria, the area was a center of various mining and processing activities, while the Slovenian alluvial plains are mainly used for extensive agriculture. A number of larger cities along the river are responsible for typical urban contaminants such as hospital wastewater effluents, industry and urbanization. To study the different sources of trace elements and its impact on the river, stream sediments were collected from 41 sampling sites along the river near its source in Austria to the Slovenian-Croatian border. The samples were further investigated by ICP-MS using two multiacid digestion methods. Specific elements such as Na, K, Mg are related to the lithological features of the study area, while anomalies of certain elements (e.g., Cd, Pb, Zn) were found at sites that could indicate anthropogenic sources and high-tech industries. For example, in Graz the contents of Cd, Pb and Zn were 0.33 mg/kg, 45,83 mg/kg and 181,00 mg/kg respectively, while in St. Michael im Lungau, where the influence of human activities is much lower, these values were 0.01 mg/kg, 15,58 mg/kg and 61,70 mg/kg for Cd, Pb and Zn, respectively. In the next phase of the project, collected sediment samples will be analyzed for mineralogical composition and individual particle characterization.

Development and validation of an HPLC-MS/MS multi-class method for the analysis of different classes of veterinary drug residues in milk and poultry feed

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The continuous utilization of veterinary drugs on livestock gives rise to various concerns, such as the need for residue monitoring, cumulative risk evaluation, antimicrobial resistance, and environmental pollution. Hence, it is vital to establish regulatory limits and sustain them using reliable analytical techniques. Despite efforts globally, creating a comprehensive analytical technique that saves time while maintaining both sensitivity and robustness for different compound classes remains an ongoing task. The objective of this investigation was to develop and validate a multi-class method utilizing HPLC-MS/MS for detecting various veterinary drug residues in poultry feed and milk. The sample preparation protocol based on the “dilute and shoot” approach previously used for multi-mycotoxin detection (Malachová et al. (2014)) was followed and further optimized in this study. Method validation for >140 analytes was conducted according to the SANTE validation guideline. Method performance characteristics such as linearity, limits of detection, limits of quantification, precision, accuracy, and repeatability were examined. Limits of quantification for >80% of the analytes in milk were between 10 and 50 µg/kg and lower, while for poultry feed regulations of MRL are still not available. Intermediate precision complied with the SANTE criterion of RSD <20% for almost 90% of the analytes for both matrices. Milk samples were affected by matrix effects with a signal enhancement, for 22% of analytes above 120% compared to solvent standards. In contrast, strong to moderate signal suppression was observed in poultry feed, a much more complex matrix, with 55% of analytes detected below 80% when compared to the solvent standards. The majority of the analytes in milk and chicken feed met the SANTE routine laboratory criteria for accuracy, with a range of 80-90% for milk and 50-60% for chicken feed, with a recovery range between 60-140%.

POSTER P.03

Fostering inclusive access to analytical instrumentation

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Analytical Chemistry encompasses a variety of obvious and hidden obstacles in the work environment for people. As a consequence, chemists with disabilities need barrier-free admission to analytical laboratories and instruments (e.g. mass spectrometers). In context of a diverse and inclusive workplace, easy accessibility and operability have to be ensured for laboratory infrastructure and analytical machines. However, current laboratory and instrument setups rarely consider the needs of disabled people from simple benchtop devices to sophisticated analytical equipment and truly operator-friendly instruments are still rare for personnel with disabilities. The result is the exclusion of competent persons from laboratory work by trivial issues, such as: critical parts of an instrument cannot be reached, software cannot be changed in format and presentation, and warning signals and alarms cannot be recognized.

Therefore, in a project funded by the Inclusion & Diversity Fund of the Royal Society of Chemistry (RSC), the current status of disabilities in the lab was investigated with the aim to evaluate supporting strategies and to promote a barrier-free access for everyone by easier accessibility and operability of analytical instruments.

For this purpose, a questionnaire consisting of two parts was developed and provided online. In part 1, the types and occurrence of disabilities in the lab with its conscious and unconscious bias was investigated. In part 2, ideas and possible suggestions to overcome disabilities were assessed. The questionnaire was completely anonymous and no personal data was collected. During the duration of the project, the questionnaire was advertised and promoted at conferences to the scientific community. A final report with a full evaluation of all findings was released online for possible stakeholders (e.g. laboratory suppliers or instrument manufacturers) to make the laboratory environment more diverse and inclusive.

Questionnaire, report, and poster are available online: <https://icpms-leoben2022.at/inclusion-in-lab>

POSTER P.04

Tracing the origin of non-metallic inclusions by elemental and isotopic fingerprints

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Non-metallic inclusions (NMIs) are microscopic particles (size range between 1 and 15 μm) inside the steel which inevitably form during steel production. Their exact formation and modification in the different production steps are not entirely clarified by today. Depending on the steel grade, NMIs affect the physical and chemical characteristics of the final products. Tracing techniques allow for tracking the sources of interfering particles and hypothesis the formation of single inclusion types over the process.

Two different tracing approaches have been investigated in this study. For the first approach, the rare earth element (REE) fingerprint in auxiliaries (e.g., casting powder, slag former, aluminum granules for deoxidation), clogging layer, and NMIs are determined. The REE patterns of the individual substances based on the REE content measured by ICP-MS are compared. Hence, the potential source of interfering inclusions can be determined since each substance is expected to have a unique REE fingerprint. An alternative and novel approach uses enriched stable isotopes to identify the source of NMIs. For this approach, which, until now, has not been applied in the field of metallurgy, the isotopic composition of one potential source of interfering NMIs is modified to a significantly different composition compared to other sources of the same element. Thus, a characteristic and unique tag is conferred on a potential input source of an NMI. Consequently, it is possible to track the evolution of these NMIs over the process by determining the isotopic ratio of single particles using spatially-resolved laser ablation (LA)-ICP-MS followed by isotope pattern deconvolution during data reduction.

Click Chemistry Modification of Metal Nanoparticles for targeted SERS

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Raman spectroscopy is a promising method for the analysis of biological materials, but it is held back by the inherent weak intensity of the Raman signals. By bringing metal nanoparticles into close contact with the biological material, the signal intensity can be increased by several orders of magnitude [1]. Usually, the contact between biological material and nanoparticle happens at random points, with nanoparticle solution and cells being mixed and measured. In contrast, probes made from antibodies and nanoparticles can be manufactured to allow for targeted measurements, with the antibody binding to antigens on the surface or in the cytosol of cells.

Three approaches for the modification of the nanoparticles are used. In the first approach, nanoparticles are coated in streptavidin using unspecific and non-covalent interactions. The streptavidin on the surface can then bind biotinylated antibodies, creating a probe [2]. In the second approach, the nanoparticle and the antibody are modified with reactive groups. These groups are *then* joined together using copper catalyzed azide alkyne click chemistry [3]. In the third approach, a bivalent polyethylene glycol linker binds to the antibody and the nanoparticle.

Different protocols for the synthesis of gold nanoparticles have been evaluated. The necessary amounts of streptavidin and BSA for the conjugation have been determined by titration and a first conjugate of nanoparticle, streptavidin and BSA has been successfully produced. As part of the RaDiaM project, these conjugates will be used to enhance Raman signals in melanoma cells, to distinguish them from healthy precursor cells and cells treated with cytostatic [4].

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POSTER P.06

High-performance liquid chromatography and mass spectrometry of chronic lymphocytic leukaemia cells reveal changes in hexosamine metabolism upon Ibrutinib treatment

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Chronic lymphocytic leukaemia (CLL) shows the highest prevalence of any adult leukemic disease, mainly affecting the elderly. CLL can be classified into distinct subtypes, with varying disease progression rate and severity of symptoms. First line treatment is often done with Ibrutinib (IBR), a small molecule Bruton Tyrosine Kinase inhibitor. [1] Little is known about the metabolic changes induced upon IBR treatment. Therefore, we investigated the metabolome of patient derived cells treated with IBR to gain insight into the molecular intricacies of disease progression and potentially developing resistance to IBR treatment. Donor cells were isolated and treated in culture, quenching of cellular metabolism and extraction of metabolites was done using ice-cold methanol. In order to increase metabolome coverage, we employed a multi-modal HPLC-MS approach featuring reversed-phase and hydrophilic interaction chromatography with subsequent positive and negative electrospray ionization on an Q Exactive™ Orbitrap mass spectrometer. A combination of several bioinformatics software solutions was employed for data evaluation and is centred around UmetaFlow – a newly developed tool providing an easy-to-use graphical user interface for OpenMS. [2] Preliminary results show regulation of energy, hexosamine and neuraminic acid metabolism, indicating oxidative stress and changes in glycosylation upon IBR treatment.

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Challenges in analytical process monitoring of biochemical separation of cotton/polyester textiles

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Cellulases are well known for more than a half of a decade. Their use has become a standard technology in the textile industry. Treating cotton-polyester blended fabrics with cellulase formulations would enable the separation of these fractions, providing an environmentally friendly method for textile recycling. However, so far, no industrial viable process has been established [1, 2]. As cotton consists of cellulose, cellulase enzymes hydrolyze the polymer into short, water-soluble oligosaccharides — and ultimately — glucose. For complete degradation nature uses three enzyme activities: endoglucanase-, cellobiohydrolase- and β -glucosidase activity. These different types of enzyme activities act synergistically and are combined in commercial enzyme formulations in various portions to achieve different effects (depilling, stonewash, total hydrolysis, etc.). The activity of these different cellulase types can be determined using specific substrates, such as CMC, Avicel, etc. The concentration of released soluble reducing sugars can be measured by the neocuproine method. It provides information about the degradation efficiency and enables to monitor the process. The total protein concentration in solution reveals enzyme stability over time and is determined using the Micro Bradford assay. The use of electrophoretic and chromatographic methods allows insights to the composition of different formulations.

In our work, we are testing and comparing different commercially available cellulase formulations from various application areas. In both, laboratory, and pilot scale experiments, we have optimized and monitored conditions for efficient cotton degradation. In this poster, we present main factors influencing cellulase activity as well as a comparison of analytical methods for process monitoring. With these findings we will contribute to the long-term goal to design an industrial viable process for cotton/polyester separation aiming for the minimization of blended fiber textile waste.

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Detection of inorganic arsenic in rice using a field test kit: a screening method with Cola extraction

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Rice, a staple food in many areas of the world, is known to take up and store arsenic during cultivation. Inorganic arsenic (iAs) can pose a health risk as it is declared as a class I carcinogen for humans by the WHO. The EU regulation for maximum levels (ML) of iAs in rice were set to 100, 200 and 250 µg iAs/kg for infant products, polished rice, and brown rice respectively (1).

To screen rice for iAs, especially in low-income countries where sample transport and analysis in a laboratory may not be available, the field kit has been shown to be a reliable alternative (2). Here we show an advancement of the previous field kit method (3), by using Cola instead of nitric acid as the extractant.

In 31 rice samples from the Austrian market, iAs was analyzed using both, HPLC-ICP-MS (reference) and the field kit with Cola extraction. A correlation diagram shows that the results obtained from the Arsenator are comparable to results from speciation analysis on the HPLC-ICP-MS ($R^2=0.806$). The field kit results with the Cola extraction showed quantification limits of about 69 µg iAs/kg, and good reproducibility for a field method ($\pm 21\%$). These results show the potential of Cola as an extractant with the field kit as a screen tool for iAs in rice.

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POSTER P.09

Analytical evaluation of the chemistry of Ti(Si)N coatings by atom probe tomography

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The nanocomposite structure of TiSiN coatings makes a detailed investigation of their microstructure and phase composition a challenging task. Atom probe tomography (APT) would be a valuable method to study the nanocomposite structure spatially-resolved, but the overlap of Si and N peaks in APT mass spectra does not allow to differentiate those. Thus, isotopic substitution of ^{14}N by ^{15}N was applied to disentangle the contributions of Si and N to the mass spectrum. Two series of model coatings, namely TiN, SiN and TiSiN single layers as well as TiN/SiN, TiN/TiSiN and SiN/TiSiN multilayer coatings were synthesized by sputter deposition using *i)* ^{14}N and *ii)* ^{15}N , respectively. The deposited coatings were systematically investigated using laser-assisted field evaporation in a LEAP 5000 XR atom probe. Special attention was paid to the resulting mass spectra and significant emphasis was laid on the identification of present ion species, subsequent peak ranging and assessment if peak overlaps could be resolved. To review the obtained compositional accuracy of the APT measurements, elastic recoil detection analysis was performed on both, the ^{14}N and ^{15}N single layer coatings. Moreover, three dimensional reconstructions of the performed measurements were further investigated with regard to homogeneity of the elemental distribution of Ti, Si, and N within the single layer model coatings. Finally, the multilayered architectures were utilized to evaluate the capability to differentiate the different investigated materials using isotopic substitution and APT analysis.

POSTER P.10

Development of a fast GC-MS/MS method for the simultaneous measurement of peroxisomal key metabolites including saturated and polyunsaturated fatty acids and one ether lipid biosynthesis intermediate

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Peroxisomes are cell organelles, which play crucial roles in detoxification. To study the fatty acid profile in human fibroblasts suffering from peroxisomal disorders or genetically modified human fibroblasts, a tailored analytical method is needed.

A novel approach for the extraction of total fatty acids after acidic hydrolysis was established. The newly developed method omits the usage of n-hexane and isooctane and facilitates fatty acid hydrolysis and extraction with a reagent consumption of less than one-milliliter per sample and subsequent GC-MS/MS measurement. For the first time, 1-chlorobutane was used for lipid extraction and enables the simultaneous extraction of six saturated long to very long-chain fatty acids, nine polyunsaturated fatty acids (PUFAs, including the FA 22:6 n-3 precursor FA 24:6 n-3), two dicarboxylic acids and the ether lipid synthesis intermediate 1-O-octadecyl glycerol (batyl alcohol) after acidic hydrolysis. The method was validated by spiking analytical standards into fibroblast suspensions. The applicability of the method was demonstrated by the measurement of primary human fibroblasts derived from five healthy individuals, five patients suffering from X-linked adrenoleukodystrophy and six Zellweger spectrum disorder patients. Batyl alcohol is suggested as readout for ether lipid synthesis in cell culture after acidic hydrolysis.

POSTER P.11

Assessment of the levels of trace elements and polycyclic aromatic hydrocarbons (PAHs) in ambient air in the city of Kampala

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Clean air is an important resource for sustaining human existence and the environment. However, there is a global rise in air pollution and the limit values for air pollutants are frequently exceeded due to anthropogenic and natural activity. Particulate matter (PM), for example dust fall, is a carrier for airborne pollutants, which can be either organic or inorganic. Therefore, dust fall samples can be used to assess the extent of pollution at a particular site. PM of diameter < 10 µm have a high probability of deposition deeper into the respiratory tract and are likely to trigger several health effects.

Uganda, particularly its capital city Kampala, is not an exception to this global issue due to poorly controlled emission sources, and insufficient environmental management policies and strategies resulting in high ambient concentrations of pollutants. This study aims to assess the levels of trace elements and polycyclic aromatic hydrocarbons (PAHs) in ambient air at selected locations in Kampala and to apportion their sources. For this purpose, dry and wet precipitation samples were collected using a Bergerhoff sampler from eight different outdoor and three indoor locations in Kampala over a period of one month. Both the water soluble and water insoluble fractions were analyzed for 48 elements using ICP-MS/MS. Water insoluble fractions were digested using microwave assisted acid digestion with HNO₃, H₂O₂ and HBF₄. PAHs will be analyzed in Uganda using GC-MS.

The provided data on the level of pollution in the city will be used to assess potential risks to human health. The study highlights the need for further continuous monitoring of air quality in Kampala, as high levels of certain trace elements can pose potential risks to human health. The findings may be useful in developing strategies to mitigate the impact of air pollution and the implementation of measures to reduce air pollution and improve air quality in urban areas.

Green facades as model systems for anthropogenic emissions of technology-critical elements

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In the course of the FWF-funded project TecEUS (P 33099-N, www.teceus.at), 292 leaf samples from two green facades and 18 river water samples were analysed for their mass fractions of 48 elements by inductively coupled plasma tandem-mass spectrometry (ICP-MS/MS [1], [2]). Special focus was set on technology-critical elements (TCEs), in particular on less-studied TCEs. The leaf samples originate from eight plant species commonly used on green facades and were taken across five storeys in four seasons. For each leaf sample, one replicate was washed with water to investigate surface dust.

Analyses of Variances (ANOVAs) revealed significant differences in elemental distribution linked to sampling month, storey, and plant species. Highest sums of standardised element contents were found in leaf samples from the lowest storey at one site, and in samples from March and of *G. macrorrhizum* at the other site. Highest mass fractions of Li were found in *A. millefolium* and of Ge in *S. heufleriana*. Low Nb/Ta ratios in some leaf samples indicate anthropogenic Ta emissions. In view of the potential public health threats from exposure to these elements, the presented data can form a so-far lacking base for future studies on the identification of environmental TCE sources.

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POSTER P.13

Electrodeposition as an encapsulation tool for atom probe tomography of Cu nanoparticles

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Atom probe tomography is a powerful method for analysis of nanoparticles, encapsulated using electro-deposition. Encapsulation films are promising approaches to enable preparation of the required tip-shaped specimen [1].

This study presents a methodology for preparing atom probe tomography specimens by encapsulating Cu nanoparticles between two different combinations of film and substrate materials, utilizing electrodeposition. Suitable electrolytes and electrodeposition processes were developed for deposition of Ni films on Co substrates, and vice versa. Subsequently, the crystallinity and phase composition of the electro-deposited films was investigated by X-ray diffraction. Prior to encapsulation, scanning electron microscopy was used to confirm deposition of nanoparticles on the substrates. Nanoparticles were then encapsulated using the above mentioned film-substrate combinations, which were considered to yield homogenous field evaporation. It is crucial to ensure a similar evaporation field for nanoparticles, encapsulation films and substrate material, as well as strong adhesion of the interfaces between the substrate, nanoparticles and the electro-deposited film. Carefully selected and matched combinations of substrates, nanoparticles and encapsulation films are used to prevent mass spectral peak overlaps. Atom probe tomography specimens, including the encapsulated Cu nanoparticles were prepared using femtosecond laser processing followed by annular focused ion beam milling. Sandwiching of the Cu nanoparticles at the interface and careful preparation facilitated their successful detection using atom probe tomography. The presence of residual micro- or nano-voids may result in specimen fracture during atom probe tomography while impurities within such voids can also cause additional peaks in the mass spectra that, could overlap with those of the nanoparticles. Specimen preparation challenges will be addressed and solutions for successful atom probe tomography of nanoparticles will be presented.

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POSTER P.14

Investigation of iron uptake in the human placenta using LA-ICPMS

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An optimal iron nutrition is essential for the healthy development of a fetus. During pregnancy, the iron is passed from the mother to the fetus via the placenta. An iron deficiency is associated with various neurodevelopmental deficits. These deficits can persist even after iron administration. Despite the important role of iron in fetal development, iron metabolism in the placenta is not fully understood. [1,2]

State-of-the-art analytical methods are required to get a deeper insight into a complex problem. LA-ICPMS together with antibody labeling has great potential to visualize different structures in tissue sections. In this preliminary study, term and preterm placenta tissue was explored. A metal-conjugated antibody panel was chosen to label different cell types which are present in the placenta. This allows the comparison of the iron distribution in the different cell types. Thus, it can be investigated which cell types might be responsible for the iron storage.

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POSTER P.15

Repurposing an Existing Natural Gas Pipeline for 100% Hydrogen Transport

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To achieve the strategy of zero-greenhouse gas emissions in Europe by 2050 to mitigate the danger of climate change, hydrogen offers the most promising and reliable solution as an efficient energy carrier. As a result, hydrogen research nowadays shows a great revolution in production techniques and applications. Nevertheless, hydrogen transport is still one of the most serious challenges facing hydrogen fuel expansion.

The phenomenon of hydrogen embrittlement (HE) is a critical issue that negatively affects metals and alloys under stress in a hydrogen environment. It occurs when hydrogen atoms adsorb on the metal surface, then diffuse into the metallic matrix and recombine to form an internal high pressure or occupy the potential sites for crack initiation and propagation resulting in a premature fracture under stress. Therefore, the existence of qualified infrastructure for hydrogen transport that overcomes HE is highly demanded. Meanwhile, establishing a new infrastructure for hydrogen transport requires an extremely high budget and a long time to be implemented.

In the Frame of the HyGrid2 project supported by the Austrian Research Promotion Agency (FFG), this research aims to study and qualify an existing natural gas pipeline for 100 % hydrogen transport. The study aim will be approached by simulating the hydrogen environment, such as hydrogen partial pressure, humidity and odorants with different tests to evaluate the HE susceptibility of the pipeline base metal and welds. The tests include constant load tests (CLT), slow strain rate tests (SSRT), ripple load tests (RLT) and fracture mechanics tests under hydrogen environments. This study will contribute to a swift implementation of a cost-effective and efficient hydrogen distribution system.

POSTER P.16

Applicability of selected pipe materials for underground hydrogen storage facilities

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In the framework of the Horizon 2020 project HyStories, the hydrogen storage possibility in old, depleted gas reservoirs and natural gas storage facilities is investigated throughout Europe. As part of this project, the work package "Materials and Corrosion" has the aim to test the applicability of selected pipe materials with respect to hydrogen embrittlement. For this purpose, carbon steels and corrosion resistance alloys are investigated, steels with tempered martensitic structure, steels with a ferritic-perlitic structure, a welded steel grade, ferritic and austenitic stainless steels and Duplex steels, were investigated by means of high-pressure, high-temperature autoclave tests and analyses of the hydrogen uptake. The autoclave tests were performed on tensile specimens loaded at 90% of the Yield Strength, and the samples were also analysed to determine the hydrogen uptake. After the tests were completed, the hydrogen uptake was analysed by Thermal Desorption Spectroscopy. There were four main gas compositions used in the autoclave tests: 120 bar H₂, 120 bar H₂ + 15 bar CO₂, 120 bar H₂ + 1 bar H₂S and 120 bar H₂ + 15 bar CO₂ + 1 bar H₂S, with and without the addition of electrolytes with various chloride concentrations. In addition, the experiments were carried out at room temperature and at 120°C. The duration of the experiments was 720 hours. From the results, it can be seen that the hydrogen uptake for carbon steels is low even under the most severe conditions. The results show that the hydrogen uptake is much higher for stainless steels compared to carbon steels. All samples tested are recommended as suitable pipe material with the exception of the Duplex stainless steels 2205 for underground hydrogen storage. The higher strength carbon steel P110 should be considered with some risk in sour gas applications.

POSTER P.17

On the hydrogen uptake of line pipe steels L80 and P110 under gaseous hydrogen charging up to 1000 bar and 200°C

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In hydrogen storage and transportation steels for pipelines and tanks come in contact with hydrogen at various pressures and temperatures. Under high pressures and temperatures, the hydrogen uptake of steels is increased, which can cause hydrogen embrittlement and lead to operation risks. To prevent hydrogen embrittlement, it is of crucial importance to investigate the used materials under the conditions encountered during their application. To investigate the hydrogen uptake behavior of line pipe steels L80 and P110 a new high pressure, high temperature autoclave test bench for constant load tests and charging experiments, with the operation range up to 1000 bar hydrogen partial pressure and 200 °C was established. Hydrogen uptake of L80 and P110 steel has been investigated with and without a constant load of 90% yield strength as function of hydrogen partial pressure (between 100 and 1000 bar) and temperature (between 25 and 200°C). Furthermore, the critical hydrogen content for causing brittle material behavior was determined. In addition, the effective diffusion coefficients have been measured by electrochemical permeation measurements to be able to simulate hydrogen uptake in form of time dependent hydrogen profiles. The diffusion coefficients resulting from electrochemical permeation measurements are $1.4 \cdot 10^{-6} \text{ cm}^2/\text{s}$ for L80 and $1.1 \cdot 10^{-6} \text{ cm}^2/\text{s}$ for P110 respectively. The hydrogen content of L80 and P110 increase with the applied partial pressure from 0.2 wt.-ppm (100 bar and 25°C) to about 1 wt.-ppm (1000 bar and 25°C). An increase in temperature up to 200°C leads to a constant and pressure independent increase of the hydrogen contents present in both materials. Independent from the material, no fracture occurred under any of the tested conditions in constant load tests with 90 % yield strength. The critical hydrogen content for L80 is 1.7 wt.-ppm and 1.0 wt.-ppm for P110 respectively.

POSTER P.18

Recent progress in a study on the development of hydrogen resistant martensitic steels: influence of Mo carbides addition and surface treatment

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High-strength martensitic steels are widely implemented in various industrial applications owing to good balance of mechanical properties. Properties of high-strength steels can be significantly impaired once the steel is exposed to hydrogen containing environment due to the susceptibility to hydrogen embrittlement (HE). In order to reduce the penetration of hydrogen in material, surface treatments such as shot-peening can be employed as hydrogen barrier and increase resistance to HE. However, understanding the HE behaviour of the material in ground condition is assumed essential to optimize further conditions of applying surface treatment. Mo can form carbides Mo_2C and Mo_6C , which can act as hydrogen trapping sites. In previous studies, the effect of Mo content on resistance of martensitic steels was reported in terms of sulfide stress cracking where formation of sulfide layer can impact hydrogen induced crack propagation. In case of sulfide-free hydrogen conditions, there is limited knowledge about the role of Mo in the commercially available martensitic steels and its effect on HE.

This study clarifies the role of Mo carbides in the hydrogen uptake of two tempered Cr-Mo martensitic steels with different chemical compositions and heat treatments. Hydrogen trapping was investigated by means of cathodic charging and Thermal Desorption Spectroscopy (TDS). Electrochemically charged Cr-Mo steels were subjected to Slow Strain Rate Tests (SSRT) to elucidate mechanical performance. The carbide distribution and microstructure of Cr-Mo steels were observed using Scanning Electron Microscopy (SEM). The results showed the level of reversibility of trapped hydrogen in the microstructure of investigated Cr-Mo steels. TDS indicated two low temperature peaks with similar activation energies in case of both alloys. Hydrogen related to these peaks referred to as diffusible hydrogen was responsible for the deterioration of mechanical properties. Electrochemical charging showed higher uptake of hydrogen for alloy with higher content of Mo. The alloys with different Mo contents showed different levels of HE susceptibility.

Characterization of Jet Fuel by Comprehensive Two-Dimensional Gas Chromatography

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Sustainable aviation fuels (SAFs) are essential to reduce the aviation industry's carbon footprint, but optimizing their production is challenging due to complex fuel composition. Fischer-Tropsch (FT) process from non-petroleum sources is a promising method for SAFs production [1]. Two-dimensional gas chromatography (GCxGC) is a powerful tool for analyzing aviation fuel composition. Composition-property based prediction modelling is used as a pre-screening tool to avoid costly and time-consuming efforts in SAF development [2]. This work aims to develop an analytical method for comprehensive SAF characterization by GCxGC and machine learning-based property prediction models. Detailed chemical composition of jet fuel samples was obtained using cryogenic modulation comprehensive GCxGC-MS. Normal column configuration was used in the analysis with nonpolar column for the 1st dimension and mid-polar column for the second dimension. The analysis revealed that the samples consisted mainly of linear and branched hydrocarbons with aromatic hydrocarbons having the least relative concentration, and compound class regions were identified in the chromatograms due to the added dimensionality of GCxGC analysis. This analytical technique can efficiently assess detailed composition of samples and has the potential to guide optimization of the FT process for improved production of SAFs with specific characteristics. The ongoing work involves exploring a reversed column configuration of GCxGC and using composition matrix for fuel property prediction with linear and nonlinear machine learning models.

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POSTER P.20

Hydrogen Applicability of Steels in Gas Storage Facilities

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Climate change is one of the major issues facing the world today. The energy sector is looking at hydrogen as a solution to minimise carbon emissions, and hydrogen can play an important role. Hydrogen energy in the future will require a transportation and storage system, depending on the demand. There is a lack of data on the behaviour of hydrogen in underground environments with materials to be used in storage and transportation facilities. Oil and gas companies tend to use carbon steel for transportation and storage facilities because of its easy availability, economic cost and the required strength. Hydrogen molecules under pressure tend to decompose to a small extent on the surface of steel and other metallic materials, and the metal can uptake hydrogen as atoms. Depending on the strength of the steel and other conditions, the absorbed atomic hydrogen tends to embrittle steels, which can lead to unforeseeable and catastrophic failures. Therefore, Materials like carbon steels, which are mentioned in the API 5CT, such as K55, L80, N80Q and C90 in an environment with a mixture of H₂, CO₂, and H₂S are used with a brine with 5% NaCl. Amount of absorbed hydrogen in the material analysed with Thermal Desorption Spectroscopy (TDS). Constant load tests and slow strain rate tests, and Fatigue and fracture Mechanics tests are performed. The aim of this research is to study the available steels from the API 5CT standards and find out if they are suitable for using underground hydrogen storage. The first results look promising, that no substantial embrittlement as reduction of a lifetime was not far expected in most steel environment systems.