ESAS 2026

Budapest, Hungary

European Symposium on Analytical Spectrometry

Budapest,
August 30 – September 3, 2026

Book of abstracts

ELTE EÖTVÖS LORÁND UNIVERSITY

SZTE UNIVERSITY OF SZEGED HUNGARY

MAGYAR KÉMIKUSOK EGYESÜLETE MKE HUNGARIAN CHEMICAL SOCIETY

ISBN 978-615-6018-42-7

Person responsible for publishing: János Szabó

Published by: Hungarian Chemical Society

Editors: Gábor Galbács, Viktor G. Mihucz, Orsolya Urbán, Gyula Kajner

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Dear Colleagues,

It is our great pleasure to welcome you to Budapest and to the European Symposium on Analytical Spectrometry 2026. On behalf of the organizing committee, we are delighted to host about 150 participants from across Europe and beyond — including colleagues from Hungary, Czechia, Poland, Austria, Germany, Brazil and more. Your presence underscores the vitality and global reach of our analytical spectrometry community.

This year's scientific programme is exceptionally rich. Over the next four days, we will hear more than 50 oral presentations — including plenary lectures, keynotes, and regular talks — alongside an impressive array of scientific posters covering the full spectrum of atomic and molecular spectrometry. The breadth of topics reflects how rapidly our field is evolving: from single particle ICP MS, PFAS and microplastic analysis, advanced mass spectrometry, and laser based techniques, to chemometrics and machine learning.

We are especially proud that many students and early career researchers are joining us this year. ESAS has always been committed to supporting the next generation of analytical scientists, and we hope that this symposium will be an inspiring and formative experience for them. To further encourage excellence, we will again award poster prizes— a tradition that highlights the creativity and dedication of our young colleagues.

We are also grateful for the strong engagement of our instrument vendors, whose technologies drive innovation in our laboratories. The presence of Wiley, Elsevier, Royal Chemical Society and Taylor & Francis reflects the close partnership between academia, industry, and scientific publishing that sustains progress in analytical chemistry.

Allow us to express our sincere thanks to all speakers, session chairs, poster presenters, and sponsors for contributing to this event. We also acknowledge the dedicated work of the organizing team at ELTE, the University of Szeged and the Hungarian Chemical Society, whose efforts made this symposium possible.

We hope that ESAS 2026 will be not only scientifically stimulating, but also personally enriching. Budapest offers a unique blend of history, culture, and hospitality — and we encourage you to also enjoy the city, reconnect with colleagues, and build new collaborations.

With this, we wish you an inspiring and memorable symposium. Thank you for being here, and we look forward to a week of excellent science and meaningful exchange.
Welcome to ESAS 2026!

Viktor G. Mihucz
co-chair

Gábor Galbács
co-chair

Conference venue: Ráday House Conference Center, 1092 Budapest, Ráday street 28.
Conference website: www.esas2026.hu

SCIENTIFIC PROGRAMME

Sunday, August 30, 2026

Short courses

15:00–16:30 D. Clases (Austria): Single particle ICP-MS analysis

17:00–18:30 B. Hufnagl (Austria): Machine learning in spectroscopy

15:00–16:30 T. Janáky (Hungary): Mass spectroscopy in proteomics

17:00–18:30 P. Fürjes (Hungary): Microfluidics in spectroscopy

Monday, August 31, 2026

11:00-11:15 **Opening ceremony**

11:15-12:00 **Plenary talk –** Volker Deckert: Three decades of nanoscale Raman spectroscopy: limits, lessons and opportunities

Oral session 1A - Machine learning and data fusion in spectroscopy
Chair: Barbara Wagner

13:00-13:40 **Keynote 1A** – E. Bulska: Omics sciences in the era of artificial intelligence: an analytical chemistry perspective

13:40-14:00 1A1 – C. Jakopin: FTIR and LIBS data fusion – a chemometric approach for the classification of polyimides in the semiconductor industry

14:00-14:20 1A2 – Y. Kim: Improving major element quantification in complex geomaterials via portable LIBS–XRF data fusion

14:20-14:40 1A3 – A. Khezr pour: Dual-domain spectral data fusion of ICP-OES and FTIR via chemometric embedding for robust environmental source discrimination and multi-scale fingerprinting

Oral session 2B - Analysis of biological and food samples
Chair: Mihály Dernovics

13:00-13:40 **Keynote 2B** – E. Baranyai: Comprehensive elemental and isotopic characterization of U.S. East Coast honeys

13:40-14:00 2B1 – Á. Dienes: Complex analytical investigation of natural and artificial sweeteners

14:00-14:20 2B2 – I. Machado: Evaluation of *in vitro* bioaccessibility of essential and toxic elements in insects by MIP-OES: integration with LC-MS/MS polyphenol profiling

14:20-14:40 2B3 – K. Solymosi: The effect of salt stress on the photosynthetic activity, pigment content, greening and ion (Na^+ and K^+) uptake of light-grown, dark-grown and greening wheat seedlings

Oral session 3A - Vibration spectroscopy
Chair: Volker Deckert

15:00-15:40 **Keynote 3A** – M. Veres: Detection of DNA hybridization with alkyne-labelling and Raman spectroscopy

15:40-16:00 3A1 – Z.H. Luo: Infrared spectroscopic measurement of isolated surfactant protein A and D for predictive quantification modelling

16:00-16:20 3A2 – K. Kotaška: Application of FTIR in medicine

16:20-16:40 3A3 – A. Deák: Optical spectroscopy of individual nanoparticles: insights into structure, dynamics, and surface chemistry at the nanoscale

16:40-17:00 3A4 – T. Alwaraa: Real-time SERS monitoring of plasmonic coupling during thiocynate-induced gold nanoparticle aggregation

Chemistry Europe session – Analysis and sensing
Chair: Katja Glatz

15:00-15:40 Meet the editor

Tuesday, September 1, 2026

09:00-09:45 **Plenary talk** - Detlef Günther: Fundamental studies using nitrogen as plasma gas for ICP-MS and as carrier gas for laser aerosols

Oral session 4A - LA-ICP-MS analysis
Chair: Detlef Günther

10:00-10:40 **Keynote 4A** – M. Holá: Quantitative LA-ICP-MS analysis of strategic minerals using tailor-made glass reference materials

10:40-11:00 4A1 – O. Lanaridi: LA-ICP-MS analysis of impurities in SiC materials: how does a microdroplet generator approach compare to standard addition?

11:00-11:20 4A2 – B. Wagner: Spectral analysis of historical inks assisted by machine learning

11:20-11:40 4A3 – T. Procházková: New glass reference materials for in-situ analysis of lithium- and uranium-rich minerals

Oral session 5B - Single particle and cell analysis
Chair: Jörg Feldmann

10:00-10:20 5B1 – D. Clases: Particles – gotta catch 'em all! - Pushing the boundaries of single particle methods

10:20-10:40 5B2 – K. Tvrdy: Single-cell LA-ICP-MS in assessing the elemental composition of the algae *G. Sulphuraria*

10:40-11:00 5B3 – B. Godlewska-Żyłkiewicz: Multi-approach assessment of migration and human exposure to ZnO nanoparticles from medical materials

11:00-11:20 5B4 – D. Eichert: Weathering impact on uranium particles from Sierra Pena Blanca, Mexico: a synchrotron-based study

Oral session 6A - PFAS and microplastic analysis
Chair: Ursula Fittschen

13:00-13:40 **Keynote 6A** – J. Feldmann: The element strikes back: atomic spectrometry meets the PFAS challenge

13:40-14:00 6A1 – R. Gonzalez de Vega: Multi-modal BaF^+-ICP-MS/MS: a comprehensive analytical platform for tracing environmental PFAS, microplastics, and inorganic fluorine

14:00-14:20 6A2 – Z. Kowalewska: Graphite furnace and fluorine determination: 2026

14:20-14:40 6A3 – B. Hufnagl: FTIR imaging from microplastics to microfibers: tackling spectral complexity

14:40-15:00 6A4 – O. Urbán: Classification of contaminated plastic microparticles using laser induced breakdown spectroscopy with machine learning algorithms

Oral session 7B - Challenges and novel technologies in ICP-MS
Chair: Markéta Holá

13:00-13:20 7B1 – É.M.M. Flores: Determination of rare earth elements by ICP-MS: new challenges and trends

13:20-13:40 7B2 – J. Karasiński: Isotopic and elemental composition analysis of historical artifacts to enhance the interpretation of past research findings

13:40-14:00 7B3 – G. Kajner: 3D-printed nebulizers for ICP-MS: feasibility, limitations, and analytical performance

14:00-14:20 7B4 – B. Lajin: Removing a bottleneck in speciation analysis with novel chromatographic eluents

Poster session 1P - Biomedical and pharmaceutical spectrometry
Chairs: Gábor Galbács, Viktor G. Mihucz

1P01 - H. Kopřivová: Spatially resolved quantification of elements in cutaneous tumors by LA-ICP-TOFMS

1P02 - K. Vaňková: Elemental mapping of dental tissues in SATB2-associated syndrome using LIBS

1P03 - Š. Kosina: Suppression of nonspecific sorption of nanoparticle-antibody conjugate in p53 protein detection

1P04 - A. Ruszczynska: ICP-MS-based elemental profiling of paired psoriatic skin biopsies: distinguishing local tissue-specific alterations

1P05 - N. Altannak: Assessment and density functional theory of bioactive compounds of *Curcuma Longa L*. root responsible for its cardio-protective and anti-cancer activities

1P06 - Z. Kowalewska: Investigation of fluorine release from dental fillings using HR-CS FMAS and HR-CS GFMAS

1P07 - B. Berlinger: Advances in the application of single-cell ICP-MS for investigating cellular metal uptake

1P08 - O. Dushna: Mass spectrometric insights into selective electrochemical defluorination of fluorinated pharmaceuticals

1P09 - M. Dernovics: Metabolomic profiling of dandelion and related food product using coupled mass spectrometry method

1P10 - M. Dernovics: Artefact or feature: the follow-up of cultivation- dependent stress response to selenium exposure of *Cardamine hupingshanensis* with UPLC-PDA-ESI-HR-AMMS-based (seleno)metabolomics

1P11 - A. Herczegh: Characterization of Hank's balanced salt solution (HBSS) for quality control using spectroscopic and chemometric approaches

1P12 - E. Fehérvári: Resolving isobaric post-translational modifications by cyclic ion mobility tandem mass spectrometry

1P13 - B. Schwartz: Unveiling the molecular complexity of shilajit supplements by high-resolution mass spectrometry

1P14 - H. Ayvaz: Near- and mid-infrared spectroscopy with chemometrics for classification and quantification of oil adulteration in oleogels

Poster session 2P - Environmental, industrial and food analysis
Chairs: Viktor G. Mihucz, Gábor Galbács

2P01 - T. Vozár: Monitoring lithium accumulation in plants using laser-induced breakdown spectroscopy

2P02 - D. Csontos: Sensitivity improvement of ELCAD-OES for the determination of some environmentally relevant elements in water samples

2P03 - A.B. Nagy: Determination of antioxidant capacity in tea leaves using the DDPH scavenging method

2P04 - D. Princz: Assessment of toxic elements in online market cocoa powders

2P05 – C. Zatykó: Toxic element profiling in fast-beauty lipsticks

2P06 – N. Apriyani: Statistical analysis of real-time concentration of air pollutants in vegan and vegetarian commercial kitchens

2P07 – Á. Freiler-Nagy: Integrated atomic spectrometric methods for multi-matrix elemental assessment of the soil–plant–animal continuum

2P08 – K. Csicskovics: Adsorption of heavy metal ions in microplastic-containing waters

2P09 – B. Bodó: Detection of halogenated pesticides on tomato fruits using laser-induced plasma spectroscopy and machine learning algorithms

2P10 - P.G.K. Hemachandra: Development of a direct sampling GFAAS method for simultaneous determination of cadmium and lead in fruit juices

2P11 - P.G.K. Hemachandra: Simultaneous determination of chromium and beryllium in fruit juices by direct sampling GFAAS

2P12 - E. Küntzelmann: Direct analysis of size fractionated airborne particles with total reflection X-ray fluorescence spectrometry

2P13 - E. Terbák: Aging the timeless pollutant: the analysis of artificially aged PET samples using positron annihilation lifetime spectroscopy

2P14 – M.Q. Hoang: The use of bacterial cellulose in the field of anti-counterfeiting using fluorescence additive

Wednesday, September 2, 2026

09:00-09:45 **Plenary talk** - Vincent Motto-Ros: How far can LIBS imaging go? A journey across scales

Oral session 8A – Laser-induced breakdown and ionization spectroscopy
Chair: Vincent Motto-Ros

10:00-10:20 8A1 – S. Blume: Comparing femtosecond and nanosecond laser-induced XUV spectroscopy (LIXS)

10:20-10:40 8A2 – D. Palásti: Laser-induced breakdown spectroscopy using kHz repetition rate pulses from a fiber laser

10:40-11:00 8A3 – K. Novotný: Several aspects of the LIBS potential as a complementary technique in geological sciences

11:00-11:20 8A4 – M. Veis: Spectroscopy across energy scales: from laser induced plasmas to cold atoms

11:20-11:40 8A5 – I. Schechter: Multiphoton electron extraction spectroscopy (MEES) and its analytical applications

Oral session 9B - Environmental and biomedical spectrometry
Chair: Edina Baranyai

10:00-10:40 **Keynote 9B** - Y-I. Lee: Microfluidic paper devices and hollow microneedles: emerging platforms for next-generation optical sensing of environmental pollutants and biomarkers

10:40-11:00 9B1 – E. Covaci: Small-sized electrothermal vaporization capacitively coupled plasma optical emission spectrometry for Cd, Cu, Pb and Zn determination in surface waters after micro-solid phase extraction

11:00-11:20 9B2 – S.H. Hosseini: Optimizing copper-doped bioactive glass compositions via ion release for antibacterial applications in bone tissue engineering

11:20-11:40 9B3 – N. Vlčková: Photochemical vapor generation of cobalt for atomic absorption spectrometry with atomization in a dielectric barrier discharge: optimization and mechanistic study

11:40-12:00 9B4 – A.A. Ambushe: Speciation analysis of arsenic, chromium and mercury in water and river sediments

Oral session 10A – X-ray and gamma-ray spectroscopy
Chair: Miklós Veres

13:00-13:20 10A1 – U.E.A. Fittschen: Laboratory based XANES and XES analysis of slag

13:20-13:40 10A2 – D. Eichert: X-RF -based studies of particulate matter on filters

13:40-14:00 10A3 – Z. Homonnay: A closer look at the speciation of iron: the power of Mössbauer spectroscopy

14:00-14:20 10A4 – K. Kovács: Iron components in various dietary supplements – a Mössbauer-spectroscopic study

14:20-14:40 10A5 – Zs. Végvári: Technical art history as an objective method for the scientific authentication of paintings

Oral session 11B - Material characterization
Chair: Ewa Bulska

13:00-13:20 11B1 – I. Tolnai: Durability studies of cementitious mixtures containing reinforcing steel

13:20-13:40 11B2 – J. Osán: Metal and selenite sorption on clays as barriers for radioactive waste repository

13:40-14:00 11B3 – B. Zsirka: Synthesis and characterization of clay mineral-based graphitic carbon nitride composite photocatalysts

14:00-14:20 11B4 – J. Kóth: Red mud - from industrial waste to functional and structural material

14:20-14:40 11A5 – V. Vágvölgyi: In/Zn-oxide – clay mineral triple composite systems as photocatalysts

Poster session 3P – Instrumentation and method development
Chairs: Gábor Galbács, Viktor G. Mihucz

3P01 – A. Gawor: The hidden language of proteins in psoriasis: a mass spectrometry perspective

3P02 – M. Svoboda: Sensitive determination of germanium using hydride generation, miniature plasma and high-resolution mass spectrometry with orbitrap analyzer

3P03 – K.N. Pap: Elemental composition and bio-based content of polymers using ICP-OES and ^{14}C techniques

3P04 – G. Coelho: Feasibility study of coupling photochemical vapor generation and high resolution mass spectrometry with orbitrap analyzer for tungsten ultra-trace determination

3P05 – Z. Lyu: Optimization of photochemical vapor generation of fluorine coupled with indirect detection by ICP-MS/MS

3P06 – D. Csontos: Graphite furnace atomic absorption spectrometric analysis of some trace elements in lithium niobate optical crystals

3P07 – L.F.P. Prado Moreira: Ultratrace determination of trimethylgermanium (TMGe) by HG-CT-ICP-MS/MS

3P08 – F. Shoeb: Imaging flow-enhanced spatiotemporal pH oscillations in a microfluidic reactor

3P09 – B. Godlewska- Żyłkiewicz: Development of a new HR-CS ETAAS method for Eu determination in LED phosphors using permanent graphite tube modifiers

3P10 – Gy. Kajner: A modular microfluidic platform for sample preparation in single particle ICP-MS analysis

3P11 – A.R. Rweyemamu: Assessment of the suitability of 3D-printed porous polymer substrates for use in liquid microsample analysis by laser induced breakdown spectroscopy

3P12 – A.R. Rweyemamu: Discrimination of aerosolized contaminants originating from burning plastics using LIBS and machine learning

3P13 – D. Palásti: A fast pulsed UV Raman microscope for microplastic imaging

3P14 – T. Drobil: Improving spatial resolution of laser-induced breakdown spectroscopy for mineralized biological structures

3P15 – D. Eichert: The importance of scientific terminology and concepts: TXRF new standard ISO 18115-4

3P16 – L. Szabó: Methodological advances in microplastic analysis of agricultural soils: preliminary results using sample preparation, automated image analysis, and Raman spectroscopy

Poster session 4P - Materials, geoscience and cultural heritage
Chairs: Viktor G. Mihucz, Gábor Galbács

4P01 – B. Żelazko: Comparative elemental analysis of eighteenth-century inks in historical handwritten documents by X-ray fluorescence spectrometry

4P02 – M. Švecova: From instability to reliability: oxidative modification of copper SERS substrates

4P03 – P. Zima: Development of (LA)-ICP-MS analytical methodology for elemental analysis of historical silver coins and assessment of isotope analysis possibilities

4P04 – E. Maťaš: Rapid IMS-MS analysis of thermal degradation in biodegradable polymers

4P05 – V. Grossová: Laser-based detection and imaging of microplastics in cave sediment matrices

4P06 – K. Csonka: investigation of the photochemical transformation of substituted benzoquinone and anthraquinone derivatives and LC–MS/MS-based identification of reaction products

4P07 – M. Kudor: Mössbauer and XRD investigations of Eu-doped goethites for novel battery electrodes

4P08 – P. Hać: Isotope dilution-assisted LC-HRMS fingerprinting of selenized yeast

4P09 – R. Sevcik: Comprehensive investigation of the carbonation reaction of lime pastes produced by modern and traditional technologies

4P10 – M. Horvath: Biocompatible composite protective thin layer based on cellulose matrix reinforcing with silica cryogel

4P11 – P. Mácová: FTIR analysis and micro-Raman mapping of organosilane-based additives in geopolymers

4P12 – V. Kóródi: Structure and thermal decomposition studies of different [hexakis(urea-o)iron(III)] complexes

4P13 – F. Herczeg: Hypothesized metasomatic alteration of olivine minerals in carbonaceous chondrite meteorites

4P14 – M. Zabielska-Konopka: Urban mining of mobile phones: determination of palladium and platinum in printed circuit boards by atomic absorption spectrometry

4P15 – M. Kmetík: Effect of environmental conditions on the stability of forensic samples studied by vibrational spectroscopy

4P16 – L. Bauer: Pollution-driven soil organic matter restructuring alters organic micropollutant sorption in agricultural soil

Thursday, September 3, 2026.

09:00-09:45 **Plenary talk** - László Drahos: Current trends in mass spectrometry

Oral session 12A - Advanced mass spectroscopy
Chair: László Drahos

10:00-10:40 **Keynote 12A** – M.A.Z. Arruda: Speciomics: integrating elemental and molecular mass spectrometry for comprehensive chemical species analysis

10:40-11:00 12A1 – S. Musil: Photochemical vapor generation coupled with DART-HRMS: identification of volatile species of transition metals and potential for their sensitive determination

11:00-11:20 12A2 – M.F. Mesko: Determination of halogens and their species by mass spectrometric techniques: sample preparation strategies

11:20-11:40 12A3 – L. Márk: Single cell imaging mass spectrometry

12:00-12:20 **Closing ceremony**

ORAL PRESENTATIONS

THREE DECADES OF NANOSCALE RAMAN SPECTROSCOPY: LIMITS, LESSONS AND OPPORTUNITIES

Volker Deckert

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Nanoscale Raman spectroscopy emerged from the ambition to combine the chemical specificity of vibrational spectroscopy with spatial resolution far below the diffraction limit. From the perspective of its early development, this lecture revisits the field beginning with aperture-based scanning near-field optical microscopy (SNOM) Raman experiments of the late 1990s and follows its evolution toward tip-enhanced Raman spectroscopy (TERS) and current near-field concepts. The emphasis is not only on milestones, but on the questions that have accompanied the field from the beginning, and still drive the field: what can genuinely be measured on the nanoscale, under which experimental conditions, and with what level of confidence? Early aperture-based approaches demonstrated that subwavelength Raman imaging and localized optical spectroscopy were possible, while also making clear the practical costs in signal, probe performance, and experimental complexity. The move toward tip-enhanced concepts expanded sensitivity and spatial resolution and changed the perception of what nanoscale Raman spectroscopy might achieve, and questions regarding reproducibility, interpretation, and methodological boundaries came up. In this lecture I will discuss how these opportunities and challenges have jointly shaped the field and continue to define its scientific value.

OMICS SCIENCES IN THE ERA OF ARTIFICIAL INTELLIGENCE: AN ANALYTICAL CHEMISTRY PERSPECTIVE

Ewa Bulska

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The integration of analytical chemistry with omics sciences represents a major advancement in biomedical research, enabling comprehensive, multi-level characterization of biological systems and their responses to pharmacological, nutritional, and pathological factors. In this framework, high-resolution analytical techniques, particularly mass spectrometry coupled with advanced bioinformatic processing, provide access to large and complex datasets describing proteomic and metabolomic changes across tissues and biological conditions. Such approaches create new opportunities for the study of disease mechanisms, biomarker discovery, safety assessment of medicinal products, and the development of precision medicine.

At the same time, the scientific and practical value of omics data depends not only on technological sophistication, but above all on the quality, comparability, and interpretability of the results obtained. For this reason, metrology rules emains a fundamental component of contemporary biomedical analytics. Measurement traceability, validated analytical procedures, appropriate calibration strategies, estimation of uncertainty, and the use of reference materials are essential for ensuring that molecular data are reliable, reproducible, and suitable for meaningful biological and clinical interpretation. This requirement becomes even more important in the era of artificial intelligence, where algorithmic performance is directly dependent on the quality and consistency of the input data. Artificial intelligence may significantly enhance pattern recognition, classification, and predictive modeling in omics research, but it cannot compensate for poor analytical design, lack of standardization, or insufficient control of measurement uncertainty.

In this sense, trustworthy AI-driven conclusions can only emerge from metrologically sound experimental foundations. From a broader scientific and industrial perspective, omics sciences offer substantial potential for translational applications, including improved drug safety evaluation, more precise patient stratification, and better understanding of complex disorders characterized by systemic molecular dysregulation. However, important limitations still remain, particularly with regard to standardization of workflows, interlaboratory comparability, reproducibility of large-scale datasets, and the conversion of molecular signatures into clinically actionable and regulatorily acceptable outcomes. Therefore, future progress in this field requires not only further analytical and computational innovation, but also a strong commitment to metrological rigor as the basis for credible results, responsible interpretation, and effective implementation in both clinical practice and industrial research.

FTIR AND LIBS DATA FUSION – A CHEMOMETRIC APPROACH FOR THE CLASSIFICATION OF POLYIMIDES IN THE SEMICONDUCTOR INDUSTRY

Cornelia Jakopin[1,2*], Eva-Maria Henn[3], Maximilian Podsednik[2], Lars Varain[2], Lukas Brunnbauer[1*], Andreas Limbeck[1]

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Fourier-transform infrared (FTIR) spectroscopy is a well-established analytical method characterized by its speed and simplicity in implementation. When combined with laser induced breakdown spectroscopy (LIBS), a method renowned for its fast elemental analysis and relatively high sensitivity, a more comprehensive multimodal framework is formed. This study demonstrates the application of this hybrid approach for polyimide classification in the semiconductor industry [1].

This methodological approach addresses inherent limitations of single technique analysis. Spectral preprocessing protocols were optimized for each technique prior to data fusion accounting for differences in baseline correction. Dimensionality reduction through targeted feature integration and principal component analysis (PCA) identified key discriminatory wavelengths and emission lines. Random forest (RF) and linear discriminant analysis (LDA) were subsequently applied for classification, enabling accurate sample discrimination and quality assessement [2].

This methodology provides a transferable framework for industrial quality control applications requiring comprehensive chemical characterization.

[1] X. Xu, M. Fei, Z. Jianmin, D. Changwen, *Anal. Methods*, 18 (2026) 1003.
[2] C.A.M. Ramirez, M. Greenop, A. Lorna, R. Ihtesham., *Appl. Spectrosc. Rev.*, 56 (2021) 733.

IMPROVING MAJOR ELEMENT QUANTIFICATION IN COMPLEX GEOMATERIALS VIA PORTABLE LIBS–XRF DATA FUSION

Yonghwi Kim*, Cécile Fabre, Jean Cauzid

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Portable X-ray fluorescence (pXRF) and laser-induced breakdown spectroscopy (pLIBS) have become integral tools for on-site geochemical analysis, enabling rapid decision-making during mineral exploration. However, the quantitative reliability of pLIBS is frequently compromised by spectrochemical matrix effects in heterogeneous geological materials, where physical and chemical variations may introduce non-linearity in emission signals. This work is carried out within the EU Horizon Europe project DeepBEAT (Deep exploration Boosted by Advanced exploration Technologies), which develops advanced analytical and geochemical technologies to improve the detection of deep-seated mineral deposits. In this study, we present a calibration framework designed to mitigate these effects by integrating pXRF compositional data as a chemical-proximity prior to guide the selection of matrix-matched reference standards.

The proposed methodology operates within a multi-dimensional compositional space defined by major lithogenic constituents. The method is based on reference samples having been measured with pLIBS and pXRF, most of which have also been analysed by laboratory wet chemistry. For each unknown sample, the XRF quantitative data is compared to that of reference samples using a Euclidean distance threshold. The algorithm then identifies the most relevant reference samples, ensuring that the calibration ensemble shares a similar chemical matrix with the target and that the unknown is interpolated rather than extrapolated. The selected reference samples are used to build a calibration line linking the LIBS signal to elemental concentrations, which is used to determine the final composition of the unknown samples.

This framework was validated using a suite of monomineralic reference samples and complex alteration rock samples from porphyry-to-epithermal systems in Greece. Analytical data were acquired using pLIBS (SciAps Z-300) and pXRF (SciAps X-250) instruments, with Standard Normal Variate normalization applied to the pLIBS spectra to mitigate fluctuations in plasma–sample coupling. Validation against laboratory ICP-OES reference concentrations demonstrated that the partial calibration approach reduced the overall mean absolute error by approximately 40% relative to conventional global models. The most pronounced improvements were observed for major matrix-forming elements (e.g., Si, Al, Ca, Fe), for which conventional global models are most susceptible to compositional bias. These findings confirm that pXRF-informed local regression effectively compensates for matrix effects in the pLIBS response across diverse lithologies. The workflow is entirely field-compatible, allowing exploration geologists to leverage previously characterized reference materials, including project-specific samples from earlier campaigns, to provide defensible, quantitative data that narrows the gap between portable sensors and laboratory-grade geochemistry for major elements.

This research was part of the project DeepBEAT. The project received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101177617.

DUAL-DOMAIN SPECTRAL DATA FUSION OF ICP-OES AND FTIR VIA CHEMOMETRIC EMBEDDING FOR ROBUST ENVIRONMENTAL SOURCE DISCRIMINATION AND MULTI-SCALE FINGERPRINTING

Ali Khezr pour

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Reliable characterization of complex environmental matrices requires analytical strategies capable of integrating complementary information from both elemental and molecular domains. However, most conventional approaches treat atomic and molecular spectroscopic data independently, limiting the depth of interpretability and reducing classification robustness in heterogeneous samples. In this study, we introduce a dual-domain spectral data fusion framework that integrates inductively coupled plasma optical emission spectroscopy (ICP-OES) and Fourier transform infrared spectroscopy (FTIR) through a unified chemometric embedding strategy. Unlike conventional sequential or independent analysis pipelines, the proposed approach constructs a joint latent feature space in which elemental signatures and molecular vibrational patterns are co-represented for enhanced discriminatory power. To achieve this, raw spectral data were preprocessed and aligned using standardized normalization and feature scaling procedures, followed by dimensionality reduction and latent structure extraction through principal component analysis (PCA). Subsequently, a supervised orthogonal partial least squares discriminant analysis (OPLS-DA) model was developed on the fused feature matrix to enable high-resolution classification of environmental samples.

The methodology was validated using soil and surface water samples collected from industrial and agriculturally impacted regions exhibiting overlapping contamination profiles. The proposed fusion model achieved 96% classification accuracy, significantly outperforming single-technique models based solely on ICP-OES or FTIR data. Beyond classification performance, the integrated framework enabled simultaneous interpretation of elemental enrichment patterns (Fe, Mn, Zn, Cu) and molecular-level perturbations associated with organic pollutant exposure, demonstrating improved mechanistic interpretability of environmental degradation processes. This work highlights the potential of cross-domain spectral fusion combined with chemometric embedding as a powerful analytical paradigm for multi-scale environmental fingerprinting and complex matrix discrimination.

COMPREHENSIVE ELEMENTAL AND ISOTOPIC CHARACTERIZATION OF U.S. EAST COAST HONEYS

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Honey represents a natural product that integrates environmental information through plant–soil–atmosphere interactions and can therefore serve as a bioindicator of its production environment. In this study, 121 honey samples collected from the eastern United States between 2017 and 2019 were analyzed to evaluate their elemental composition and isotopic characteristics for environmental assessment and origin determination. Elemental concentrations of 27 elements were determined using ICP-OES and ICP-MS following acid digestion, while MC-ICP-MS measured strontium and lead isotope ratios after chromatographic separation.

Potassium was identified as the dominant element, accounting for the majority of the total mineral content, reflecting its strong botanical origin. Aluminium showed spatial variation associated with regional soil characteristics, while toxic elements were generally present at low concentrations, with only a single sample exceeding established health limits. Multivariate statistical analysis (PCA, CDA) demonstrated that elemental composition enabled clear differentiation by botanical origin, whereas geographical discrimination was limited at broader scales but improved at finer spatial resolutions. Elemental profiling alone was not sufficient for reliable identification of adulteration due to high natural variability among samples. The measured 87Sr/86Sr ratios reflected large-scale geological patterns; however, their applicability for precise provenance determination was constrained by overlapping ranges, heterogeneous foraging areas, and agricultural influences. Lead isotope ratios indicated predominantly anthropogenic sources, consistent with legacy emissions.

These results confirm that honey acts as a complex geochemical archive integrating environmental and anthropogenic signals. The combined application of elemental and isotopic analysis provides valuable information for environmental monitoring, food safety, and traceability, although limitations remain for high-resolution geographic assignment.

COMPLEX ANALYTICAL INVESTIGATION OF NATURAL AND ARTIFICIAL SWEETENERS

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The market for commercial sweeteners has been expanding rapidly, encompassing products that range from minimally processed natural substances to entirely synthetic compounds. This diversification creates growing difficulties in verifying authenticity and determining origin. Traditional analytical methods typically depend on single-parameter measurements, which are often inadequate for distinguishing between samples with overlapping compositional characteristics influenced by plant source, processing level, and formulation techniques. In present work, a comprehensive analytical strategy was employed to investigate a wide selection of commercially available sweeteners. The approach combined elemental analysis using inductively coupled plasma optical emission spectrometry, stable carbon isotope ratio determination, radiocarbon-based assessment of biogenic carbon content, and attenuated total reflectance Fourier-transform infrared spectroscopy supported by multivariate chemometric evaluation.

The elemental composition patterns revealed consistent differences among sweetener groups, reflecting both their raw material origins and the extent of processing. At the same time, $\delta^{13}C$ measurements offered additional insight into the nature of the carbon sources. Radiocarbon analysis proved particularly valuable, as it allowed clear differentiation between contemporary biogenic carbon and fossil-derived carbon—an essential distinction in the case of highly refined or synthetic sweeteners that cannot be reliably classified using stable isotope data alone. Chemometric models based on FTIR spectra showed strong potential as rapid screening tools, enabling accurate classification of samples and helping to identify those requiring more detailed and resource-intensive isotopic investigations. By integrating elemental, isotopic, and spectroscopic datasets, a coherent and interpretable classification system was achieved, reflecting both processing intensity and origin-related characteristics. Overall, this study demonstrates the advantages of combining complementary analytical techniques and proposes a transferable framework for authenticity verification, quality assurance, and risk-based monitoring of sweeteners within complex food matrices.

Acknowledgements
Ágota Dienes was supported by the the KDP-2023 program of the Ministry for Culture and Innovation from the source of the National Research, Development and Innovation Fund and the PhD Excellence Scholarship from the Count István Tisza Foundation for the University of Debrecen.

EVALUATION OF *IN VITRO* BIOACCESSIBILITY OF ESSENTIAL AND TOXIC ELEMENTS IN INSECTS BY MIP OES: INTEGRATION WITH LC-MS/MS POLYPHENOL PROFILING

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In recent years, insects have gained increasing attention as a sustainable alternative protein source, providing not only high-quality proteins but also essential nutrients such as minerals and bioactive compounds. However, they may also bioaccumulate toxic elements from the environment. Therefore, assessing the bioaccessible fraction of both essential and toxic elements is crucial from a food quality perspective. Bioaccessibility is defined as the fraction released from the food matrix into the gastrointestinal tract and potentially available for absorption.

In this study, the *in vitro* bioaccessibility of aluminium, copper, iron, lead, manganese, and zinc was evaluated in three insect species (*Chromacris speciosa*, *Diloboderus abderus*, and *Gryllus assimilis*) collected in Uruguay. Samples were lyophilized, homogenized, and subjected to a two-step simulated gastrointestinal digestion (gastric and intestinal phases) based on the international INFOGEST protocol. Total element concentrations in samples and digestion residues were determined after microwave-assisted acid digestion.

Elemental analysis was carried out by microwave-induced plasma optical emission spectrometry (MIP OES), using an Agilent 4210 system. Instrumental parameters were optimized for each element, and analytical performance allowed reliable determination of bioaccessible fractions. The obtained results were consistent with previous findings reported for similar European species.

Additionally, a set of eight polyphenolic compounds (caffeic, chlorogenic, 4-hydroxybenzoic, gallic, sinapic, ferulic, p-coumaric and syringic acids) was targeted and determined by LC-MS/MS following microwave-assisted extraction in a methanol:water mixture. Method development included optimization of extraction and mass spectrometric parameters to ensure adequate sensitivity and selectivity. This complementary approach aims to explore potential correlations between polyphenol content and elemental bioaccessibility.

Overall, this study proposes an integrated analytical strategy combining elemental analysis and targeted metabolite profiling to better understand the nutritional and functional properties of edible insects as sustainable food sources.

THE EFFECT OF SALT STRESS ON THE PHOTOSYNTHETIC ACTIVITY, PIGMENT CONTENT, GREENING AND ION (Na^+ AND K^+) UPTAKE OF LIGHT-GROWN, DARK-GROWN AND GREENING WHEAT SEEDLINGS

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High soil salinity is an increasing threat to agricultural productivity, which is already affecting more than 1.1 billion hectares of soil worldwide. Salts primarily interact with underground organs like roots but can also affect directly the leaves of young seedlings germinating in the soil in case of tsunamis, saltwater flooding or seawater seepage to agricultural lands.

Our recent studies on young light-grown, dark-grown or greening wheat (*Triticum aestivum* L. Mv. Béres) seedlings have clearly demonstrated that floating their excised leaves on 600 mM NaCl:KCl (1:1) solution for 4 h differently affected the structure and function as well as the light-induced transformation of their plastids [1]. The so-called etioplasts of dark-germinated seedlings were the most prone to the salt stress treatment in the dark, with spectacular swelling of their inner membranes called prothylakoids, while this swelling was absent from the chloroplast membranes of the light-grown green leaves and of transitional etio-chloroplasts of greening dark-grown samples after they established a functional photosynthetic apparatus [1]. Detailed investigations based on 77K fluorescence spectroscopy of chlorophyllous pigments in the leaves of dark-grown seedlings exposed to various salt types and concentrations revealed that the inhibition of greening, chlorophyll (Chl) biosynthesis and the prothylakoid swelling is associated mostly with high concentrations of Na^+ [2]. Therefore, using ICP-MS we compared ion uptake by light-grown, dark-grown and greening wheat leaves treated with the above solution in the dark for 4 h or in the light (in case of light-grown seedlings). Interestingly, dark-grown seedlings had the lowest Na^+ concentrations among the salt stressed samples. Further ultrastructural and functional analyses were performed to understand how salinity affected gas exchange, photosynthetic parameters and photosynthetic pigments in the different studied samples. Our data outline which plant developmental stages are more susceptible to salt stress, provide advice on salts to be used as environment-friendly ice-melting compounds on roads, and in the long-term might contribute to the development of sustainable agricultural protocols for growing plants on salt affected lands, and to the breeding of salt-resilient crops.

Acknowledgements
This work was financed by the NKKP Advanced Grant 153509 of the National Research, Development and Innovation Office (NRDIO).

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DETECTION OF DNA HYBRIDIZATION WITH ALKYNE-LABELLING AND RAMAN SPECTROSCOPY

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DNA hybridization is a technique used in molecular biology to measure the degree of genetic similarity between DNA sequences. It involves the mixing of a known single-stranded probe DNA sequence with the sample DNA; followed by the denaturation of the sample DNA and the re-establishment of the hydrogen bonds (hybridization) with the probe strand. Successful hybridization means that the probe and sample strands are complementary, and it is a clear confirmation that the sequence in question is present in the sample DNA. In most cases, hybridization is detected by well-known polymerase chain reactions and other techniques.

Here we report on a Raman spectroscopy-based method in which the probe strand is labeled with an alkyne group and the hybridization is detected through the changes in the parameters of the alkyne Raman peak, occurring during the hydrogen bond formation [1].

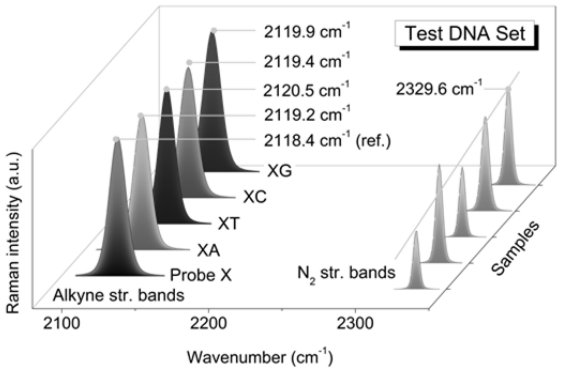

Figure 1. Curve-fitted alkyne Raman bands (C≡C stretching vibrations) of the DNA set for SNV detection, and molecular nitrogen Raman bands (N≡N stretching vibrations) used as an internal reference (N2 gas). The data for the fitting are obtained from baseline-corrected experimental Raman spectra of the oligonucleotides.

It was found that the variation of the peak position allows the distinction between the complete and imperfect hybridizations of the probe and sample DNA strands, and so the identification of mutations in the sample strand (Figure 1). Therefore, our method is capable of the detection of single-nucleotide variants or SNVs (substitution of a single nucleotide at a specific position in the DNA sequence). On the other hand, probes tagged with different alkyne groups having distinct Raman signals can be used for simultaneous detection of multiple DNA sequences in the sample.

Acknowledgments
The work was supported by the EU H2020 FET-Open 712821 NEURAM project, and the NKFIH-468-3/2021 NAPLIFE, VEKOP-2.3.3-15-2016-00002 and TKP2021-NVA-04 grants of the National Research, Development and Innovation Office of Hungary.

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INFRARED SPECTROSCOPIC MEASUREMENT OF ISOLATED SURFACTANT PROTEIN A AND D FOR PREDICTIVE QUANTIFICATION MODELLING

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Respiratory distress syndrome (RDS) can arise from surfactant deficiency. Surfactant quality can be rapidly assessed using the lecithin-to-sphingomyelin (L/S) ratio [1]. Infrared spectroscopy, combined with machine learning models, offers a promising route to quantify the L/S ratio rapidly at the bedside. Human lung surfactant samples also contain surfactant proteins A (SP-A) and D (SP-D) that are known to be dysregulated in RDS [2]. It is therefore imperative that these proteins are spectroscopically characterised to understand how their spectra interact with lipid components of surfactant so that both can be rapidly quantified.

We now report the first attenuated total reflection Fourier transform infrared (ATR-FTIR) spectroscopic study of dried recombinant human SP-A and recombinant fragment of human SP-D (Figure 1A.) that were originally purchased stored in Tris-HCl buffer with salts. The buffer components gave rise to spectral features overlapping the protein spectrum so buffer exchange was performed using distilled water, and the dried protein spectra were subsequently acquired (Figure 1A). The purified SP-A and SP-D share some spectral peaks with the human derived surfactant samples as well as S and L as denoted by P underneath the dashed line in Fig. 1B. The buffer components which had strong peaks in the 1650 cm^{-1} to 1300 cm^{-1} were not present indicating their complete removal after dialysis.

In summary, the results show that the presence of protein peaks in the human derived sufactant samples match with those observed in SP-A and SP-D. This will help build a robust machine learning calibration model for the quantification of lipids and proteins in human surfactant samples.

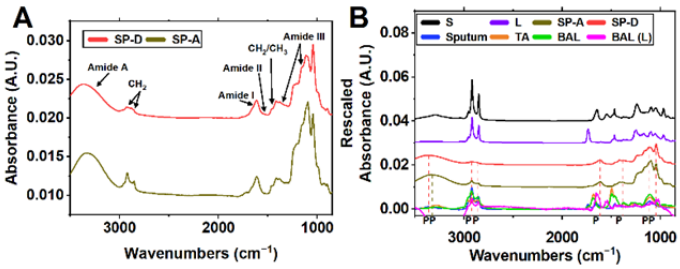

Figure 1. (A) ATR-FTIR spectra of dried SP-A and SP-D (B) Comparison of S and L spectra with dried sputum, tracheal aspirate (TA), bronchoalveolar lavage (BAL) and neat liquid BAL (BAL (L)) from healthy human volunteers. P below the dashed line denotes peaks attributed to proteins (SP-A and SP-D).

Acknowledgments
The authors would like to acknowledge funding support received from the UK EPSRC grant EP/S03109X/1 and NIHR Southampton BRC Perioperative and Critical Care Theme.

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APPLICATION OF FTIR SPECTROSCOPY IN MEDICINE

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Fourier transform infrared (FTIR) spectroscopy has evolved into a key analytical technique in medical laboratories, particularly where rapid and reliable chemical characterization of solid and semi-solid biological samples is required. Its high structural specificity, minimal sample preparation requirements, and compatibility with very small sample amounts make FTIR spectroscopy well suited for both routine diagnostics and advanced biomedical research. This contribution demonstrates selected medical applications of FTIR spectroscopy, with a particular focus on the analysis of biological concretions of organic and inorganic origin [1–4].

In concretion analysis, FTIR spectroscopy is considered a reference method for the identification of urinary stones. It enables robust discrimination among major mineral phases such as calcium oxalates (whewellite, weddellite), calcium phosphates (apatite, brushite), urates, and struvite, including mixed and layered compositions commonly encountered in clinical samples. In our laboratory, approximately 360 urinary stone samples are analyzed annually, with calcium oxalates being the predominant components (whewellite ~75 %, weddellite ~38 %), followed by phosphates (~20 %) and urates (~15 %). In addition to common stone types, FTIR spectroscopy allows reliable identification of rare and atypical urinary concretions, including cystine, pyrophosphate or cyanoacrylate-based materials, as well as concretions originating from other organs and tissues, such as the gastrointestinal tract, endocrine glands, cartillages and tendons, lungs, or testes.

In summary, FTIR spectroscopy serves as a powerful bridge between analytical chemistry and clinical diagnostics. Its versatility, speed, and high informational value make it a valuable tool for both routine medical analysis and advanced research applications, confirming its important role in modern medicine.

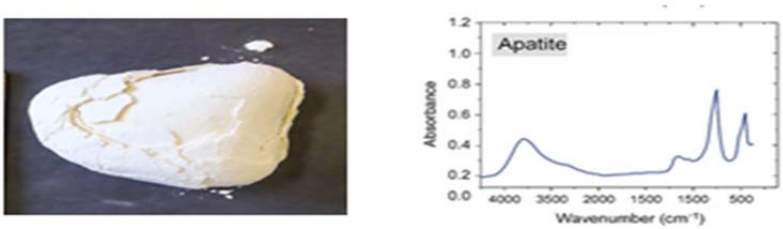

Figure 1. Representative photo and FTIR spectra of apatite concrement

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OPTICAL SPECTROSCOPY OF INDIVIDUAL NANOPARTICLES: INSIGHTS INTO STRUCTURE, DYNAMICS, AND SURFACE CHEMISTRY AT THE NANOSCALE

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Understanding nanoscale materials requires characterization techniques that can access the behaviour of individual nano-objects rather than ensemble averages. Single-particle spectroscopy directly probes the optical response of individual nanostructures, enabling detailed investigations of structure–property relationships at the nanoscale.

In this presentation it is demonstrated how single-particle optical spectroscopy can be used to extract information about the nanoscale molecular coverage, arrangement and local environment around nanostructures - insights often inaccessible through ensemble measurements. Detailed analysis of plasmonic nanoparticles' scattering spectra can reveal how molecules accumulate at the particles' surface [1,2]. Fine-tuning of this modification process can translate into spatially modulated colloidal interactions, allowing directional control during the self-assembly of nanoparticles, which can be also monitored in-situ by spectroscopy at the individual particle level [3,4]. The spectroscopic approach can be also utilized to follow the structural evolution of photocatalytical active oxide-semiconductor/gold heteroparticles [5,6] and to characterize the SERS-performance of nanostructured surfaces [7].

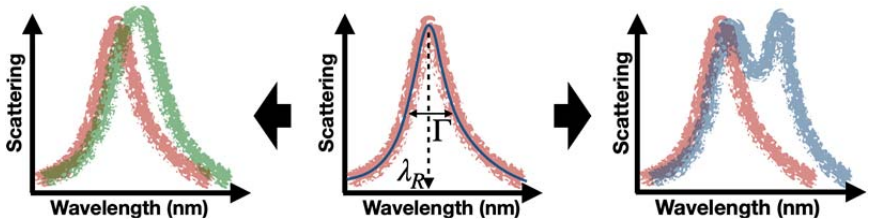

Figure 1. Optical changes of the scattering spectrum upon molecule adsorption or particle-assembly formation

Acknowledgements
Projects OTKA FK 142148 and NKKP Advanced 153064 received support from the Ministry of Culture and Innovation of Hungary from the National Research, Development, and Innovation Fund (NRDI).

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REAL-TIME SERS MONITORING OF PLASMONIC COUPLING DURING THIOCYNATE-INDUCED GOLD NANOPRTICLE AGGREGATION

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Gold nanoparticle (AuNP) aggregation is one of the most effective strategies for enhancing surface-enhanced Raman scattering (SERS) through the generation of plasmonic hot spots. Understanding the mechanisms governing aggregation and the resulting plasmonic interactions is therefore essential for the development of highly sensitive sensing platforms. In this work, we investigate the interaction of thiocyanate ions (SCN^-) with 30 nm colloidal AuNPs in the presence of potassium thiocyanate (KSCN) and sodium thiocyanate (NaSCN), focusing on their adsorption geometry and influence on SERS activity.

As the most chaotropic anion in the Hofmeister series, SCN^- exhibits a dual functionality. First, it promotes nanoparticle aggregation while preventing irreversible agglomeration, enabling controlled formation of interparticle junctions that act as plasmonic hot spots. Second, due to its intrinsic Raman activity, SCN^- serves as an internal SERS probe, allowing real-time monitoring of hot-spot formation without the need for additional reporter molecules. Assuming that the nanoparticles preserve their size and morphology during aggregation, we attribute the observed SERS enhancement primarily to interparticle spacing and plasmonic coupling.

Spectra in Figure 1. reveals two peaks for SCN^- at 2120 cm^{-1} and 2150 cm^{-1} for different configurations with enhancement factors of approximately 70- and 40-fold, respectively.

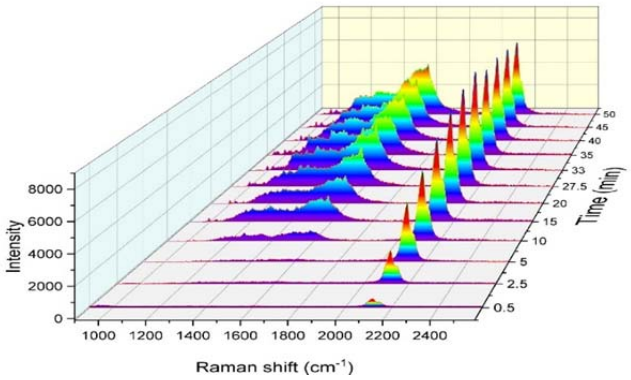

Figure 1. Evolution of the SERS signal for KSCN salt (37.5 mM) in 30 nm gold colloid with time duration 50 minutes.

FUNDAMENTAL STUDIES USING NITROGEN AS PLASMA GAS FOR ICP-MS AND AS CARRIER GAS FOR LASER AEROSOLS

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Laser Ablation Inductively Coupled Plasma Spectrometry (LA-ICP-MS) is one of the most widely applied techniques for trace element analysis and routinely applied in geology, environmental and materials sciences and is entering the biomedical research, especially imaging of various tissue samples. Some of the imaging capabilities has become possible by using the latest generation of time-of-flight mass spectrometers (TOFMS) in combination with low dispersion laser ablation cells.

Latest developments have focused on substituting the well-known argon plasma source by a nitrogen plasma, which substantially reduces Argon interferences and opens new opportunities of operation. Some experiments and their outcomes on such the nitrogen plasma source will be presented and compared to the conventional argon plasma.

The benefits of the nitrogen plasma in combination with low-disperson ablation cells open new capabilities in terms of aerosol carrier (e.g. nitrogen) to the inductively coupled plasma. The determination of the transport efficiency of laser aerosols have become possible and will be reported for nitrogen and helium. Furthermore, imaging techniques allow to investigate non-stoichiometric effects, which will be discussed in the presentation.

Furthermore, a change of the orientation of the ICP (nitrogen and argon plasma) has been realized and a downwards pointing plasma prototype instrument has been realized in our lab. Results of the new capabilities of sample introduction of micron-sized samples will be presented.

QUANTITATIVE LA-ICP-MS ANALYSIS OF STRATEGIC MINERALS USING TAILOR-MADE GLASS REFERENCE MATERIALS

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Strategic raw materials play a key role in current and future energy technologies, including Li-bearing minerals for battery production and U-rich phases relevant to nuclear-energy and geochronological applications. Reliable elemental and isotopic analysis of these materials is essential for resource evaluation, processing and understanding the origin of ore deposits. In U-rich minerals such as uraninite, U-Pb dating provides information on the timing of mineralisation, which is crucial for genetic models of ore formation and exploration of new resources.

LA-ICP-MS is a powerful tool for in situ analysis of geological and technological materials, but accurate quantification is affected by laser-sample interaction, aerosol generation, transport efficiency and matrix-dependent elemental fractionation. Reference glasses such as NIST SRM 610 provide excellent reproducibility, but their composition and ablation behaviour do not fully represent Li-rich aluminosilicates or U/Pb-rich phases. This mismatch may cause signal stability, calibration slope and quantitative accuracy.

This contribution evaluates the analytical performance of newly developed tailor-made glass reference materials in LA-ICP-MS applications relevant to strategic minerals. Li-rich glasses were tested for the quantification of petalite, spodumene and Li-rich micas, while U/Pb-rich glasses were considered for future applications in the analysis and dating of U-rich minerals. The focus is placed on the practical use of these materials as calibration standards, supported by SIMS imaging for the assessment of sample homogeneity and comparison with LA-ICP-MS results.

Special attention was paid to laser-material interaction and its effect on quantification. Ablation experiments using a 193 nm ArF excimer laser showed that Li-rich matrices require higher fluence for stable and reproducible ablation than NIST SRM 610. At low fluence, Li-rich glasses and natural minerals produced shallow or poorly reproducible craters, whereas higher fluences provided stable signals and well-defined crater geometries. The comparison between NIST SRM 610, tailor-made glasses and natural minerals demonstrates that matrix-relevant calibration can improve quantitative LA-ICP-MS analysis of strategic raw materials and supports the development of application-specific reference materials for geochemical and technological samples.

Acknowledgements
This work was supported by the Slovak Research and Development Agency APVV-22–006, the Horizon Europe project Li4Life under grant agreement No. 101137932, and by the CICRR infrastructure, financially supported by the Ministry of Education, Youth and Sports of the Czech Republic under project No. LM2023041.

LA-ICP-MS ANALYSIS OF IMPURITIES IN SiC MATERIALS: HOW DOES A MICRODROPLET GENERATOR APPROACH COMPARE TO STANDARD ADDITION?

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Semiconductors based on SiC are the leading alternatives to the traditionally used Si ones, owing to characteristics that can contribute to the production of optimized electronic devices in terms of efficiency, power, temperature and chip size [1]. The manufacturing of high-purity SiC is of critical importance since the level of impurities present can affect corrosion of SiC incorporated in electronic devices, thereby hampering its ability to maintain its structural integrity in extreme conditions [2].

The analysis of contaminations in technologically relevant materials is usually performed with ICP-MS, after preliminary conversion of the solid sample into a solution [3]. In the case of SiC this approach is extremely challenging due its inert nature. Alternatively, direct analysis of the solid material is possible with the aid of GD-MS or SIMS [4]. The advantage of these analytical methods is that they allow for spatially resolved investigations; however, the lack of certified reference materials (CRMs) required for accurate quantification can pose a significant limitation.

In this work, we present the combination of a microdroplet generator (MDG) with LA-ICP-MS for the quantification of elemental contamination levels on the surface and in the bulk of SiC wafers and grains. The major advantage of using an MDG is that we circumvent the need for a CRM, which in most cases is not available anyway. The microdroplets generated from a standard solution are delivered to the plasma through a tube with the aid of flowing gases (Ar, He) which dry the droplet during its transportation, thereby resulting in the formation of a dried residue with defined mass and composition. To account for variations in the ablation process, the target analyte signals are normalized to a major component, which is Si for SiC materials. When MDG is combined with LA-ICP-MS, various areas ranging from a few μm^2 up to several mm^2 can be measured with adjustable resolution, thereby elemental distribution information can be derived.

Herein, we compare the combination of an MDG with LA-ICP-MS to a standard addition approach, for the spatial quantification of elemental contaminants (Al, Zn, Cu, Pb, W, Ti) on the surface and in the bulk of SiC wafers and grains. The two standard addition approaches rely on the coating of the SiC samples with a thin polymer film containing the target analytes with known concentrations. Thin film deposition was conducted either *via* spraying [5] or spin coating [6] of respective standard solutions.

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SPECTRAL ANALYSIS OF HISTORICAL INKS ASSISTED BY MACHINE LEARNING

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A non-destructive analytical workflow was developed for the investigation of historical manuscripts written with iron-gall inks. The methodology combines indicator-paper sampling, laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS), and machine-learning (ML) data processing. Instead of direct sampling of valuable documents, chemical information was transferred from manuscript surfaces to specially prepared indicator papers acting as carriers of elemental signatures.

The indicator papers are then analysed using LA-ICP-MS to provide spatially resolved, multielemental data with high sensitivity and minimal material consumption. However, as the interaction between the ink components and the indicator substrate is governed by complex, nonlinear chemical processes, the measured signals cannot be directly interpreted as the composition of the original inks.

Machine-learning models were therefore trained using experimental datasets obtained from reference materials and historical samples, in order to decode this indirect analytical information. These models enabled the reconstruction of the elemental composition of the source inks and improved discrimination between different writing media.

The methodology was applied to manuscripts dating from the 11th to the 20th century, yielding information relevant to conservation assessment, ink discrimination, and studies of document history. The results demonstrated that combining the use of specific indicator papers and LA-ICP-MS with machine learning is a powerful approach for safely analysing documents.

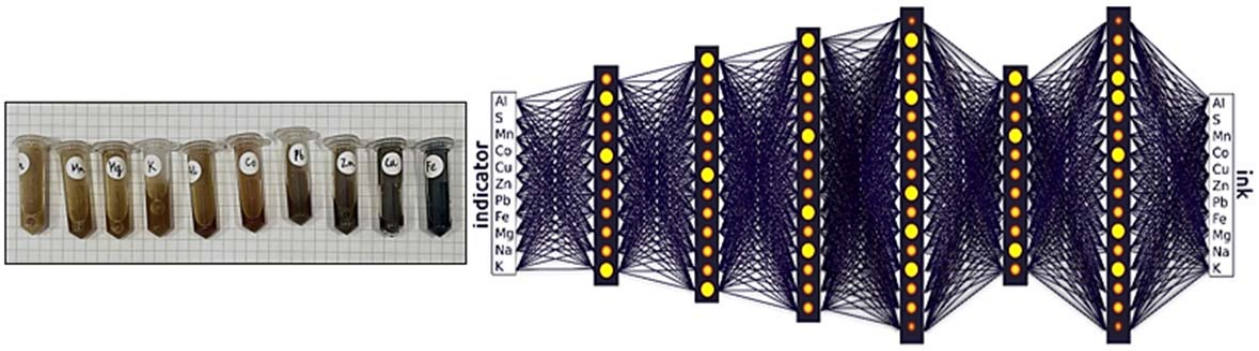

Figure 1. The picture of model ink solutions used to create mock-ups for indicator-paper sampling prior to LA-ICP-MS measurements and ML data processing

NEW GLASS REFERENCE MATERIALS FOR IN SITU ANALYSIS OF LITHIUM- AND URANIUM-RICH MINERALS

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Laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) is widely used for the determination of elemental and isotopic composition in geological materials. However, accurate quantification remains challenging when suitable matrix-matched reference materials are not available. This limitation is particularly relevant for lithium- and uranium-rich minerals, where commonly used reference glasses, such as NIST SRM 610, differ substantially in major-element composition and analyte concentration from natural samples.

This work presents the development and characterization of new silicate glass reference materials tailored for in situ analysis of Li- and U/Pb-rich mineral systems. The glasses were prepared in collaboration with the FunGlass research centre and designed to extend the calibration range beyond currently available commercial materials. Two compositional series were developed: Li-rich glasses intended for the analysis of Li-bearing minerals such as petalite, spodumene and Li-rich micas, and U/Pb-rich glasses aimed at applications involving U-rich minerals such as uraninite.

The prepared materials were characterized using a combination of bulk and microanalytical techniques. Major and trace element compositions were determined by XRF, ICP-OES and LA-ICP-MS, while micrometre-scale homogeneity was evaluated by LA-ICP-MS spot analyses and elemental mapping. Complementary micro-XRF measurements were used to verify the spatial distribution of selected elements. For U/Pb-rich glasses, SIMS measurements were applied to assess Pb isotope ratios and isotope homogeneity, which are essential for potential geochronological applications.

The results demonstrate that the prepared Li-rich glasses exhibit good microscale homogeneity for most investigated elements and show strong potential for LA-ICP-MS quantification of Li-bearing minerals. The U/Pb-rich glasses provide a promising basis for the development of reference materials suitable for in situ elemental and isotopic analysis of U-rich phases. Overall, the study shows that tailor-made glass standards represent a flexible and effective route toward improved calibration strategies in LA-ICP-MS and complementary in situ analytical techniques.

Acknowledgements
This work was supported by the Slovak Research and Development Agency APVV-22–006, the Horizon Europe project Li4Life under grant agreement No. 101137932, and by the CICRR infrastructure, financially supported by the Ministry of Education, Youth and Sports of the Czech Republic under project No. LM2023041.

PARTICLES – GOTTA CATCH 'EM ALL! PUSHING THE BOUNDARIES OF SINGLE PARTICLE METHODS

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Single particle ICP-MS has transformed our ability to interrogate complex particulate systems, offering highly sensitive and information-rich access to particles in a one-by-one fashion. Yet its applicability remains constrained by inherent limitations. These become particularly evident when targeting particles at both ends of the analysable size range, when particles have heterogeneous compositions or chemically relevant molecular identities. At the same time, the increasing scale and complexity of single particle datasets place growing demands on data treatment, interpretation and analytical confidence.

This presentation explores emerging strategies to expand the analytical scope of single particle analysis beyond these boundaries. These include approaches to retrieve molecular signatures and physical particle properties before particles are destroyed during ICP-MS analysis. In particular, complementary optical and spectroscopic methods, including in-line microscopy, Raman spectroscopy and optical trapping-based approaches, are introduced as routes to access particle-resolved information on size, morphology and chemical identity. In parallel, ICP-TOFMS and new data-processing pipelines are highlighted as powerful tools for screening complex samples for relevant particle populations and enabling in-depth characterisation.

By combining rapid elemental screening with orthogonal particle-resolved techniques, these approaches open new avenues for the analysis of biologically, environmentally and industrially relevant particles in complex real-world samples with greater selectivity, accuracy and interpretative depth. Rather than viewing ICP-MS as a standalone endpoint, this presentation advocates an integrated analytical strategy for deciphering complex particulate systems.

SINGLE-CELL LA-ICP-MS IN ASSESSING THE ELEMENTAL COMPOSITION OF THE ALGAE *G. SULPHURARIA*

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The unicellular thermo-acidophilic microalgae *Galdieria sulphuraria* (*G. sulphuraria*) attracted interest in biotechnology for various applications, as they not only produce bioactive compounds, but also can be used for the bioremediation of wastewater sources and the recovery of precious metals from industrial side streams. Due to their resilience under harsh conditions and their ability to utilize various metabolic pathways, *G. sulphuraria* are adaptable to different process conditions [1].

Currently, elemental quantification of cells in suspension, is typically performed via ICP-MS in the form of a bulk measurement. However, this method does not provide information pertinent to the individual cells but only average elemental content of the cell population. Thus, the assumption needs to be made, that the population of the cells is homogeneous and the average values are representative of the entirety of cells. As there are biological variations to be expected, the elemental concentration within the individual cells is of particular interest. Within recent years, Single Cell ICP-MS was developed, which is able to quantify the elemental composition of single cells in solution. However, the critical aspect is the introduction of single cells into the instrument to avoid multiple cell events. Another challenge is the precipitation of the cell mass over time, which influences the homogeneity of the solution. Furthermore, the instrumentation is not equipped to handle high loads of solid materials, which leads to nebulizer blockage [2, 3]. Single-cell analysis utilizing LA-ICP-MS is an emerging approach that has been reported for elemental quantification in mammalian [4] and human cell lines [5].

Herein, we present the development of a LA-ICP-MS method for the direct quantification of P, Mn and C content within single *G. sulphuraria cells* of the SAG 107.79 cell line. The algae are deposited on a 1x1 cm SiC wafer and subsequently immobilized using a cooling Peltier element within the laser chamber. This method creates a thin ice film containing the spatially separated cells. This approach enables the determination of elemental composition at the level of individual cells using LA-ICP-MS. Using ice films instead of other immobilisation methods allows for simple sample preparation, as no cell separation or laborious immobilization methods are needed. Method validation is performed by comparing population-averaged LA-ICP-MS results with bulk ICP-MS measurements [2, 4, 5].

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MULTI-TECHNIQUE APPROACH FOR ASSESSMENTS OF MIGRATION AND HUMAN EXPOSURE TO ZnO NANOPARTICLES FROM MEDICAL MATERIALS

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The use of metal-based nanomaterials has improved the optical, physicochemical, and biological properties of a wide range of medical and consumer products. Zinc oxide nanoparticles (ZnO NPs) are among the most widely used nanomaterials due to their ability to absorb ultraviolet (UV) radiation, high catalytic and photochemical activities, antibacterial properties, and low cost. Therefore, ZnONPs are widely used in personal care products such as cosmetics and sunscreens, as well as in sportswear, food packaging, medical products, wound healing agents, and drug delivery systems. However, the risks and benefits of using nanomaterials in medical disposable materials have not yet been fully recognized.

The presentation will show an analytical protocol developed to investigate the migration and transformation of ZnO NPs from medical products (face masks, typing tape, and polymeric fabric) into simulated biological fluids, such as artificial saliva and sweat, mimicking oral and dermal exposure to zinc species. For this purpose, a multi-technique analytical approach was employed.

Single-particle inductively coupled plasma mass spectrometry (sp ICP-MS) was used to determine the nano- and dissolved forms of zinc in migration solutions. The analytical characteristics of the sp-ICP Ms method, such as detection limits of the particle size, particle number concentration, and element mass concentration, were performed, and the zinc migration, including zinc ions and nanoparticle form, from the medical product was assessed. To complete and confirm the results obtained by sp ICP-MS, Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM) coupled with Energy-Dispersive X-ray spectroscopy (EDX), as well as X-ray diffraction (XRD) were applied.

The obtained data were used to assess human exposure to commercially relevant medical materials, such as typing tape, polymeric fabric, and face masks, that contain ZnO NPs. Exposure assessment considered both particulate and dissolved fractions, recognizing that transformation processes may affect bioavailability and toxicity of nanomaterials.

WEATHERING IMPACT ON URANIUM PARTICLES FROM SIERRA PENA BLANCA, MEXICO: A SYNCHROTRON-BASED STUDY

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The Sierra Peña Blanca (SPB) geological formation, in the state of Chihuahua, Mexico, contains about 40% of the country's uranium. Extensive uranium exploitation campaigns and mining activities have been taking place there until the early 1980s, when mining activities in the region closed. The extracted and unprocessed uranium ore, confined in a repository, and the ore in open-pit mines were left exposed to climatic conditions, with subsequent weathering, erosion and deposition phenomena. Obviously, such weathering also and primarily affects the geological formations, with their rocks submitted to their sedimentary rock cycle, leading to decomposition, alteration and fragmentation of the rock, which in turn allow for their subsequent erosion and displacement. The SPB formation is also an endorheic basin, and the area's hydrology favors the mechanical transport of the material exposed in the mines through the main streams to the Laguna del Cuervo. Consequently, characterizing the source and the transport of uranium in the environment is important both for health and environmental purposes, as is the evaluation of the potential contaminations from acid drainages generated by mining processes.

This work [1] investigates the transport of uranium by surface water through the main streams from the deposits in SPB to Laguna del Cuervo, concentrating on the fine sand fraction. Uranium particles were extracted by optical fluorescence from the fine sand, and were extensively characterized by a correlation of laboratory- and synchrotron-based techniques.

The uranium particles' density was quantified using gamma spectrometry, and their 238U activity established. Their morphology and elemental composition were analyzed using Focused Ion Beam electron microscopy and Scanning Transmission Electron Microscopy. The mineral phases associated with the fluorescent particles were characterized by X-ray diffraction and X-ray Absorption Spectroscopy (XANES and EXAFS). In particular, uranium oxidation state was thoroughly determined. Finally, XRF micro computed tomography was applied to reveal the 3D distribution of uranium, and other elements (e.g., Si, Ca, Fe, Sr) in the selected particles, the largest dimension of which not exceeding 55 micrometers. The data collected allowed to retrieve the uranium particles mineralogy, with uranophane as the most abundant U mineral present in a matrix, and its impact on 238U activity. They also shed some light on the transport of uranium minerals from SPB by surface water, and their potential toxicity.

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THE ELEMENT STRIKES BACK: ATOMIC SPECTROMETRY MEETS THE PFAS CHALLENGE

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Per- and polyfluoroalkyl substances (PFAS) are traditionally analysed by molecular mass spectrometry, with LC-MS/MS forming the basis of environmental monitoring and regulatory compliance. While these methods provide highly sensitive quantification of selected compounds, they often capture only a fraction of the fluorinated species present in environmental and biological systems and offer limited insight into fluorine mass balance, fluorinated polymers, volatile fluorinated compounds, or particulate fluorinated materials.

Recent developments are enabling a shift from molecule-centred to fluorine-centred analysis. This lecture will present emerging approaches based on atomic spectrometry and complementary fluorine-specific techniques that directly target fluorine irrespective of molecular structure. Particular emphasis will be placed on HR GFMAS, tandem ICP-MS/MS and negative-ion ICP-MS for fluorine detection and quantification.

The analytical toolbox will be extended by gas chromatography coupled to atomic emission detection (GC-AED) for volatile fluorinated compounds and by ^{19}F-NMR spectroscopy for direct structural characterization and quantification of fluorinated materials. Together, these approaches provide orthogonal information that complements conventional LC-MS workflows and contributes to fluorine mass balance assessments.

Applications will include the characterization of fluoropolymer micro- and nanoparticles by single-particle negative-ion ICP-MS (SP-nICP-MS), spatially resolved fluorine bioimaging in tissues using laser ablation ICP-MS (LA-ICP-MS), and the detection of previously overlooked fluorinated compounds and materials in environmental samples.

The lecture will demonstrate how fluorine-specific analytical methodologies are transforming our ability to investigate PFAS and other fluorinated substances. By combining elemental, structural, molecular, and particle-based information, these approaches provide new opportunities to quantify the unknown fluorine fraction and address some of the most pressing analytical challenges in environmental fluorine science.

MULTI-MODAL BAF^+-ICP-MS/MS: A COMPREHENSIVE ANALYTICAL PLATFORM FOR TRACING ENVIRONMENTAL PFAS, MICROPLASTICS, AND INORGANIC FLUORINE

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The reliable quantification and speciation of fluorine remain an analytical bottleneck in environmental chemistry due to the element's high ionisation potential and poor ionization efficiency in standard argon plasmas. While monitoring the polyatomic BaF^+ ion via tandem mass spectrometry (ICP-MS/MS) provides a viable alternative strategy, achieving matrix-independent accuracy requires mitigating complex plasma chemistry and transport phenomena. To resolve these challenges, this study presents a multi-modal analytical platform that standardizes BaF^+ signal generation across three sample introduction techniques: Liquid Chromatography (LC), Laser Ablation (LA), and Single Particle (SP) ICP-MS/MS. This unified framework enables the concurrent tracking of distinct fluorine fractions, ranging from molecular per- and polyfluoroalkyl substances (PFAS) and particulate fluorinated microplastics (MPs) to solid-bound inorganic fluorine.

Investigations into the system dynamics indicate that BaF^+ efficiency is governed primarily by aerosol formation and transport behaviour within the sample introduction interface, rather than intrinsic plasma chemistry alone. Modifying the sample introduction interface with a low-flow system eliminated the transport biases that typically compromise conventional pneumatic nebulization. For solid-state spatial analysis, an integrated dual LA-ICP-MS/MS and LIBS system delivers high-resolution fluorine mapping, enabling simultaneous optical and mass spectrometric profiling of both atomic (F 685.6 nm) and molecular (CaF 603 nm) emission lines alongside the mass shifted isotopes. Finally, by operating the platform in SP-ICP-MS mode, we demonstrate the high-throughput screening, sizing, and counting of individual fluorinated microparticles in complex matrices. Ultimately, this work delivers a validated strategy for non-target environmental monitoring, effectively bridging total fluorine screening and precise molecular speciation.

GRAPHITE FURNACE AND FLUORINE DETERMINATION: 2026

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During the previous ESAS conference, a talk was presented on the determination of fluorine using graphite furnace-based techniques [1]. The current presentation aims to show new results in the field, based on almost 20 new papers. The present role of graphite furnace-based techniques will be evaluated, the existing needs and limitations identified, and the possible directions of development determined.

The major topic will be the determination of fluorine in organic form using high-resolution continuum source graphite furnace molecular absorption spectrometry (HR-CS GFMAS). The important area of researchers' interest during the considered period was the analysis of extractable organic fluorine (EOF) as a sum parameter in the per- and polyalkyl substance (PFAS) mass balance approach [2-4]. Gallium [3-5] or calcium monofluoride [2] was used as the target molecule. Calcium monofluoride was also successfully used for the determination of unknown forms of organic fluorine in alkylate (a gasoline component) produced using HF technology [6].

The results of research will show the unknown face of the graphite furnace technique and sometimes „strange" phenomena, for example:

- increase of F-related signal with an increase of pyrolysis temperature,
- possible positive effect and usefulness of forming carbonaceous residue (usually recognised as a nightmare in direct analysis of high-carbon materials),
- lower losses of volatile organic F compounds/increase of F-related signal with increase of drying phase time,
- higher losses of less volatile F compounds in comparison with more volatile compounds

The major problem in the determination of organic forms of fluorine was a species-dependent signal. Huge efforts were undertaken to equalise the signals of fluorine species by optimising the analytical procedure [3-4] or by using external mineralisation [5]. However, the results were not always/fully effective.

A graphite furnace was also used for electrothermal evaporation of solid samples into an inductively coupled plasma-triple quadrupole mass spectrometer for measurement of fluorine via $^{138}Ba^{19}F^{+}$ [7].

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FTIR IMAGING FROM MICROPLASTICS TO MICROFIBERS: TACKLING SPECTRAL COMPLEXITY

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Microplastics analysis by chemical imaging techniques such as µFTIR has rapidly advanced with the integration of machine learning. However, the intrinsic variability in particle size, shape, and morphology—particularly for microfibers—introduces significant challenges for spectroscopic identification. Physical phenomena such as Mie scattering, resonant Mie scattering, and total absorbance can substantially distort infrared spectra, leading to misclassification, inaccurate particle contours, and fragmentation artifacts in automated workflows.

Machine learning offers a powerful alternative to conventional spectral library searches by capturing complex, non-linear relationships in spectroscopic data. Nevertheless, its performance strongly depends on the representativeness of training datasets and the ability to account for physically altered spectra. Recent approaches demonstrate that scattering and absorbance effects can be effectively modeled, improving robustness in the identification of both particles and fibers in environmental and textile-related samples.

In this presentation, we will explore examples of how the size and shape of microplastics and microfibers alter the appearance of IR spectra. Based on sampled polymer spectra, we will showcase how total absorbance and scattering effects can be modelled using machine learning. We will further discuss application cases of microfiber analysis in environmental samples and in residues from textile washing.

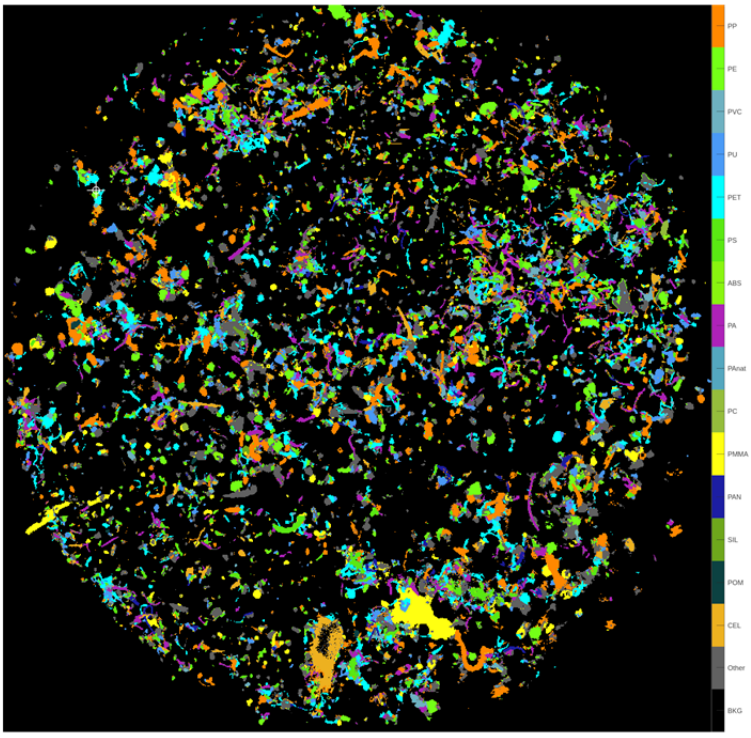

Figure 2: A complex environmental sample containing microplastics and microfibers

CLASSIFICATION OF CONTAMINATED PLASTIC MICROPARTICLES USING LASER INDUCED BREAKDOWN SPECTROSCOPY WITH MACHINE LEARNING ALGORITHMS

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The identification of microplastic particles is an important analytical task that could be particularly well-suited to LIBS. Whereas the usual Raman microscopy or hyperspectral imaging systems require specific labels or are very time consuming, LIBS offers fast measurements without any complex sample preparation steps [1]. LIBS is a laser- based atomic emission spectroscopy technique, but it can also give molecular information in the form of diatomic emission bands. With crater diameters as small as a few tens of micrometers, even truly microscopic particles are easily measureable.

The spectrum of samples collected from the environment is heavily influenced by the matrix it was collected from, making it much harder to identify the polymer type. There are ways to combat this, like the cleaning of the particles themselves before measurement or treating the collected spectra to emphasise polymer characteristics (feature selection). The sorting can be done with a variety of multivariate statistical approaches (e.g. principal component analyis, linear discrimination analysis, classification tree, etc.) [2,3].

In this project we set out to investigate how the classification of microplastic particles exposed to different environmental (synthetic seawater, industrial sewage sludge) or biological (synthetic gastric juice, artificial saliva) matrices can be performed. To improve the accuracy of the discrimination, several physical and chemical cleaning procedures were tested. We also assessed the performance of various feature selection approaches.

Acknowledgements
This work was funded by the National Research, Development and Innovation Office (NKFIH) of Hungary through projects OTKA K 146733, 2024-1.2.3-HU-RIZONT-2024-00032 and GINOP-2.3.3-15-2016-00040. O. Urbán and G. Galbács also thankfully acknowledge the support received from the Austrian Research Promotion Agency (FFG) in the frame of the Important Project of Common European Interest (IPCEI) on Microelectronics and Communication Technologies.

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DETERMINATION OF RARE EARTH ELEMENTS BY ICP-MS: NEW CHALLENGES AND TRENDS

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Rare earth elements (REE) have been used in industrial, geological, medical, and agricultural applications. For this reason, the mineral reserves exploration has increased significantly in the last years, which can naturally lead to an increase of the concentration of these elements in soil, water, and consequently in living beings. Given possible exposures, REE has been listed as "New and Emerging Risks to Occupational Safety and Health" by the European Agency for Safety and Health at Work (EU-OSHA). Nowadays, there is a need for suitable methods for the determination of rare earth elements (REE) in many matrices and some of the analytical techniques used for this purpose are neutron activation analysis (NAA), inductively coupled plasma optical emission spectrometry (ICP OES) and inductively coupled plasma mass spectrometry (ICP-MS). Inductively coupled plasma mass spectrometry can be considered as the most suitable technique for the determination of REE, enabling good sensitivity and multielement capability. The determination of REE by ICP-MS has been generally performed using nebulization systems, making necessary the use of high efficiency sample preparation methods with low acidity in final digests to minimize interferences. Additionally, it is well known that the digestion of some matrices having a high content of carbon as, e.g., crude oil, graphite, blood, bcarbon nanotubes, is not a simple task, making necessary very frequently the use of time-consuming sample preparation methods. Some options include the direct analysis by ETV-ICP-MS or using a high efficiency digestion system. Nowadays, there is a trend for the development of methods requiring lower reagent consumption, less analytical steps and lower waste generation combined with high efficiency of digestion. In addition, it is important obtaining digests that are suitable for determination techniques avoiding excessive dilution or higher blank levels. Taking into account the difficulties involved in REE determination in high carbon content matrices, modern methods and trends in sample preparation for food and biological samples will be discussed for further ICP-MS determination.

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ISOTOPIC AND ELEMENTAL COMPOSITION ANALYSIS OF HISTORICAL ARTIFACTS TO ENHANCE THE INTERPRETATION OF PAST RESEARCH FINDINGS

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The analysis of isotopic ratios and elemental composition is a key technique supporting provenance studies of archaeological artifacts (such as bronzes and ceramics) and the reconstruction of artwork histories. However, the representativeness of the results used to interpret an object's features is rarely addressed. A major limitation is that, due to the unique and irreplaceable value of historical objects, sampling is highly restricted, typically to a single sample from the entire artifact.

Although non-destructive methods seem ideal, they also involve significant technical and interpretative limitations. Therefore, compromise analytical strategies must be developed that both preserve the artifact and provide reliable, meaningful data.

So far, no studies have systematically evaluated how single-point sampling affects the reliability of data intended to represent an entire object. In this project, historical bronze and lead artifacts were analyzed: 16th-century stained-glass cames (18 samples), a 1st-century BCE bronze axe blade (21 samples), eight samples from a 17th-century Lebanese sarcophagus, and, with the cooperation of the National Maritime Museum in Gdańsk, 12 samples from a 17th-century naval cannon recovered from the Swedish galleon Solen, sunk during the Battle of Oliwa in 1627.

All samples were digested using microwave-assisted closed-vessel systems, then analyzed for elemental composition by ICP-MS and for lead isotopic ratios by MC-ICP-MS. The results were processed using dedicated statistical methods and uncertainty estimation.

The main aim of the study was to assess how well a single sample can represent the isotopic and elemental composition of an entire object, and to determine the level of uncertainty required for such data to be considered reliable.

3D-PRINTED NEBULIZERS FOR ICP-MS: FEASIBILITY, LIMITATIONS, AND ANALYTICAL PERFORMANCE

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The increasing popularity of single-particle ICP-MS has led to growing interest in alternative, high-efficiency sample introduction systems (SISs). Consequently, a number of studies have been published, aiming to develop novel SISs and methodologies to maximize transport efficiency [1,2]. Simultaneously, manufacturers have introduced product lines specifically for single particle analysis usually comprising of a single-pass spray chamber and a pneumatic nebulizer operated at 10-30 µL/min sample uptake rates. Nevertheless, both commercial and experimental approaches remain far from ideal, and an optimal solution to the sample introduction problem has yet to be established. Additive manufacturing is a rapid and cost-effective tool to produce analytical devices, enabling fast iterative prototyping and accelerating the development of improved SISs.

In this study two different types of pneumatic nebulizers (concentric and flow focusing) were developed and manufactured using 3D printing (material jetting) as alternatives to commercially available micronebulizers. First, the printing accuracy and piece-to-piece reproducibility of the nebulizers were evaluated using micro-computer tomography (µCT). Next, the aerosol output of the different designs was characterized under various flow conditions using an optical particle counter (OPC). Finally, their analytical performance was assessed in both conventional and single-particle ICP-MS measurements using standard solutions and nanoparticle suspensions. For comparison, all experiments were also performed using a commercially available pneumatic nebulizer (MicroMist) too.

Results have shown that the performance of these 3D printed nebulizers was comparable to that of the commercial ones, making them an equally valid, but significantly cheaper (>1000 vs 3.7 USD/piece), and therefore potentially even disposable alternative for (single particle) ICP-MS analysis.

Acknowledgements
This work was partially funded by the National Research, Development and Innovation Office (NKFIH) of Hungary through projects OTKA K 146733. The authors also thankfully acknowledge the support received from the Austrian Research Promotion Agency (FFG) in the frame of the Important Project of Common European Interest (IPCEI) on Microelectronics and Communication Technologies.

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REMOVING A BOTTLENECK IN SPECIATION ANALYSIS WITH NOVEL CHROMATOGRAPHIC ELUENTS

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Speciation analysis of hydrophobic compounds with ICPMS (inductively coupled plasma mass spectrometry) detection has been limited by the use of the organic ICPMS mode which has been practiced over decades. Despite the fundamentally element-dependent and molecule-independent signal response of this detector, there is a clear correlation between the hydrophobicity of compounds and their limits of detection, with the most common example being detection limits for the arsenolipids which are frequently reported at 10-100-fold higher levels than hydrophilic arsenic species. We have been actively working in previous years on addressing this limitation by introducing novel chromatographic approaches in speciation analysis. Herein, we present our progress in this area while focusing on the introduction of hexanediol as a major step forward along the path towards complete elimination of the need for the organic ICPMS mode. We show that the use of hexanediol as a novel chromatographic eluent allows unprecedented levels of convenience and sensitivity in speciation analysis for hydrophobic compounds including natural compounds and organic pollutants. We present a real-world application where we show how this development unlocks previously inaccessible areas in arsenolipid research.

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HOW FAR CAN LIBS IMAGING GO? A JOURNEY ACROSS SCALES

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Laser-induced breakdown spectroscopy (LIBS) imaging has evolved significantly over the last decade, progressively extending the range of spatial scales accessible to elemental imaging while preserving its core strengths: multi-element capability, sensitivity to light elements, and operation under ambient conditions [1,2].

Recent advances in high-repetition-rate laser sources, fast detectors, and optimized scanning strategies have enabled a major increase in acquisition throughput. As a result, LIBS imaging can now cover surfaces reaching several hundreds of square centimeters while maintaining micrometric spatial resolution on the order of 10 µm. Such capabilities are particularly well suited to the investigation of chemically complex and highly heterogeneous samples, as encountered in geosciences, materials science, and industrial environments, where spatial variability plays a central role (c.f. figure 1). In parallel, continued developments in beam shaping, focusing optics, and signal optimization have pushed LIBS imaging toward higher spatial resolution. Lateral resolutions approaching the micrometer scale (~1 µm) are now achievable, allowing the investigation of fine microstructures, interfaces, and heterogeneous phases that were previously inaccessible to conventional LIBS imaging.

By bridging high-throughput, large-area mapping and ultra-high spatial resolution through complementary instrumental implementations of LIBS imaging, this presentation illustrates how LIBS imaging has become a scale-transcending technique. This journey across scales highlights how instrumental innovation and analytical ambition jointly define how far LIBS imaging can truly go.

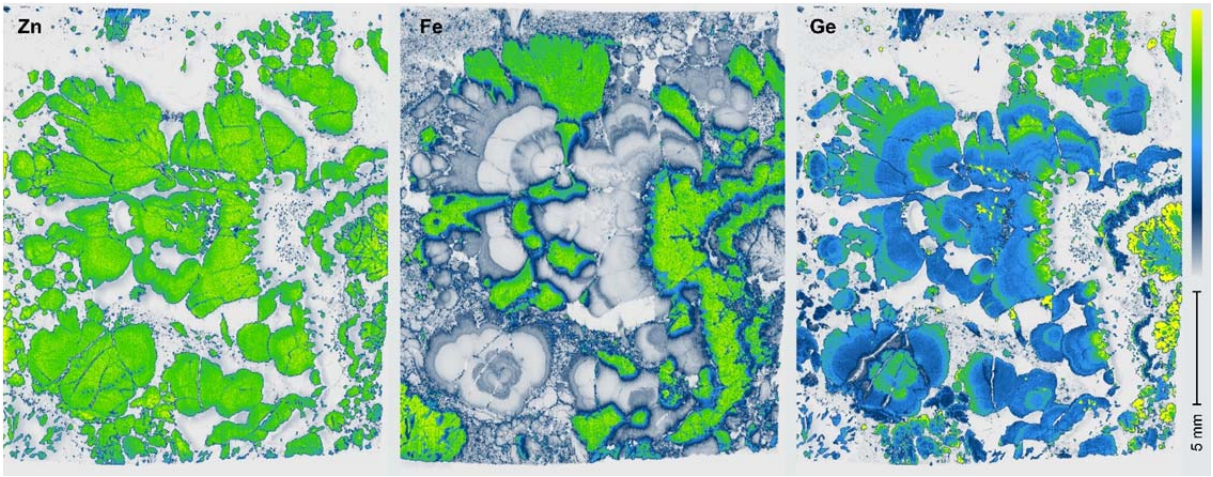

Figure 1. Elemental LIBS images of zinc (Zn), iron (Fe), and germanium (Ge) in sphalerite, revealing distinct chemical zonations.

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COMPARING FEMTOSECOND AND NANOSECOND LASER-INDUCED XUV SPECTROSCOPY (LIXS)

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In contrast to laser-induced breakdown spectroscopy (LIBS), measuring after a delay as long as a few microseconds, laser-induced XUV spectroscopy (LIXS) takes advantage of emissions from the very first instant of the pristine plasma. This process exhibits stable and intense line and recombination emissions in the XUV-range. Therefore, common challenges for precise measurements (e.g. quantification efforts) in LIBS caused by signal intensity fluctuations due to matrix effects and plasma-flicker noise are improved, as shown for ns excitation [1].

A femtosecond laser (pulse length ~100 fs) interacts fundamentally different with matter than a nanosecond laser. Of the many photons needed for ionization of the sample, less are absorbed via inverse Bremsstrahlung and more in a Franck-Condon multiphoton absorption (MPA) process. In combination with the higher peak power – and therefore higher initial plasma temperature (> 10 eV) – atoms are selectively ionized to a higher degree while at the same time thermal dissipation and equilibration are reduced. This specificity in excitation leads to a reduced background and the highly ionized atoms overwhelmingly emit the desired XUV-radiation. Thus, fs-LIXS promises to lead to “cleaner” spectra with sharper separation of the emission lines.

The capabilities of a fs-LIXS setup in comparison to ns-LIXS will be discussed. Samples of pure elements, as well as composite samples serve as model systems to highlight the different capabilities.

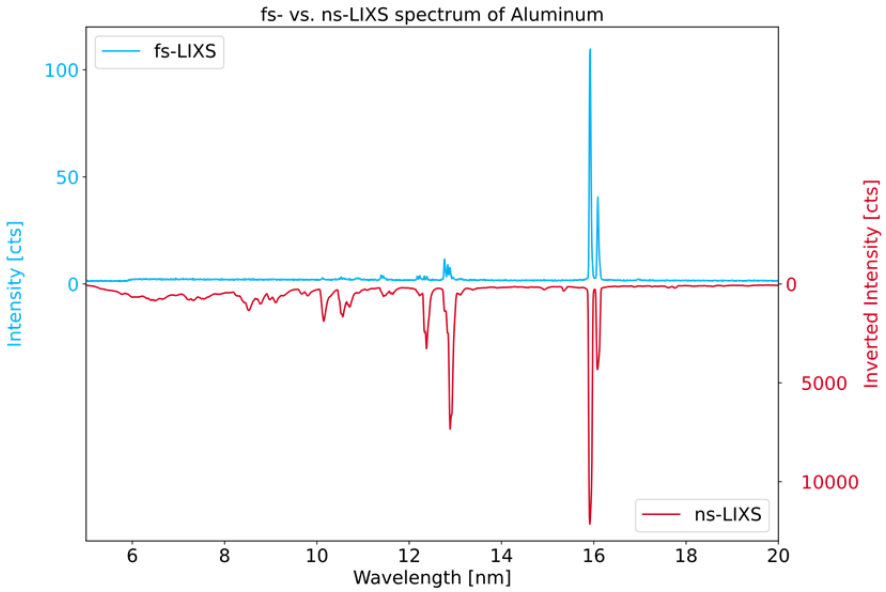

Figure 1. ns-LIXS (1064 nm, 6 ns, 450 mJ, single pulse) spectrum in red and fs-LIXS (800 nm, 100 fs, 700 µJ, 100 pulses) spectrum in blue of pure aluminum.

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LASER-INDUCED BREAKDOWN SPECTROSCOPY USING KHz REPETITION RATE PULSES FROM A FIBER LASER

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Laser-induced breakdown spectroscopy (LIBS) is a quickly evolving, laser based elemental analytical technique. Due to the developments of the recent decade, LIBS become a well-established analytical method, applied in both laboratorial and industrial environments [1]. One of the limitations of LIBS comes with the relatively low repetition rate (20 Hz) of the traditionally used solid state lasers. One candidate to replace these lasers and increase the throughput of such systems is the fiberlaser. Modern, master oscillator power amplifier (MOPA) based fiberlasers are capable of emitting pulses up to the MHz rate, while the pulse energy still adequate for plasma generation [2]. Their unique features (high repetition rate and tuneable pulse shape) for single and double pulse measurements have been discussed in the literature in detail recently [3-4].

In this current study our focus is the investigation of plasmas generated by continuous, high repetition rate pulses from a fiberlaser. As lasersource a variable pulse duration and pulse repetition rate MOPA laser with 80W power output and 1064 nm emission wavelength (JPT M7, VONJAN Technology GmbH, Wessling, Germany) was used, while low alloy steel standards (BAS) served as samples. The laser emitted low energy (0.4 mJ) pulses at 200 kHz pulse repetition rate, while the pulse duration was varied between 50 and 500 ns. The plasma emission was recorded by high performance LTB spectrometers (Butterfly, Demon) in several spectral regions, which included iron, chromium and manganese lines.

Utilizing the variable pulse duration of this laser source, it was possible to assess the effects of changing the fluence, while the irradiance was kept at the same value. Among the investigated parameters are the emission intensity, peak width and self-absorption characteristics of major and minor components, as well as the plasma temperature. While the effects for the peak intensity are quite well correlated with the fluence, but the relationship between it and the other peak parameters seems to be more complicated.

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SEVERAL ASPECTS OF THE LIBS POTENTIAL AS A COMPLEMENTARY TECHNIQUE IN GEOLOGICAL SCIENCES

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Among the main advantages of the LIBS method is often cited its ability to detect virtually all elements of the periodic table, including light elements. However, this potential is still underestimated in practice, even though detecting light elements can provide crucial information in many cases. A typical example is geological materials, for which LIBS appears to be an ideal complementary technique for routinely used methods such as EMPA or XRF, precisely because of its capability to detect light elements. Moreover, in combination with high spatial resolution, it is well suited for identifying various inhomogeneities, different geological phases and mineralization, as well as for studying weathering and other processes. Since a large amount of data is often generated by the wide range of measured spectra, data processing with sophisticated chemometric and artificial intelligence methods poses new challenges. These aspects will be demonstrated through several cases in the presentation. A dual-imaging method combining LA-ICP-MS and LIBS was applied to produce images revealing the distribution and possible migration of elements and isotopes in a uranium ore sample [1]. The next work demonstrates the potential of LIBS as a complementary technique to EMPA for distinguishing and characterizing uranium mineralization. Due to its ability to detect oxygen and hydrogen, LIBS enables estimation of uranium oxidation states, which can play an important role in monitoring the potential mobilization of uranium in the environment [2].

Differences in elemental fingerprints allowed the identification of various forms of selenium mineralization, including, for example, berzelianite, umangite, Ni-tyrrelite, ferroselite, eskebornite, and bukovite. In all cases, the spatial distributions of the identified phases were consistent with reference method maps, confirming the validity of the fingerprint-based approach. The fingerprinting strategy further demonstrates that LIBS is applicable beyond inorganic systems. This is illustrated using a LIBS-based analytical method that reliably distinguishes different types of microplastics in complex karst sediment matrices. However, polymers with similar chemical compositions exhibit partially overlapping spectral features, making their discrimination more challenging. These findings highlight the need for expanded spectral libraries, advanced data processing, and multivariate classification strategies, including machine learning techniques, to improve polymer-specific resolution.

Overall, the presented case studies demonstrate the broad applicability of LIBS as a complementary analytical tool that significantly enhances the information value of material characterization. Future progress in this field is expected to be driven by the continued development of advanced chemometric methods and the rapidly evolving landscape of deep learning and artificial intelligence.

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SPECTROSCOPY ACROSS ENERGY SCALES: FROM LASER INDUCED PLASMAS TO COLD ATOMS

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Calibration-free laser induced breakdown spectroscopy provides quantitative elemental analysis [1] including light elements (B, C, S, P, etc.) particularly in the VUV range [2]. Systematic ablation allows for mapping and depth profiling [3] which is essential for geological samples, space research [4], and for the analysis of deposited material (D, T, He) on the wall of fusion reactors [5,6]. Using of ps lasers is advantageous for finer resolution and heat dissipation, but the plasma is generally short-lived with a lower temperature [7] which limits the detection of H. Different LIP re-excitation schemes such as Resonant LIBS [8], ps/ns double pulse LIBS or electric discharge enhancement [9] were explored. The recently developed LIBS-AL for analysis of liquids [10,12] led to diagnostics of the plasma dynamics at liquids/gas interface which utilizes techniques such as shadowgraphy [11] and time of fligh expansion at the ns timescale. These techniques are planned to be employed in our current experiments with ultracold ^{87}Rb gas [13].

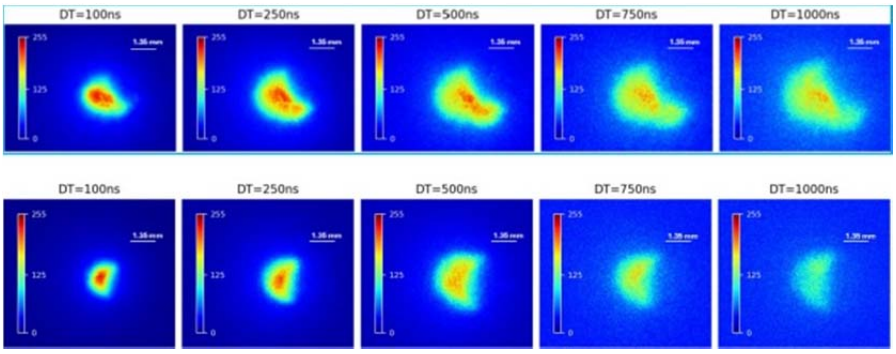

Figure 1. Temporal evolution of laser induced plasma, adapted from [11]

Acknowledgments
Funding came from the Scientific Grant Agency of the Slovak Republic (VEGA-1/0815/25, 2/0120/25), the Slovak Research and Development Agency (APVV-22-0548, APVV-23-0281).

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MULTIPHOTON ELECTRON EXTRACTION SPECTROSCOPY (MEES) AND ITS ANALYTICAL APPLICATIONS

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Multiphoton Electron Extraction Spectroscopy (MEES) is an ambient-condition analytical spectroscopy based on resonant multiphoton ionization under high electrical field. Short, tunable UV laser pulses interact with molecules, and the emitted photoelectrons are collected. The integrated photocharge is recorded as a function of laser wavelength, producing spectra rich in sharp resonance peaks that originate from electronic and vibronic transitions. In Solid MEES, surfaces of solids, liquids, films, powders, swabs, and other substrates are analyzed directly, without vacuum and with little or no sample preparation. In Gas MEES, the same principle is transferred to volatile and semi-volatile molecules in a flow cell at atmospheric pressure, enabling online trace gas detection. Compared with conventional spectroscopies such as absorption, reflection, fluorescence, Raman, FT-IR, and FT-NIR, MEES provides a higher peak density, high signal-to-noise ratio, and high spectral quality density. These properties give MEES strong molecular fingerprinting power, high sensitivity, and an ability to handle complex matrices and mixtures.

The recent development of Gas MEES extends the method from surfaces to direct on-line gas analysis. This method was applied to BTEX compounds, benzene, toluene, ethylbenzene, and xylenes, which are important environmental and industrial pollutants. Gas MEES provided distinct spectral signatures for each BTEX compound, including the individual xylene isomers, and allowed online real-time detection in ambient air. The LODs are in the PPT range, comparable to canine olfactory system. The additivity of MEES spectra also supports quantitative analysis of mixtures without chromatographic separation, suggesting a route to compact and selective real-time sensors for air quality monitoring.

The analytical applications of MEES are not limited to gas sensing. Solid MEES has shown exceptional performance in trace detection and mapping of explosives on surfaces. Nitro-, nitrate-, and nitroso-containing explosives exhibit characteristic resonance signals, allowing rapid detection on swabs, in dry-transfer security protocols, and in plastic explosives such as Semtex. Sub-pmol analytical detection limits and spatial imaging of traces, including explosive residues in fingerprints, demonstrate the value of MEES for security screening and forensic analysis. More broadly, the combination of ambient operation, high sensitivity, spectral selectivity, and chemical imaging makes MEES a promising platform for environmental monitoring, industrial safety, homeland security, forensic science, quality control, and future medical diagnostics based on volatile biomarkers.

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MICROFLUIDIC PAPER DEVICES AND HOLLOW MICRONEEDLES: EMERGING PLATFORMS FOR NEXT-GENERATION OPTICAL SENSING OF ENVIRONMENTAL POLLUTANTS AND BIOMARKERS

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The development of highly sensitive, low-cost, and portable sensing technologies is of increasing importance for environmental monitoring and healthcare diagnostics. This presentation highlights two emerging analytical platforms—microfluidic paper devices and hollow microneedles—that offer innovative solutions for the efficient sampling and optical detection of environmental pollutants and biological biomarkers. First, a microfluidic paper-based surface-enhanced Raman spectroscopy (SERS) platform was developed for the simultaneous detection of endocrine-disrupting compounds, bisphenol A (BPA) and bisphenol S (BPS), in plastic toys and thermal receipts. The sensing substrate consists of molecularly imprinted nanogels decorated with silver nanoparticles, where selective recognition cavities are combined with a wrinkled nanostructure capable of generating dense plasmonic hot spots. This synergistic design enabled highly selective and ultrasensitive detection, achieving sub-picomolar limits of detection of 0.38 pM for BPA and 0.37 pM for BPS.

Second, high-resolution hollow microneedles were fabricated using digital light processing (DLP)-based 3D printing and biocompatible resin for minimally invasive extraction of interstitial fluid (ISF). The obelisk-shaped microneedles demonstrated efficient fluid collection from agarose tissue phantoms and porcine skin, highlighting their suitability as a sampling platform for point-of-care diagnostics. As a proof of concept, the extracted fluid was analyzed using paper-based analytical devices (PADs) for the colorimetric determination of bilirubin and cortisol. The resulting system exhibited excellent sensitivity, linearity, and analytical performance, demonstrating its potential for wearable and minimally invasive health monitoring.

Together, these studies illustrate the versatility of microfluidic paper devices and hollow microneedles as next-generation platforms for environmental and biomedical sensing, providing promising pathways toward portable, user-friendly, and cost-effective analytical technologies.

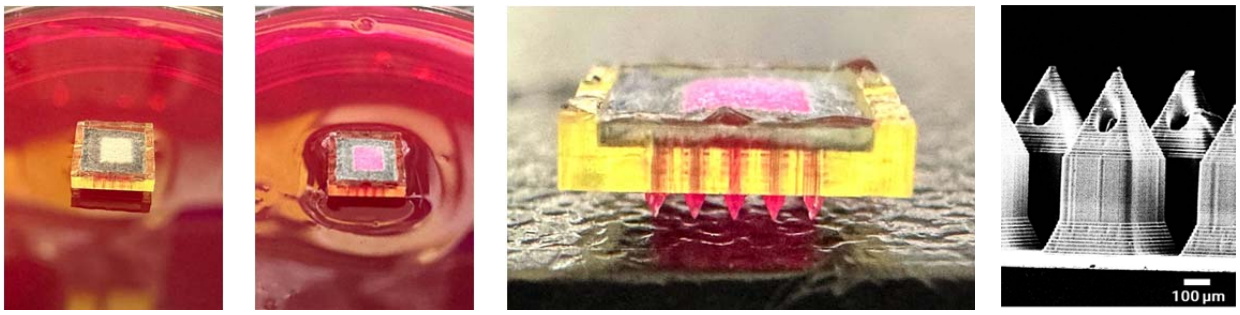

Figure 1. In vitro demonstration of ISF extraction and optical sensing using the microneedle-integrated paper-based analytical device (MN–PAD)

SMALL-SIZED ELECTROTHERMAL VAPORIZATION CAPACITIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY FOR Cd, Cu, Pb AND Zn DETERMINATION IN SURFACE WATERS AFTER MICRO-SOLID PHASE EXTRACTION

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The development of highly sensitive, resource-efficient and portable analytical methodologies for environmental monitoring remains a major challenge in modern analytical chemistry [1–3]. The determination of hazardous and priority hazardous metals in surface waters is particularly challenging due to their typically low concentrations, which often require laboratory-based instrumentation such as ICP-OES, ICP-MS, or GFAAS, frequently coupled with additional preconcentration procedures. In this work, a tandem system powered by a photovoltaically charged battery was developed for *on-site* river water sample preparation by micro-solid phase extraction (μ-SPE) on dithizone-functionalized C18 cartridges and subsequent *ex-situ* determination of Cd, Cu, Pb and Zn by small-sized electrothermal vaporization capacitively coupled plasma optical emission spectrometry (SSETV–μCCP–OES). The μ-SPE system provided a 100-fold enrichment of metals from river water samples and enabled simultaneous multielement determination from 10 μL eluates using a low-power (15 W) and low-argon-consumption (150 mL min^{-1}) microplasma. The proposed method demonstrated accurate determination of metals through the analysis of certified reference materials and achieved detection limits at the ng L^{-1} level. In addition, assessment using the AGREEprep [4] and RGB12 [2] metrics confirmed the favorable green and white analytical characteristics of the method, highlighting the potential of the proposed approach as a resource-efficient alternative to conventional laboratory-based techniques for trace metal monitoring in surface waters.

Acknowledgements
This work was supported by a grant of the Ministry of Education and Scientific Research in Romania, CNCS/CCCDI-UEFISCDI, contract no. 15PED/2025, project number PN-IV-P7-7.1-PED-2024-0091, within PNCDI IV.

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OPTIMIZING COPPER-DOPED BIOACTIVE GLASS COMPOSITIONS VIA ION RELEASE FOR ANTIBACTERIAL APPLICATIONS IN BONE TISSUE ENGINEERING

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In the field of bone tissue engineering, implant-associated infections remain a major hurdle. Therefore, this study focuses on incorporating 0–20 mol% (labeled as CuX%) copper(II) oxide (CuO) ions into bioactive glasses (BGs) to introduce antibacterial properties without compromising their inherent bioactivity. To precisely track the dissolution kinetics of the glass network and accurately measure trace elements in the liquid phase, Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) was introduced, leveraging high-temperature argon plasma to excite atoms and enable precise, simultaneous multi-elemental analysis at trace levels. Through this technique, the release profiles of Si^{4+} and Cu^{2+} ions along with pH variations were monitored over 24 hours of immersion in Simulated Body Fluid (SBF), while the glass's antibacterial efficiency against *Escherichia coli* and its long-term bioactivity were evaluated using statistical methods and Scanning Electron Microscopy (SEM).

ICP-OES demonstrated the concentration-dependent release of Cu^{2+} ions, with Cu5% and Cu8% reaching 58 ± 2.75 ppm and 61 ± 3.60 ppm after 24 h in SBF, corresponding to increases of 117.8% and 121.1% relative to Cu3%. Meanwhile, a more controlled glass dissolution was shown by observing the decrease in the Si(IV) release, from 30 ± 2.4 ppm in Cu0% to 23.2 ± 2.65 ppm for Cu5%. The 58–61 ppm release of Cu^{2+} corresponded to the highest antibacterial performance against E. coli, with Cu5% achieving 75 ± 3.5% antibacterial efficiency, that is more than 2-fold higher than the antibacterial efficiency of the Cu0% (****$p < 0.0001$). Although, higher CuO concentrations further decreased the antibacterial properties of Cu-doped BGs. Furthermore, SEM imaging validated the distinct bioactivity of the glass by confirming the robust formation of a hydroxyapatite layer on the optimal Cu5% composition after 14 days. Ultimately, these findings demonstrate a controlled ion release profile and establish Cu5% as the ideal, well-balanced composition that successfully merges superior antibacterial performance with excellent in vitro bioactivity for bone regeneration applications.

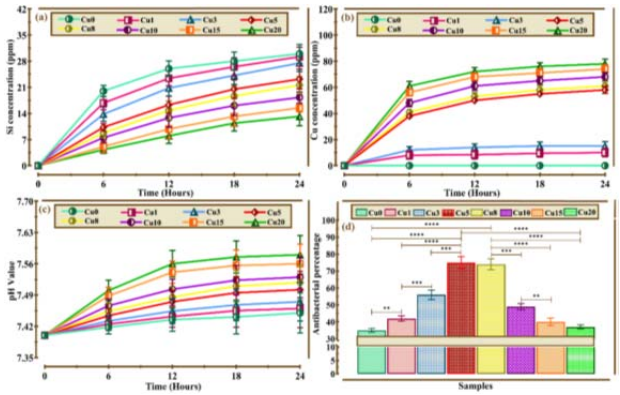

Figure 1. ICP-OES and antibacterial analysis of BGs, a) Si concentration, b) Cu concentration, c) pH value, d) Antibacterial percentage for Cu-BGs.

PHOTOCHEMICAL VAPOR GENERATION OF COBALT FOR ATOMIC ABSORPTION SPECTROMETRY WITH ATOMIZATION IN A DIELECTRIC BARRIER DISCHARGE: OPTIMIZATION AND MECHANISTIC STUDY

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Photochemical vapor generation (PVG) enables, analogous to chemical vapor generation (CVG), efficient and matrix-free analyte introduction into the detector. Whereas CVG is dominantly applied to hydride forming elements and mercury, PVG is applicable to a broader range of elements, including also transition metals and nonmetals.

PVG conditions for Co were adopted from our previous study employing a thin-film flow-through photoreactor: 10% (v/v) formic acid with 1 M sodium formate as a photochemical medium, sample flow rate of 3.8 mL·min^{-1}. The efficiency of PVG step under these conditions was previously quantified to be 20%, while $Co(CO)_4H$ was identified as the volatile species produced.

In this work, atomization of volatile Co species in the dielectric barrier discharge (DBD) plasma atomizer with detection by atomic absorption spectrometry (AAS) was optimized and its mechanism was studied. The T-shaped planar DBD atomizer was powered by a high AC voltage with 28.5 kHz sinusoidal modulation. Argon (200 mL·min^{-1}) was found as the best discharge gas and the optimum high voltage was 25 kV. Since atomization of volatile compounds in plasmas and flames proceeds via reaction with hydrogen radicals, the effect of H_2 addition to Ar discharge gas was studied. The addition of 10 mL·min^{-1} H_2 resulted in a twofold increase in the Co signal.

Laser induced fluorescence (LIF) was used to determine the atomization efficiency and visualize the spatial distribution of free Co atoms in the DBD atomizer, employing a Nd:YAG pumping laser coupled to a dye tunable ns laser. Free Co atoms were excited by 304.4 nm and the atomic fluorescence was detected at 340.5 nm using an ICCD camera. The effects of DBD voltage, discharge Ar flow and H_2 addition on the Co signal were studied by PVG-DBD-LIF. This approach yielded qualitatively similar trends and results. The atomization efficiency was quantified to 30±5%, which is comparable to the atomization of the same DBD atomizer used for Bi and Pb hydrides produced by CVG. Free Co atoms were present only in the central part of the plasma plume indicating their fast decay. The life-time of excited Co atoms, measured by a picosecond laser system, was 0.35 ns, significantly shorter than the values typically observed for CVG of hydride forming elements, e.g., 2.8 ns for Bi. Analytical figures of merit for Co analysis were also determined. The sensitivity reached 34 s·µg^{-1} Co, the limit of detection was 3.8 ng·mL^{-1} and the calibration function was linear up to 200 ng·mL^{-1} Co.

Acknowledgments
This research has been supported by the Czech Science Foundation, projects 23-05974K and 26-22432S, by the Charles University Grant Agency (project no. 614225) and by the Czech Academy of Sciences (Institutional research plan RVO: 68081715).

SPECIATION ANALYSIS OF ARSENIC, CHROMIUM AND MERCURY IN WATER AND RIVER SEDIMENTS

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Speciation of arsenic (As), chromium (Cr) and mercury (Hg) in water and river sediments serves as a vital tool for assessing water quality since the actual toxicity, mobility, bioaccumulation, and reactivity of As, Cr and Hg depend on their chemical forms. In this study, microwave assisted extraction and ultrasonic extraction methods were used to achieve a safe, simple, and fast method for quantification of different chemical species of As, Cr and Hg in river sediments. Total concentrations of these elements in water and river sediments were determined by inductively coupled plasma-mass spectrometry (ICP-MS), whereas speciation analyses were conducted by high performance liquid chromatography (HPLC) hyphenated to ICP-MS. Herein discussion will be focused on the following points with the objective of developing efficient analytical methods for speciation analysis of As, Cr and Hg in water and river sediments that include synchronic extraction and speciation of As and Cr in river sediments and water [1, 2], as well as speciation and bioavailability of Hg in river sediments [3]. The developed analytical methods were applied for quantitative speciation of As, Cr and Hg species in water and river sediment samples. The effects of industrial pollution and mismanagement of municipal wastewater will be discussed. A thermo-desorption studies of Hg in river sediments using a Zeeman direct Hg analyser to investigate the behaviour of Hg release from sediments will also be discussed [4].

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LABORATORY BASED XANES AND XES ANALYSIS OF SLAG

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Identifying the solid-state characteristics — such as oxidation states and the local coordination environment of neighboring atoms — is crucial across diverse disciplines including catalysis, nuclear science, geochemistry, and the growing field of critical element recovery from industrial waste. X-ray Absorption Fine Structure (XAFS) spectroscopy is particularly valuable because it can be applied to nearly all elements and provides bulk-sensitive information. In recent years, laboratory-based XANES (X-ray Absorption Near Edge Structure) measurements have experienced a resurgence [1]. This stems from significant advancements in instrumentation, detector technology, X-ray sources, and optical components. The increasing demand in condensed matter research for analyzing amorphous or non-crystalline materials in routine lab settings has further fueled this trend.

Understanding the speciation of metal ions in slags is essential for minimizing environmental leaching and for designing efficient recovery processes for critical materials. These metal ions can be present at elevated concentrations — e.g. Fe reaches ca. 20 wt.% in electric arc furnace (EAF) slags, while Cr can constitute up to 15 wt.% in ferrochromium slags. Laboratory XANES spectra offer rich insights into the chemical forms of these metals. Key spectral features, such as pre-edge peak energy and intensity, main edge position, whiteline height, and post-edge oscillations are often diagnostic. Linear combination fitting is commonly employed to quantify the relative proportions of different species [2]. Errors can be introduced by damping of the spectral features due to leak (stray or parasitic) radiation. This radiation leads to a systematic reduction of the absorbance, which is stronger when the absorbance is high *e.g.* at strong absorption bands like the whiteline in the XANES, reducing characteristic features. In our work we estimate errors and magnitudes of leak radiation with respect to Fe speciation in EAF slags [3] and discuss the options to characterize samples limited by low concentration of the analyte (<1-2 wt.%) and sample amount (<5 mg) by XES.

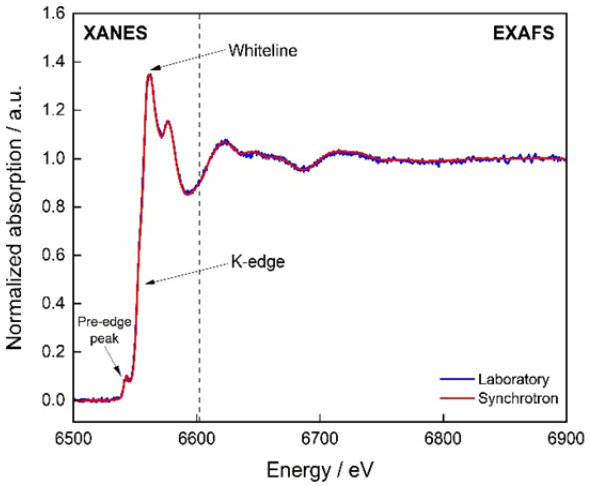

Figure 1. XAFS spectrum of Mn(IV) oxide measured as a pellet in transmission mode with a laboratory setup (easyXES-100, blue) and at the BAM*line* endstation at BESSY II (red) [3].

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X-RAY FLUORESCENCE-BASED STUDIES OF PARTICULATE MATTER ON FILTERS

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Under the European Green Deal, the zero-pollution action plan (Directive (EU) 2024/2881) targets to improve air quality by 2030, with a focus on particulate matter (PM), especially PM2.5. It also introduces an obligation to monitor additional pollutants such as ultrafine particles and sets new thresholds for potentially toxic elements such as Pb, Cd, As, Ni and Hg that national environmental agencies must regulate to. Hence are needed additional PM monitoring, characterization and controls which in turn requires reliable and accurate elemental analysis techniques underpinned by calibration procedures employing fit-for-purpose reference materials (RMs). Unfortunately, suitable RMs for PM on filters are crucially lacking, with no adequate concentration ranges for PMs covering the targeted applications. In addition, both for environmental, safety and economic reasons, analytical scientists are increasingly leaning towards green analytical chemistry. This concept aims at providing environmentally friendly alternatives to established analytical practices, developing cost-saving opportunities and ensuring laboratory personnel safety whilst preserving the classic analytical figures of merit (e.g., accuracy, sensitivity, selectivity).

Within these two frameworks, X-ray Fluorescence (XRF) may find an opportunity to establish itself. XRF-based techniques present interesting advantages, with simultaneous elemental analysis of qualitative, quantitative or screening character. Total Reflection X-ray Fluorescence (TXRF), as an example, enables experimentalists to simultaneously determine the elemental compositions with detection limits in the low picogram range. As for XRF microscopy or tomography, they provide spatially resolved information of the sample surface or deep volume composition, respectively, typically at the micrometer scale. When a synchrotron is used as an X-ray source, elemental sensitivity down to the femtogram range (TXRF) and spatial resolution at the nanometer scale (μ-XRF) may be achieved. Moreover, XRF is usually regarded as a greener, sustainable analytical technique in comparison to other wet analytical methods.

Here, we illustrate the potential of XRF-based techniques to the study of particulate matter on filters. We present data from a set of calibration samples characterized with XRF under grazing incidence conditions allowing for quantification procedures for PMs captured on air filters at environmentally relevant levels. The quantification yields uncertainties comparable with those obtained by other elemental analysis techniques. We also present results from a PM source apportionment study, using a combination of XRF-based techniques, including X-ray absorption spectroscopy (XANES) and imaging.

Acknowledgments
This work was supported by the COST Innovator Grant IG18130 “AIR-CAL” supported by COST (European Cooperation in Science and Technology), and by the Italian Ministry of University and Research within the framework of the “Research Projects of National Relevance, PRIN 2022”, project "SMART-AIR" 2025-2027, CUP: D53C24003250006.

A CLOSER LOOK AT THE SPECIATION OF IRON: THE POWER OF MÖSSBAUER SPECTROSCOPY

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The speciation of iron in various systems can be crucial for the function iron in that particular system has. This is much more than the oxidation state; further details may have to be explored about the electron structure of iron. Mössbauer Spectroscopy has great sensitivity to these details through measuring the hyperfine interactions.

The isomer shift, the quadrupole splitting, and the magnetic splitting together as derived from the evaluation of a Mössbauer spectrum provide a fingerprint of an iron-containing compound. However, measuring these parameters is sometimes hindered by dynamic effects which, on the other hand, give extra information on the material under study.

Relaxation phenomena sometimes, e.g., for urea complex salts of iron(III), result in badly broadened spectra with little extractable chemical information.

Electron hopping sometimes, e.g., in magnetite and chromium-overdoped iron-chromite, results in averaged valence state of iron a chemist often call electron delocalization, not bothering about the time scale of this process.

Doping of goethite with lanthanide ions results in substantial change in the magnetic structure of goethite.

These examples will be discussed and shown what one may lose or gain due to these dynamic phenomena; how the speciation of iron can be described in more detail as with any other spectroscopic method.

IRON COMPONENTS IN VARIOUS DIETARY SUPPLEMENTS: A MÖSSBAUER-SPECTROSCOPIC STUDY

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Iron deficiency anaemia affects roughly one billion of individuals globally [1], and it is one of the top ten worldwide health issues [2]. To prevent and treat iron deficiency, various iron containing dietary supplements and pharmaceuticals are used and developed.

Present study focuses on the iron speciation in Fe dietary supplements containing either inorganic [Fe(II) sulphate or Fe(III) pyrophosphate] or organic Fe in form of salt [e.g., Fe(II) fumarate] and chelates with amino acids such as Fe(II) bisglycinate. Oxidation state and relative amounts of the different Fe compounds was determined by the help of Mössbauer-spectroscopy. According to our main results, most of the Fe(II) containing dietary supplements contain Fe also in the oxidized (+3) state that could influence the bioavailability of the Fe. Both Fe(II) and Fe(III) compounds were identified with the help of literature data [3].

The speciation of Fe before and after the incubation with simulated gastric (pH=1.5) and duodenal gastric (pH=6.8) juice was also determined by Mössbauer spectroscopy indicating the possible redox transformations of Fe after oral administration in the intestinal tract. Significant changes could be found in the chemical environment of Fe due to the incubation in both acidic and neutral gastric juices. Moreover, a relatively high oxidation rate could be found after duodenal incubation which may lead to Fe(III)-oxide formation.

Hopefully the results presented can help to understand the effectiveness of Fe containing dietary supplements applied in Fe deficiency anaemia.

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TECHNICAL ART HISTORY AS AN OBJECTIVE METHOD FOR THE SCIENTIFIC AUTHENTICATION OF PAINTINGS

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The authentication of paintings remains one of the most sensitive questions in the art market, where visual judgement, connoisseurship, and provenance research may be influenced by subjective expectations, financial interests, and the desire to believe in authenticity. This presentation introduces Technical Art History as an interdisciplinary approach that combines art historical interpretation with material, optical, and chemical analysis. It argues that the examination of material structure, pigment composition, surface morphology, and technological characteristics should form an essential starting point in the authentication process.

The presentation focuses on the work of the Painting Examination Laboratory in Budapest, which has applied this combined method to the scientific examination of 19th- and 20th-century paintings for 18 years. Through selected case studies, the presentation demonstrates how analytical methods can reveal chronological inconsistencies that remain invisible to the naked eye. Particular attention is given to the historical development of painting materials, the industrial transformation of colour production, and the diagnostic importance of historically datable pigments and modern material traces.

Forged or falsely attributed paintings will be discussed in order to show how stylistically convincing works can be questioned through material evidence. These cases demonstrate that visual inspection alone is not sufficient for reliable authentication. Scientific analysis can reveal chronological contradictions and technological impossibilities that fundamentally alter the interpretation of a painting.

Technical Art History provides a reproducible and verifiable framework for painting authentication. By bringing provenance, art historical context, and material evidence into a single interpretative system, it helps distinguish historically possible artworks from later imitations and supports a more objective understanding of artistic production.

DURABILITY STUDIES OF CEMENTITIOUS MIXTURES CONTAINING REINFORCING STEEL

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The design of radioactive waste repositories relies on a multiple barrier system to prevent the release of radionuclides into the environment. The engineered barrier system follows the principle of defense in depth, whereby each barrier is capable of independently retaining radioactive materials, ensuring that the failure of one barrier does not compromise the integrity of the others. The engineered barrier system includes the cementitious structural components and walls of intermediate-level radioactive waste repositories, as well as reinforced concrete elements that provide structural stability. Although repository design requirements vary between countries, a common objective is to ensure the long-term integrity of these structures - potentially for several hundred years - to prevent the migration of radioactive waste into the environment [1-2].

Within the framework of EURAD-2, various cementitious compositions were optimized for near-surface radioactive waste disposal based on their mechanical performance, chemical durability, and long-term stability. Cylindrical specimens prepared using CEM II/B 42.5N and CEM I 42.5R cements were investigated to evaluate their mechanical and microstructural properties, as well as the reactivity at the surface between embedded reinforcing steel and the cementitious matrix. The durability of the cement specimens was assessed through leaching tests performed in two different aqueous solutions in accordance with ASTM C1308-21 protocol. The leachates were analyzed by inductively coupled plasma optical emission spectrometry (ICP-OES) to quantify the release of major cement constituents, including Si, Al, Fe, and Mg. Following the leaching experiments, post-mortem scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (SEM-EDX) were conducted to investigate the interactions between the cement matrix and the reinforcing steel. Mechanical tests performed before and after the leaching experiments demonstrated compressive strengths exceeding typical average values for all investigated cement formulations. Detailed experimental results will be presented during the conference.

Acknowledgments
The work was co-funded by the EURAD-2, European Union under Grant Agreement No. 101166718.

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METAL AND SELENITE SORPTION ON CLAYS AS BARRIERS FOR RADIOACTIVE WASTE REPOSITORY

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The preferred method for final disposal of high-level radioactive waste (HLW) is a deep geological repository, which will provide passive multibarrier isolation of radioactive materials. The engineered barrier system comprises the waste form, the canister, and backfilling materials, while the host rock serves as the natural barrier. Due to their beneficial physico-chemical properties and high cation exchange capacity, bentonites are considered as a potential backfill material in several waste storage concepts. Boda Claystone Formation (BCF) has been selected for a potential host rock of the HLW repository in Hungary. Several of the safety approaches for the geological disposal of HLW rely on the strong uptake of radio-contaminants by clay minerals. Key cations and oxyanions such as Co^{2+}, Ni^{2+} and SeO_3^{2-} were selected chemically representing radionuclides dissolved from HLW.

Uptake of ions by bentonites and clay-rich rocks was studied by recording sorption and desorption isotherms on powdered samples suspended in synthetic porewater with Ni^{2+}, Co^{2+} and SeO_3^{2-} ions added at different concentrations. Radionuclide retention of B75/BCV bentonites (Czechia) and BCF albitic claystone was evaluated at different temperatures (25°C, 40°C, 80°C). For the liquid phase, radiotracers are usually applied in order to cover a large concentration range. The high-concentration part (0.001-10 mM) of the isotherms for the ions of interest was recorded by means of ICP-OES using inactive chemicals. The obtained results are consistent with sorption isotherms based on batch experiments involving radiotracers.

Comparison of the obtained sorption and desorption isotherms indicate irreversibility of sorption for Ni^{2+} and Co^{2+} ions at the highest concentrations. This behaviour was supported by modelling considering an 80% Ca-montmorillonite content. The experimental isotherm was underestimated for high concentrations indicating and additional uptake mechanism through formation of a new phase. Based on the results, B75/BCV bentonite bind the ions of interest to a similar extent as the BCF albitic claystone, contributing to the retention of cationic radionuclides [1,2]. Ni^{2+} sorption showed an increase with temperature, but no significant temperature difference was observed for selenite immobilization.

Total-reflection X-ray fluorescence (TXRF) was applied for elemental analysis of the solid phases. The powdered clays were analyzed in the suspension form using powdered geological standard reference materials for validation. The elemental composition of bentonite and albitic claystone samples obtained by suspension TXRF was in line with conventional XRF results of pelletized samples.

Acknowledgments
The research was co-funded by the European Union under Grant Agreement No. 101166718 (EURAD2).

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SYNTHESIS AND CHARACTERIZATION OF CLAY MINERAL-BASED GRAPHITIC CARBON NITRIDE COMPOSITE PHOTOCATALYSTS

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Heterogeneous photocatalysis could be an effective approach in the removal of a wide range of environmental pollutants. Its use is particularly attractive in environmental technologies, as it could combine green chemistry principles with efficient pollutant degradation. Current research focuses on developing photocatalysts with improved natural sunlight utilization potential, thereby enhancing their practicality and potential for applications. Graphitic carbon nitride (g-CNx) is a non-toxic, environmentally friendly *n*-type semiconductor with a band-gap of ca. 2.7 eV (459 nm). Major disadvantages are the fast recombination of photoinduced electrons and holes, low quantum efficiency, low specific surface area and poor quantum yield. Some of these could be countered by appropriate synthesis control and composite formation. Kaolin is an abundant, natural and inexpensive raw material, with miniscule intrinsic photocatalytic activity and potential for being catalyst-support. Photochemically active graphitic carbon nitride can be in-situ synthesized onto a clay mineral surface, significantly enhancing their catalytic performance and potentially improving catalyst recoverability after use in heterogeneous photocatalysis.

In our work, graphitic carbon nitride-metakaolin composite photocatalysts were synthesized from urea precursor and a commercially available kaolin, at different annealing temperatures (450-600 °C) and initial urea masses (15-20 g). Successful synthesis of nitrogen-rich g-CNx was verified by X-ray diffraction (XRD) and infrared spectroscopy (FTIR). Structural alteration of kaolinite to metakaolinite was identified as thermal dehydroxylation took place at elevated temperatures (> 400°C). Graphitic carbon nitride content and thermal stability were determined by thermal analysis (TG-DTG) and CHN analysis, while specific surface area (BET-SSA) was determined by nitrogen adsorption. Optical band gaps were determined by UV-Vis-DRIFT, validating the affinity to absorb part of the visible sunlight. In presence of kaolinite, the in-situ thermal polycondensation of g-CNx was significantly affected as its yield decreased with increasing kaolin content. The specific surface area of the composites could be improved. Photo-induced catalytic activity was investigated by the degradation of 4-nitrophenol test compound and the evolution of hydroxyl radical using a coumarin radical scavenger compound, in UV (λ_{max} = 365 nm) artificial solar irradiation.

RED MUD - FROM INDUSTRIAL WASTE TO FUNCTIONAL AND STRUCTURAL MATERIAL

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Red mud, a hazardous by-product of the aluminum industry, represents a significant environmental challenge but also a potential secondary resource. In this work, its valorization was investigated through two complementary approaches focusing on environmental remediation and material development. First, the photocatalytic activity of red mud was explored for the removal of organic pollutants from wastewater under visible light irradiation. The degradation behavior of model dyes (methylene blue, Congo red, crystal violet) and organic pollutants (cortisone, corticosterone, and naproxen) was studied, and the mechanisms of adsorption and photocatalytic degradation were analyzed using UV–VIS, fluorescence, and FTIR spectroscopy. [1, 2]

In parallel, red mud was utilized as a component in geopolymer composites synthesized via a low-energy sol–gel route with high Al/Si molar ratios (>2.5). Structural characterization by ^{27}Al MAS NMR, XRD, and thermal analysis confirmed the formation of composite phases, while mechanical strength and water solubility measurements evaluated their performance. The results demonstrate that red mud can be effectively transformed into functional materials for environmental and structural applications, contributing to sustainable waste recycling. [3]

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In/Zn-OXIDE – CLAY MINERAL TRIPLE COMPOSITE SYSTEMS AS PHOTOCATALYSTS

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Conventional water treatment technologies are often not effective enough to remove organic components such as pesticides and pharmaceutical residues. This is when alternative solutions, which although smaller in capacity and often more expensive, can be more effective. One option is the use of heterogeneous photocatalysis, where the photocatalytic nature of metal-oxides (e.g. TiO_2, ZnO) can be exploited to degrade organic contaminants. The efficiency of single component oxides can be increased by using mixed oxides, where a composite system of two or more metal oxides is formed. This can improve surface properties (e.g. specific surface area, pore structure), reduce photocorrosion and aggregation, and increase photon utilization, thus shifting the operating range from the UV to the visible range [1-3]. A proper surface structure of oxide composites can be achieved if the oxides are not only physical mixtures, but their formation occurs in parallel from the precursor salts given during the heat treatment preparation.

In this work, In-modified ZnO mixed oxide composites and their deposition onto clay mineral surfaces were studied. The applied clay minerals (kaolinite, halloysite) act as catalyst supports to prevent the aggregation of oxides, in addition, have moderate but detectable intrinsic photocatalytic nature [4, 5].

Metal oxides were prepared from precursor salts by precipitation and thermal treatment. In order to determine the composition with the most effective photocatalytic character, samples with different oxide-to-mineral ratios were prepared. Two different clay minerals were used as catalyst support, differing in hydration, morphology and photocatalytic activity. The phase composition of the samples was verified by XRD and the surface molecular structure was studied by FTIR-ATR spectroscopy. Thermogravimetry (TGA) was used to monitor the thermal decomposition processes. The photocatalytic activity was investigated in aqueous medium with coumarin, a ·OH radical scavenger test compound. The concentration of 7-hydroxycoumarin produced from coumarin was measured by fluorimetry. Since the photocatalytic activity is strongly dependent on porosity, N_2 adsorption experiments were carried out to determine specific surface area and pore size.

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CURRENT TRENDS IN MASS SPECTROMETRY

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Mass spectrometry continues to advance at an accelerating pace, driven by sustained gains in sensitivity, speed, and resolving power – and, increasingly, by the computational methods used to interpret its data. This lecture surveys the developments reshaping the field, following the analytical workflow from instrumentation through ionization and computation to a rapidly widening range of applications.

A new generation of analyzers and hybrid platforms has largely dissolved the long-standing trade-off between acquisition speed and resolution, while miniaturized and portable instruments extend analysis into field and point-of-care settings. Ion mobility has matured from a specialist technique into a routine, added dimension of separation, enabling isomer resolution, structural characterization, and collision cross-section determination. Ambient and direct ionization approaches now permit real-time, preparation-free measurement in contexts ranging from food safety and forensics to intraoperative diagnostics, and imaging mass spectrometry resolves the spatial distribution of molecules across tissues and materials.

The most rapid change, however, is computational. Machine learning has moved beyond purpose-built tools for individual tasks toward foundation models: large, self-supervised architectures that learn generalizable representations of mass spectra and can be fine-tuned for many downstream problems. In proteomics, such models increasingly unify tasks that were previously addressed separately, from spectral interpretation and identification to the prediction of analyte properties and data quality. In small-molecule and metabolomics analysis, learned spectral representations, generative approaches that infer structures directly from spectra, and novel models are reshaping the identification of unknown compounds. Together with the spread of systematic, high-coverage data-acquisition strategies across the full breadth of omics, and the move toward single-cell and clinical applications, these trends are collectively redefining the scope and reach of modern mass spectrometry.

SPECIOMICS: INTEGRATING ELEMENTAL AND MOLECULAR MASS SPECTROMETRY FOR COMPREHENSIVE CHEMICAL SPECIES ANALYSIS

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Speciomics is an emerging analytical framework that extends chemical speciation toward comprehensive characterization of chemical species using omics-based strategies. Adapted from the biological sciences, the term speciome refers to the complete set of chemical species present in a system, whereas speciomics encompasses methodologies designed to characterize this chemical space via integrated elemental and molecular measurements [1].

A key challenge in speciomics is the simultaneous acquisition of elemental and molecular information. This can be achieved by coupling Inductively Coupled Plasma Tandem Mass Spectrometry (ICP-MS/MS) with Electrospray Ionization High-Resolution Mass Spectrometry (ESI-HRMS) on a liquid chromatography platform. This approach combines element-selective detection with accurate-mass molecular identification, enabling correlation between elemental signatures and molecular structures [2].

To demonstrate the capabilities of this multimodal platform, two biological models were investigated: (i) soybean callus cultures exposed to metallic nanoparticles used for preservation and (ii) a murine colorectal cancer model. HILIC-HPLC was coupled online with ICP-MS/MS and ESI-HRMS/MS to characterize heteroatom-containing compounds (mainly P- and S-metabolites) and metallobiomolecules associated with Cu, Fe, Mn, and Zn.

The workflow enabled the putative annotation of numerous element-containing molecular species through retention time alignment, elemental detection, and highHR-MS. In the plant model, coordinated changes in metal homeostasis and heteroatom-containing metabolites were observed following nanoparticle exposure [3]. In the colorectal cancer model, treated with a novel therapeutic compound [4], alterations in copper-containing species demonstrated how integrated elemental and molecular information provides more insights into metal-associated metabolic pathways.

These results highlight speciomics as a natural evolution of speciation analysis, integrating complementary spectrometric techniques into a unified workflow for multidimensional, species-resolved characterization of complex chemical systems.

Acknowledgements
FAPESP (Fundação de Amparo à Pesquisa do Estado de São Paulo), São Paulo, Brazil; CAPES (Coordenação de Pessoal do Ensino Superior, Brasília, Brazil), CNPq (Conselho Nacional de Desenvolvimento Científico), Brasília, Brazil, FAPERGS (Fundação de Amparo à Pesquisa do Estado do Rio Grande do Sul), and Instituto Nacional de Ciência de Tecnologia em Bioanalítica Lauro Kubota – INCTBio-LK.

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PHOTOCHEMICAL VAPOR GENERATION COUPLED WITH DART-HRMS: IDENTIFICATION OF VOLATILE SPECIES OF TRANSITION METALS AND POTENTIAL FOR THEIR SENSITIVE DETERMINATION

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Photochemical vapor generation (PVG) is an emerging alternative sample introduction technique for analytical atomic spectrometry, combining advantages of efficient separation of analyte from matrix and significantly higher introduction efficiency than possible with conventional pneumatic nebulization of solutions. Volatile analyte species are synthesized during UV irradiation of an aqueous photochemical medium typically containing low-molar mass carboxylic acids, such as formic or acetic acid. Its applicability has gradually been expanded to many transition metals, which produce volatile metal carbonyls from formic acid-based media. For the past eight years, our group has played a significant role in the development of new PVG-based analytical methods for the determination of transition metals, such as Mo, W, Ni, Ru, Ir, Rh, and Re. Using inductively coupled plasma mass spectrometry (ICP-MS) as a detector, limits of detection down to the pg L^{-1} (ppq) level have been achieved for some analytes, and analytical applications have been demonstrated for complex sample matrices, including seawater, dietary supplements, and auto catalytic converters.

In order to thoroughly understand the PVG mechanism and the role of generated free radicals and aquated electrons, it is crucial to identify the final volatile products. The majority of volatile species have been identified using gas chromatography mass spectrometry (GC-MS). However, despite the high PVG yields, this approach has not succeeded in identifying photochemically generated volatile species of Ru, Os, Ir, and Rh. Based on the use of HCOOH, these were presumed to be less stable metal carbonyls with the general formula $M_x(CO)_yH_z$.

This presentation will provide an overview of our recent key PVG studies and our successful attempts to identify photochemically generated volatile Ru, Os, Ir, and Rh carbonyls or hydridocarbonyls using an ambient ionization technique, direct analysis in real time (DART), coupled with high-resolution mass spectrometry (HRMS) with an Orbitrap analyzer [1,2]. Additionally, the feasibility of coupling PVG and DART-HRMS for the sensitive and spectral interference-free W determination will be highlighted and its analytical performance will be compared to that obtained with ICP-MS.

Acknowledgments
This research has been supported by the Czech Science Foundation (project 26-22432S) and by the Czech Academy of Sciences (Institutional research plan RVO: 68081715).

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DETERMINATION OF HALOGENS AND THEIR SPECIES BY MASS SPECTROMETRIC TECHNIQUES: SAMPLE PREPARATION STRATEGIES

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The determination of halogens and their species is essential for understanding their roles in areas such as nutrition, human health, environmental sciences, and toxicology. Although significant advances have been made in analytical instrumentation, most analytical procedures still require samples to be converted into solution prior to introduction into the measurement system. Traditional digestion methods, which generally involve large amounts of concentrated reagents, are often labor-intensive and time-consuming. Furthermore, the resulting digests frequently require dilution before analysis, which can negatively affect detection limits. Even microwave-assisted closed-vessel digestion methods may suffer from incomplete sample digestion. In the case of halogen analysis, additional challenges arise from possible analyte losses caused by the formation of volatile and unstable species under acidic conditions. Consequently, increasing attention has been directed toward the development of greener analytical approaches that reduce reagent consumption, minimize waste generation, simplify analytical workflows, and provide efficient sample digestion. Equally important is ensuring that the final digest is compatible with the selected analytical technique. In view of these limitations, recent advances in sample preparation strategies for food, biological, and environmental samples, with emphasis on the determination of halogens and their species by inductively coupled plasma mass spectrometry and ion chromatography coupled to mass spectrometric detection will be discussed. Particular attention will be given to the use of dilute reagent systems, combustion-based sample preparation methods, and emerging technological developments in this area.

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SINGLE CELL IMAGING MASS SPECTROMETRY

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Single-cell imaging mass spectrometry (IMS) represents a cutting-edge frontier in spatialomics, enabling the high-resolution mapping of molecular distributions at individual cell level. This technology is essential for understanding the molecular heterogeneity of biological systems, particularly in neurobiology and oncology, where distinct cellular subpopulations often dictate physiological or pathological outcomes.

The implementation of single-cell IMS faces significant technical difficulties, such as the small physical dimensions of cells (typically 5–10 μm), extremely low sample volumes in the nanoliter range, and the low abundance of many bioactive targets. Despite these challenges, innovative methodologies have been developed to bridge the gap between histology and molecular analysis. One such approach involves pre-filling specific neurons with fluorescent dyes (like FITC or DAPI) and MALDI matrix before cryosectioning, allowing for targeted laser ablation and ionization. This method has successfully mapped neuropeptides, such as FMRFamide, in the central nervous system of *Helix pomatia* with a cellular spatial resolution of approximately 5 μm.

Continued advancements in laser focusing are pushing spatial resolution limits further, making single-cell "omics" an increasingly powerful tool for personalized medicine and fundamental biological research.

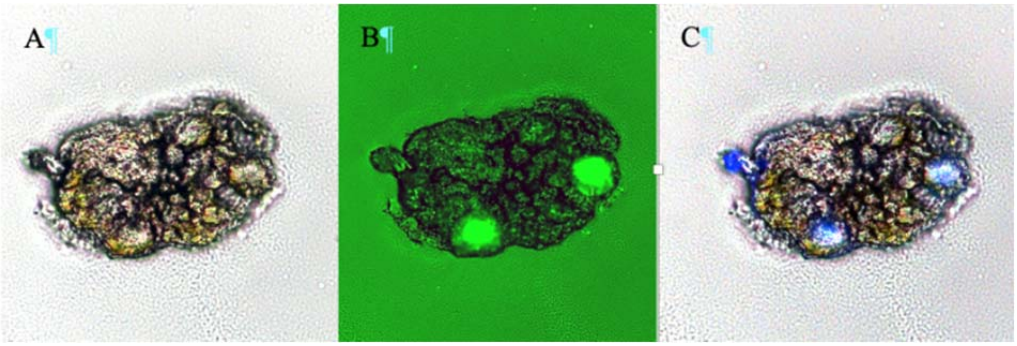

Figure 1. Microscopic image of a tissue section of *Helix pomatia's* nervous system (A); localization of neurons loaded with FITC fluorescent dye and CHCA matrix (B); MALDI-TOF IMS results for FMRFa (m/z 599.1) indicated in blue (C).

POSTER PRESENTATIONS

SPATIALLY RESOLVED QUANTIFICATION OF ELEMENTS IN CUTANEOUS TUMORS BY LA-ICP-TOFMS

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Clinical diagnosis of skin cancer is currently based on histological evaluation of surgically removed tissue. Accurate identification of tumor type, assessment of malignancy, and determination of tumor margins are essential for effective treatment. With the increasing incidence of skin cancer, there is a growing need for additional analytical approaches [1,2]. Elemental analysis is a promising option, as pathological changes in tissues are often associated with compositional differences [3]. In this work, laser ablation–ICP-TOF-MS (LA-ICP-TOFMS) was used for quantitative, spatially resolved analysis of cutaneous tumors.

In this study, thin tissue sections of malignant melanoma, basal cell carcinoma, and squamous cell carcinoma were quantitatively analyzed together with healthy skin samples for comparison. Elemental maps were obtained and evaluated to compare differences between tumor types and healthy tissue. Quantification was performed using gelatin-based matrix-matched standards for major (Ca, Mg, Na, P) and trace elements (Fe, Cu, Zn, Sr, Mn). Mg and Zn were elevated in tumors, which may be related to changes in metabolism and the tumor microenvironment. The obtained elemental maps provide additional information about tissue heterogeneity that is not accessible by conventional histology. This approach demonstrates the potential of LA-ICP-TOFMS as a complementary tool for studying cutaneous tumors and that it may contribute to understanding of their chemical composition.

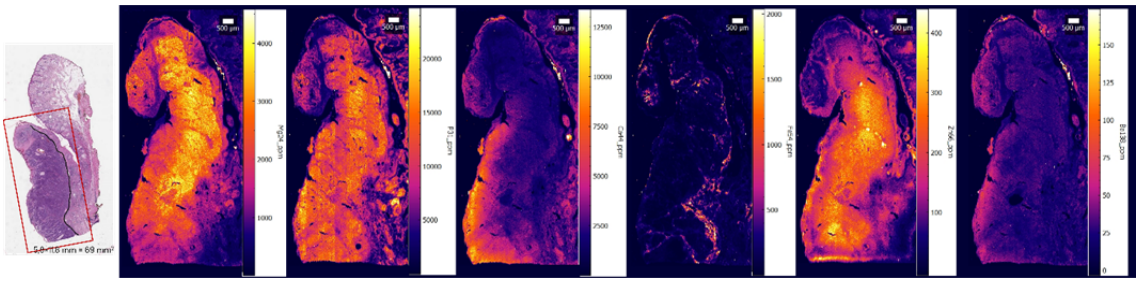

Figure 3. Quantitative LA-ICP(TOF)MS elemental maps of basal cell carcinoma.

Acknowledgements
HK (Brno Ph.D. Talent Scholarship Holder – Funded by the Brno City Municipality) acknowledges the support via the grant VUT-J-25-8897. PP gratefully acknowledges the support of the Czech Science Foundation (no. 25-16166S) and GAUK (no. 1193819).

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ELEMENTAL MAPPING OF DENTAL TISSUES IN SATB2-ASSOCIATED SYNDROME USING LIBS

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SATB2-associated syndrome (SAS), characterized by craniofacial abnormalities and structural dental defects including missing teeth and structural defects, is a rare genetic disorder. Although the SATB2 protein is a proven regulator of odontogenesis, the consequences of its deficiency for biomineralization have not yet been fully elucidated. This study, therefore, focuses on elemental analysis of hard dental tissues in patients with confirmed SATB2 gene haploinsufficiency [1].

Analysis of changes in elemental composition was performed using laser-induced breakdown spectroscopy (LIBS), an atomic emission technique based on laser ablation that enables rapid detection of multiple elements, making it suitable for examining hard tissues [2]. The LIBS method also enables spatially resolved mapping of the distribution of biogenic elements (Mg, Ca, P, Na, K, Sr) in the form of two-dimensional elemental maps.

The study involved a comparison of two human teeth with SATB2 deficiency with a pair of control teeth. To improve spatial resolution, key measurement parameters of the LIBS method were optimized. This optimization enabled the measurement of selected tooth sections with a different spatial resolution (20 μm) than that used for whole teeth (30 μm), allowing for a more detailed evaluation of the local characteristics of dental tissues.

The results revealed an imbalance in the elemental composition of the affected teeth. Elevated magnesium levels indicate the presence of immature mineral phases. Furthermore, reduced strontium levels indicate impaired enamel and dentin maturation, underscoring the important role of the SATB2 protein in the mineralization process of human teeth. Intensity profile analysis revealed significant differences between control and patient samples.

Acknowledgements
This work was supported by the projects by the Czech Science Foundation (no. 25-16166S) and CEITEC VUT/FSI-J-26-9058.

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SUPPRESSION OF NONSPECIFIC SORPTION OF NANOPARTICLE-ANTIBODY CONJUGATE IN P53 PROTEIN DETECTION

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Immunoanalytical techniques are an important tool in disease research and diagnostics. These methods utilize a highly specific interaction between antigen and a labelled antibody. In this work 60nm gold nanoparticles were used as labels and subsequently detected using LA-ICP-MS. Utilization of nanoparticle-antibody conjugates with this detection method increases the sensitivity of the immunoassay. However, it also results in an increase in background signal due to nonspecific interactions. These interactions are caused by hydrophobic attraction, electrostatic attraction, species cross-reactivity etc. [1]. Hence optimization of sample preparation is necessary to minimize these effects.

This research is focused on optimizing the dot-blot method for detection of the p53 protein in cellular lysates. The key optimized parameters were membrane material and sample volume. Additionally, the lower limit of the working range of the immunoassay was determined. The work also investigated the underlying causes of the observed effects and led to an improvement of the repeatability of the method.

Acknowledgments
This research was supported by the Grant Agency of Masaryk University project No. MUNI/C/0147/2026

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ICP-MS-BASED ELEMENTAL PROFILING OF PAIRED PSORIATIC SKIN BIOPSIES: DISTINGUISHING LOCAL TISSUE-SPECIFIC ALTERATIONS

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Psoriasis is a chronic inflammatory skin disorder associated with complex biochemical alterations, including potential disruptions in elemental homeostasis. However, reliable data on elemental composition in psoriatic skin remain limited due to analytical challenges related to small biopsy mass and matrix complexity.

This work applies an inductively coupled plasma mass spectrometry (ICP-MS) to quantitative elemental profiling of human skin biopsies. Paired samples of psoriatic lesions and clinically uninvolved skin from the same patients were analysed, alongside control skin from individuals without psoriasis. A dedicated sample preparation protocol for low-mass tissue was developed and validated using certified reference materials. Particular attention was given to elements associated with inflammatory processes and oxidative stress (Zn, Mn, Mg, Fe, Mo). Statistical evaluation was based on nonparametric methods, including paired comparisons, correlation analysis, and multivariate exploration (principal component analysis).

Elemental profiles differentiated psoriatic lesions, uninvolved skin, and control samples. The most pronounced differences were observed in paired intra-individual comparisons, demonstrating that within-patient normalisation reduces interindividual variability and improves sensitivity to local biochemical changes. Comparisons with control skin provided additional biological context.

The results indicate that elemental alterations in psoriatic skin are primarily associated with local tissue processes rather than systemic inflammation. The applied ICP-MS approach provides a robust analytical framework for low-mass biopsy material and highlights the importance of paired-sample design of elemental dysregulation.

ASSESSMENT AND DENSITY FUNCTIONAL THEORY OF BIOACTIVE COMPOUNDS OF CURCUMA LONGA L. ROOT RESPONSIBLE FOR ITS CARDIO-PROTECTIVE AND ANTI-CANCER ACTIVITIES

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Cardiovascular diseases (CVDs) and cancer remain major global health challenges and are among the leading causes of mortality worldwide, including in Kuwait. Medicinal plants are important sources of bioactive compounds with therapeutic potential. This study aimed to identify the phytochemical constituents of Curcuma longa L. root extract and evaluate their potential cardio-protective and anti-cancer activities using integrated computational approaches.

Phytochemical profiling of Curcuma longa root extract was performed using gas chromatography–mass spectrometry (GC–MS). The identified compounds were evaluated through molecular docking against selected cardiovascular and cancer-related targets, including HMG-CoA reductase, phosphoinositide 3-kinase (PI3K), cyclin-dependent kinase 6 (CDK6), and HER2 kinase receptors. Protein–ligand interactions were analyzed to determine binding stability. Biological activity prediction and pharmacokinetic properties were assessed using PASS prediction and SwissADME tools, while density functional theory (DFT) calculations were conducted to investigate electronic and quantum chemical characteristics associated with ligand reactivity.

GC–MS analysis identified seventeen phytochemical constituents with retention times ranging from 7.57 to 32.70 min. The major compounds detected were 2-oxo-cyclooctaneacetic acid (30.88%), curlone (20.99%), and tumerone (13.85%). Molecular docking revealed favorable binding affinities for α-curcumene, caryophyllene, bergamotene, cyclohexene derivatives, tumerone, curlone, and (6R,7R)-bisabolone against the selected targets, with interaction profiles comparable to reference drugs. PASS and SwissADME analyses indicated promising biological activities, acceptable drug-likeness, and favorable pharmacokinetic properties. DFT analysis demonstrated that curlone and tumerone possessed stable electronic configurations and favorable reactivity profiles.

The findings suggest that bioactive compounds from Curcuma longa may serve as promising lead candidates for the development of cardio-protective and anticancer agents. However, further experimental validation through in vitro and in vivo studies is required to confirm these computational predictions.

INVESTIGATION OF FLUORINE RELEASE FROM DENTAL FILLINGS USING HR-CS FMAS AND HR-CS GFMAS

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Dental health depends on providing the body with an appropriate amount of fluoride, which affects the structure of dental tissue and reduces the development of caries by inhibiting bacterial plaque growth. However, excessive fluoride intake leads to fluorosis of bones and teeth.

Fluorides are supplied to the body with food (beverages) and due to the use of fluoride-enriched oral hygiene products (toothpaste, mouthwashes). Another option is an application specially designed dental fillings that can gradually release fluoride. The choice of filling material depends on the amount and dynamics of fluoride release into the oral environment and can be adjusted to the patient's condition and needs, taking into account existing risk.

This study aimed to investigate the release of fluoride from nine dental fillings into a 0.9% NaCl solution simulating saliva. The tool for determining fluorine was high-resolution molecular absorption spectrometry with a continuous-radiation source and a flame or graphite furnace (HR-CS FMAS or HR-CS GFMAS).

Preliminary tests using a relatively insensitive flame technique allowed selection of determination conditions for three target molecules: GaF, CaF, and SrF, which enable fluorine determinations at levels above 2, 8, and 7 mg/L, respectively (limit of quantification). The trials to measure F via absorption of NaF were unsuccessful.

The most important measurement technique was HR-CS GFMAS with GaF as the target molecule. Optimisation of the measurement conditions enabling fluorine determinations from 0.03 to 100 mg/L (in all tested samples) was performed. The possibility of matrix effects resulting from leaching, apart from fluorine, other filling material components (including Sr, Ba, Al, Si, P, B, Ca and K) was checked. The accuracy of the HR-CS GFMAS method was verified by comparative testing of selected samples using the HR-CS FMAS and/or potentiometry with a fluoroselective electrode.

Fluoride release studies were conducted at 37 °C in independent experiments of 1, 3, 5, 7, 30 and 90 days. The maximum concentration of fluoride leached from a given dental material was from 0.5 to 80 mg/L. Fluoride release kinetics also strongly depended on the filling material (e.g., from about 10% to about 60% of the maximum value after one day of incubation).

The HR-CS GFMAS technique proved an excellent tool for studying fluoride release from dental fillings. In half of the tested samples, the cheap, fast, and simple HR-CS FMAS technique with GaF as the measurement molecule proved sufficiently sensitive.

ADVANCES IN THE APPLICATION OF SINGLE-CELL ICP-MS FOR INVESTIGATING CELLULAR METAL UPTAKE

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Single-cell inductively coupled plasma mass spectrometry (SC-ICP-MS) has emerged as a powerful tool for the quantitative investigation of metal uptake at the level of individual cells. By measuring thousands of cells separately, the technique provides unique information on cell-to-cell heterogeneity that remains inaccessible by conventional bulk analytical approaches [1, 2].

In our recent studies, SC-ICP-MS was applied to investigate the uptake of metal-containing compounds and nanoparticles in mammalian cell systems. Cellular accumulation of platinum-based anticancer drugs, including cisplatin and carboplatin, was quantified in healthy and cancerous cell lines, revealing substantial heterogeneity in intracellular platinum content [3]. The uptake behavior of novel cobalt-, ruthenium- and rhodium-based complexes was also evaluated. Furthermore, cellular uptake of 13 and 20 nm gold nanoparticles was investigated, demonstrating the applicability of SC-ICP-MS in nanoparticle research and highlighting the influence of particle size on cellular accumulation.

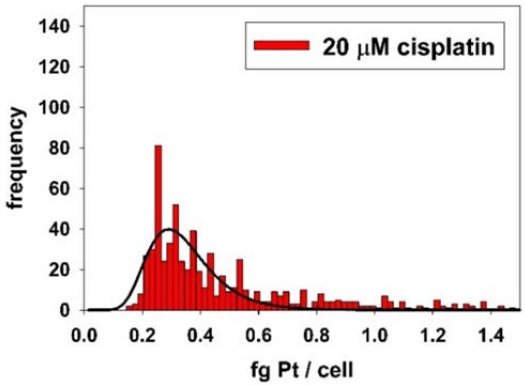

Figure 1. Intracellular platinum masses measured by SC ICP-MS in C26 cells exposed to 20 μM cisplatin.

Current work extends beyond the quantification of intracellular metal content and focuses on the interpretation of uptake distributions obtained by SC-ICP-MS. Distribution-based approaches may provide deeper insight into cellular heterogeneity, the presence of distinct subpopulations, and the relationship between metal uptake and biological response. These results demonstrate the versatility of SC-ICP-MS in metallodrug development, nanoparticle research and mechanistic studies of cellular metal uptake.

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MASS SPECTROMETRIC INSIGHTS INTO SELECTIVE ELECTROCHEMICAL DEFLUORINATION OF FLUORINATED PHARMACEUTICALS

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Fluorinated pharmaceuticals, including widely used fluoroquinolone antibiotics such as levofloxacin and ciprofloxacin, as well as the kinase inhibitor ripasudil, play a crucial role in modern medicine due to their broad-spectrum antibacterial activity and therapeutic effectiveness. Fluoroquinolones are extensively prescribed for the treatment of urinary, respiratory, and gastrointestinal infections, leading to their continuous introduction into the environment through wastewater, agricultural runoff, and improper disposal. These compounds have been detected in various aquatic systems, including rivers, lakes, and groundwater, over a wide concentration range.

Their environmental persistence is primarily attributed to the presence of strong C–F bonds, which exhibit high bond dissociation energy and resistance to conventional biological and chemical degradation processes. As a result, fluorinated pharmaceuticals tend to accumulate in aquatic environments, contributing to the development of antibiotic resistance and posing potential risks to ecosystems and human health. These challenges highlight the urgent need for effective and selective analytical strategies capable of monitoring their transformation and degradation pathways.

This study presents a mass spectrometry-centered approach for investigating the electrochemical defluorination of fluorinated pharmaceuticals in aqueous media. Electrochemical reduction was carried out at a glassy carbon electrode under hydrogen evolution conditions, enabling efficient cleavage of C–F bonds without the use of catalysts or organic solvents. The electrochemical process was validated using high-resolution liquid chromatography-mass spectrometry and potentiometric detection of fluoride ions with an ion-selective electrode. Mass spectrometric analysis confirmed a highly selective degradation pathway, leading predominantly to a single defluorinated product. In the case of levofloxacin, the parent ion (m/z 362) was converted into a dominant product (m/z 340), confirming C–F bond cleavage followed by deprotonation. Notably, no fluorinated intermediates or multiple stable by-products were detected. Simultaneously, potentiometric monitoring enabled real-time tracking of fluoride ion release, providing quantitative confirmation of defluorination efficiency. The integration of electrochemical treatment with mass spectrometry offers detailed molecular-level insight into transformation mechanisms.

The developed approach demonstrates high efficiency, selectivity, and environmental compatibility compared to conventional degradation methods, which often generate multiple uncontrolled by-products. The method was successfully validated in real water samples, highlighting its applicability for environmental monitoring and water treatment. This work emphasizes the critical role of mass spectrometry in elucidating selective degradation pathways of persistent fluorinated pharmaceuticals and provides a robust analytical platform for sustainable environmental applications.

METABOLOMIC PROFILING OF DANDELION AND RELATED FOOD PRODUCT USING COUPLED MASS SPECTROMETRY METHOD

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Plants produce numerous bioactive secondary metabolites that can enter the body through food or medicine. The great chemical diversity of these compounds, their varying concentrations, and their composition—which is also influenced by cultivation and production technologies—present a significant analytical challenge. As knowledge of phytochemistry expands, methods for compound identification and quantification continue to evolve. Mass spectrometry is a fundamental tool in the study of plant-related products, enabling the precise measurement of a compound's molecular mass and the analysis of its fragmentation patterns.

Dandelion (*Taraxacum officinale* (L.) Weber ex F.H. Wigg) is a plant widely distributed throughout the Northern Hemisphere; its roots and leaves have long been used in folk medicine, and its bioactive metabolites are the subject of ongoing research. In addition to its medicinal significance, it can also be used as a food source. To date, more than 200 small-molecule secondary metabolites have been identified from various tissues of the plant.

In our study [1], metabolomic profiling of the dandelion root-leaf drug, dandelion flowers, and a commercially available liqueur made from the latter was performed using a UPLC-ESI-IMS-QTOF-MS system. 84 compounds were identified, 30 of which were identified using authentic standards. The most characteristic molecular families were caffeic acid derivatives (20 compounds), flavonoids (including 21 quercetin and isorhamnetin derivatives), and hydroxylated derivatives of long-chain carboxylic acids. Furthermore, Taraxinositol A and B molecules were successfully identified, their MS/MS fragment spectra were recorded, and their fragmentation patterns were proposed, which had previously been found only in the related species *T. coreanum*. 24 compounds were identified for the first time in this plant species, and the presence of 13 of them was confirmed using authentic standards. During our quantitative analysis, we determined that the technology used in liqueur production is poorly suited for extracting the bioactive metabolites of dandelion flowers from the plant, so modifications to the production technology were proposed. The maturation of the liqueur was also monitored over a two-month period, during which maturation-specific metabolites (e.g., the sulfated form of esculetin) were identified. In the second month—with a few exceptions—a decrease was observed in the amount of secondary metabolites, so we determined that the optimal maturing time for the product is 1 month.

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ARTEFACT OR FEATURE: THE FOLLOW-UP OF CULTIVATION-DEPENDENT STRESS RESPONSE TO SELENIUM EXPOSURE OF CARDAMINE HUPINGSHANENSIS WITH UPLC-PDA-ESI-HR-AM MS-BASED (SELENO)METABOLOMICS

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Cardamine hupingshanensis is a microelement hyperaccumulator plant species of the Brassicaceae family [1]. This plant is indigenous to the Yutangba region (Enshi, Hubei Province, China), where the naturally high selenium content of the soils renders this plant one of the highest natural selenium containing plants in the world, reaching the concentration of 4 g Se kg^{-1} dry weight. [2] In its natural habitat *C. hupingshanensis* shows no visible signs of any stress and represents one of the most abundant plant species of the region.

Scientific and commercial valorization interests in this plant to serve as a high-selenium raw material for feeding and dietary supplement purposes have led to the controlled cultivation of *C. hupingshanensis* in greenhouse conditions where artificial cultivation media (e.g., vermiculite and perlite) have been usually addressed. As a clear contrast to natural cultivation, the biomass of *C. hupingshanensis* derived from the artificial cultivation conditions presented the symptoms of high abiotic stress such as reduced plant height and the accumulation of anthocyanins.

In order to provide the metabolomic description of the altered plant homeostasis, a UPLC-PDA-ESI-HR-AM MS instrumental setup was applied to map the main differences in the phenylpropanoid pathway and in the selenium metabolism of *C. hupingshanensis* [3]. The appearance of novel (glutathione biosynthesis-related) selenometabolites and a distinct set of novel acylated anthocyanins supports the hypothesis that the artificial cultivation parameters triggered a clear abiotic stress event, which should be traced to the transcriptomics and proteomics levels to evaluate whether a formerly hidden adaptation behavior (feature) or solely the artificial cultivation-derived event (artefact) is faced.

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CHARACTERIZATION OF HANK'S BALANCED SALT SOLUTION (HBSS) FOR QUALITY CONTROL USING SPECTROSCOPIC AND CHEMOMETRIC APPROACHES

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Hanks' Balanced Salt Solution (HBSS) has been designed to maintain mammalian cells within a narrow physiological pH range (7.0–7.4) during short-term incubations. The primary functions of HBSS include maintaining osmotic pressure, providing inorganic ions for cellular metabolism, and buffering pH primarily via the $H_2PO_4^-/HPO_4^{2-}$ system, with the H_2CO_3/HCO_3^- buffer serving as an optional complementary component in formulations that contain bicarbonate. The COVID-19 pandemic necessitated in-house HBSS production due to supply chain disruptions, creating an additional burden for pharmaceutical and research laboratories, which also had to develop rapid quality assurance (QA) methods for these solutions. Conventional infrared (IR) spectroscopic analysis faces several challenges when applied to HBSS due to the IR-active components present in very low concentrations, thus, making signal-to-noise ratios problematic and spectral overlap as many peaks for D-glucose, hydrogencarbonate, and phosphates overlap in the 1121–1001 cm^{-1} range. Through principal component analysis (PCA), this study successfully differentiated between five commercially available HBSS variants and one home-made sample. Notably, the PCA analysis was sensitive enough to separate samples based on slight variations in their glucose, carbonate, and phosphate content. Testing on home-made solutions with intentionally altered compositions showed that PCA and linear discriminant analysis could clearly differentiate most samples. While the system struggled to distinguish between ±5-10% changes in HCO_3^- specifically, it successfully flagged the absence of constituents and general shifts in glucose levels. Nuclear Magnetic Resonance (NMR) was used as a complementary tool to provide further information. Thus, ^1H NMR detected D-glucose resonances (α and β anomers) and phenol red, while ^{31}P NMR was used for the quantitative determination of phosphate. In this latter case, recovery rates above 70% were obtained with ~20-minute acquisition times, whereas near-complete recovery required measurements of approximately 50 minutes. An additional advantage of the ^{31}P NMR measurements is that the phosphate chemical shift can subsequently be used to estimate the pH of the samples. Moreover, NMR had the ability to detect impurities such as THF, acetone, acetonitrile, ethanol, ethyl acetate, acetic acid, and isopropanol in traces in the home-made and some commercially available solutions. ATR-FTIR combined with chemometrics is an excellent, rapid method for the quality control and screening of cell culture buffer solutions. This combination provides a straightforward way to monitor composition and ensure solution integrity complemented by NMR measurements if there are no budgetary and time constraints. In conclusion, while NMR remains necessary for the or the accurate determination of phosphate, (even when using benchtop instruments), the combination of ATR-FTIR and chemometric modeling offers a practical solution for pharmaceutical and research laboratories that need to validate in-house or commercial batches of HBSS.

RESOLVING ISOBARIC POST-TRANSLATIONAL MODIFICATIONS BY CYCLIC ION MOBILITY TANDEM MASS SPECTROMETRY

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Post-translational modifications (PTMs) significantly influence the structure, biological function, and activity of proteins; therefore, their precise characterization is essential. Mass spectrometry is a key tool for the investigation of PTMs. Citrullination or deimination is an irreversible PTM, associated with many neurodegenerative (Alzheimer's disease, Multiple sclerosis, Parkinson's disease) and autoimmune (Rheumatoid arthritis) diseases. During citrullination, an arginine (Arg, R) is converted to a citrulline (Cit, X) residue, accompanied by a +0.984 Da mass shift. [1] Protein citrullination is an enzyme-catalyzed process. In contrast to citrullination, protein deamidation is a spontaneous modification, which is also associated with a mass increase of +0.984 Da. Deamidation is associated with protein aging; however, it can also occur during sample preparation, making the identification of *in vivo* modified proteins even more challenging. Deamination occurs mostly on asparagine (Asn, N) and less frequently on glutamine (Gln, Q) residues, leading to an isomeric mixture of *L,D*-aspartyl (Asp, D) and *L,D*-isoAsp products. Due to the same mass increment, citrullination and deamidation cannot be reliably distinguished even by high resolution mass spectrometry.

Our aim was to develop a robust mass spectrometry-based methodology which can differentiate between citrullination and deamidation within a peptide motif. For this, various model peptides were synthetized and analyzed by cyclic ion mobility (cIM) tandem mass spectrometry (MS/MS). Cyclic ion mobility is an advanced ion mobility technique that enables improved ion separation within a closed-loop ion mobility cell, improving resolution and structural characterization. Using this method, we successfully separated deamidated, citrullinated, as well as doubly modified peptides containing both modifications. MS/MS sequencing was also used to verify the citrullination. The neutral loss of isocyanic acid (H-N=C=O, 43 Da mass difference) from citrulline residues either from peptide precursors or fragment ions can be used as an efficient diagnostic MS/MS marker. [2] Our results demonstrate the advantages of cyclic ion mobility mass spectrometry to distinguish highly challenging isomeric and isobaric species.

Acknowledgements
This work was supported by the Lendület (Momentum) Program of the Hungarian Academy of Sciences (HAS, MTA). The sponsorship of Gedeon Richter Talentum Foundation in framework of Gedeon Richter Excellence PhD Scholarship of Gedeon Richter is greatly acknowledged. The grant was awarded to Eszter Fehérvári.

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UNVEILING THE MOLECULAR COMPLEXITY OF SHILAJIT SUPPLEMENTS BY HIGH-RESOLUTION MASS SPECTROMETRY

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Shilajit is a natural, mineral-rich exudate formed over centuries from the decomposition of plant material in mountainous regions, particularly the Himalayas. It has long been used in traditional medicine systems, such as Ayurveda, and is commonly marketed as a dietary supplement with purported benefits including enhanced vitality, improved cognitive function, and general health support. Despite its widespread use and growing commercial availability, the chemical composition of shilajit-based products remains insufficiently characterized, raising questions about their consistency, authenticity, and alignment with marketing claims.

In this study, we investigated three commercially available shilajit-containing dietary supplements from different manufacturers—two in capsule form and one as a viscous liquid. The primary aim was to determine whether bioactive compounds and organic constituents could be reliably identified and to assess whether the advertised composition of these products corresponds to their actual molecular profiles. To achieve this, we developed an ultrahigh-performance liquid chromatography (UHPLC) method coupled with high-resolution tandem mass spectrometry (HRMS/MS), applying an untargeted analytical approach to capture a broad range of molecular features.

Our results revealed notable differences among the products. One sample exhibited a highly diverse and complex chemical composition, containing a wide array of detectable organic compounds, potentially including bioactive constituents associated with shilajit. In contrast, the other two products showed significantly lower chemical diversity. Interestingly, although two samples appeared significantly different upon visual inspection, their molecular complexity were found to be similar based on mass spectrometric analysis. This highlights the limitations of visual assessment and underscores the importance of advanced analytical techniques in supplement characterization. Overall, our findings demonstrate that substantial variability exists among commercially available shilajit products, both in terms of chemical complexity and potential bioactive content. These results emphasize the need for rigorous analytical validation to ensure product quality, authenticity, and transparency, particularly in the context of dietary supplements with claimed health benefits.

Acknowledgements
This work was supported by the Lendület (Momentum) Program of the Hungarian Academy of Sciences (HAS, MTA).

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NEAR- AND MID-INFRARED SPECTROSCOPY WITH CHEMOMETRICS FOR CLASSIFICATION AND QUANTIFICATION OF OIL ADULTERATION IN OLEOGELS

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Edible oleogels are promising structured-lipid alternatives to conventional solid fats, but the replacement of high-value oils with lower-cost vegetable oils creates important authenticity concerns. This focused study investigated two complementary oil-adulteration applications: qualitative classification of authentic and oil-adulterated oleogels by soft independent modelling of class analogy (SIMCA), and quantitative determination of sunflower-oil substitution in extra-virgin-olive-oil-based oleogels by partial least-squares regression (PLSR). Spectra were acquired using benchtop mid-infrared (Mid-IR), benchtop near-infrared (NIR), and handheld NIR instruments; NIR measurements were performed with 1 and 6 mm transflectance pathlengths.

For the SIMCA study, 96 authentic reference oleogels and 64 oil-adulterated oleogels were evaluated (n = 160). The adulterated samples were prepared using argan oil or extra virgin olive oil as the high-value oil, sunflower or corn oil as the lower-cost adulterant, and rice bran wax or beeswax as the gelator. Samples were randomly divided into calibration (n= 120) and independent validation (n = 40) sets. The benchtop Mid-IR model used the 3411–2630 and 1791–912 cm^{-1} regions with mean centering and an 11-point second derivative, and achieved 100% correct classification in both calibration and validation, with an interclass distance of 9.05. NIR models also provided strong discrimination: validation accuracies were 97.5 and 95.0% for benchtop NIR at 6 and 1 mm, respectively, and 97.5% for both handheld-NIR pathlengths. The Mid-IR band near 1083 cm^{-1} and NIR combination-band regions near 4792–4833 cm^{-1} contributed strongly to class separation.

For the PLSR study, 51 extra-virgin-olive-oil-based oleogels were prepared with a constant 10% rice bran wax phase and a 90% total oil phase. Within the oil phase, sunflower oil progressively replaced extra virgin olive oil from 0 to 50% in 1% increments. All Mid-IR and NIR platforms produced useful quantitative models. Benchtop Mid-IR gave a standard error of prediction (SEP) of 2.53%, rPred = 0.97, and RPD = 5.70. The best performance was obtained with benchtop NIR at 6 mm, giving SEP = 0.86%, rPred = 0.99, and RPD = 16.67; the corresponding 1 mm model gave SEP = 0.99% and RPD = 14.45. Handheld NIR retained rPred = 0.98, with SEP values of 1.96–2.19% and RPD of 6.57-7.34, demonstrating practical potential for rapid field screening. Overall, SIMCA reliably detected lower-cost oil adulteration across representative oleogel formulations, while PLSR accurately quantified sunflower oil in the selected extra-virgin-olive-oil matrix, supporting a non-destructive screen-then-quantify strategy for oleogel quality control.

Acknowledgement
This work was supported by TÜBİTAK under Project No. 2240126.

MONITORING LITHIUM ACCUMULATION IN PLANTS USING LASER-INDUCED BREAKDOWN SPECTROSCOPY

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Lithium (Li) is a naturally occurring element, but it is not considered essential for life. In recent years, growing battery production has increased environmental concern over Li contamination. Li accumulation in edible plant tissues may also pose a possible risk to human health through entry into the food chain. This points to the need for rapid and reliable analytical methods for detecting Li in plant tissues. Laser-induced breakdown spectroscopy (LIBS) has recently emerged as a promising tool, offering rapid, multi-element detection with minimal sample preparation and potential for in situ measurements [1].

In this study, radish (*Raphanus sativus* L.) plants were grown in hydroponic solutions contaminated with lithium. Pre-germinated radish sprouts were exposed for 72 h to two different lithium contaminated solutions ($LiNO_3$ and LiCl) of three concentrations (3.5, 7, and 14 mg/L Li) with a control solution of 0 mg/L Li. At harvest, plants were washed from the solution, measured for length of plants and weighed for fresh weight. Plants were divided into two parts, one for elemental analysis (LIBS) and the second for plant pigments determination. The first part of the plant material was dried, moulded, and fixed onto a glass slide with epoxy resin for LIBS analysis. The second part of the fresh plants was used for chlorophyll and polyphenol content analysis.

LIBS results indicate a strong accumulation of Li in the radish plant tissue (Figure 1). On the other hand, important nutrient elements, such as Mg, Ca, Na or K, were not influenced by the presence of lithium during growth. The 14 mg/L of lithium significantly lowered chlorophyll content and fresh weight and caused visible black spots – necrotic lesions.

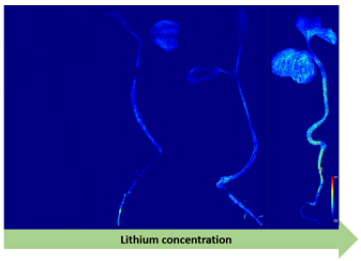

Figure 1. Lithium accumulation in $LiNO_3$ treated plants.

Acknowledgements

This work was carried out with the support of grant no. CEITEC VUT/FSI-J-26-9056. JK acknowledges the support of grant no. FSI-S-26-9044.

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SENSITIVITY IMPROVEMENT OF ELCAD-OES FOR THE DETERMINATION OF SOME ENVIRONMENTALLY RELEVANT ELEMENTS IN WATER SAMPLES

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The electrolyte cathode atmospheric glow discharge (ELCAD) is a DC plasma developed for the optical emission spectrometry (OES) determination of elements in solution samples [1], and soon after applied to the analysis of natural and waste waters [2]. The main advantage of ELCAD is the possibility of direct introduction of solution samples, after adjustment of the sample pH. For this purpose, various inorganic acids were applied in former studies, such as for instance HCl and HNO_3 [1,2]. The drawback of the ELCAD-OES method is the relatively low sensitivity, due to quenching of analyte signals. The high spectral background besides the molecular bands of certain plasma species (N_2, NO, NH) may overlap with the most important resonant lines of the analytes, present in the UV-range. The elimination/decrease of these spectral interferents is important for attaining higher analytical sensitivity.

In the present investigation, alternative and conventional acids (e.g., HNO_3, HCl, HBr, HAc) were applied for the acidification of samples to attain enhanced sensitivity for the ELCAD-OES determination of a couple of environmentally relevant elements (Cd, Cu, Hg, Ni, Pb, Zn). The glass capillary design of ELCAD with a tungsten anode was applied for this study, equipped with a CCD spectrometer (Maya2000Pro). The method is investigated for sample pH, flow rate, plasma observation height, GD voltage–current characteristics, and vertical analyte distribution, to get a closer look into likely plasma mechanisms in the presence of the studied sample medium. The recorded spectra of the samples were corrected for background emission, based on the spectra of acidic blanks. Depending on the type of acid and analyte, the limit of detection (LOD) values can be improved by a factor of 1.5-3.2, reaching values as low as 0.1-1.9 mg/L at a GD operating current of 65 mA. The calibration curves for the study analytes were linear up to 90-120 mg/L. The recovery of the optimized method was tested in spike experiments of water samples of different salinity (e.g., lake, river).

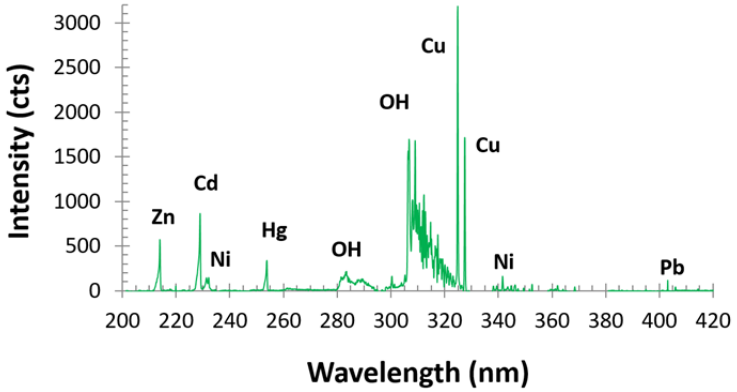

Figure 1. Background corrected ELCAD-OES spectra recorded with a standard acidified with HBr (pH=1.54).

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DETERMINATION OF ANTIOXIDANT CAPACITY IN TEA LEAVES USING THE DDPH SCAVENGING METHOD

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This study investigated the antioxidant capacity of different tea leaves using the DPPH (2,2-diphenyl-1-picrylhydrazyl) radical scavenging assay coupled with UV–Vis spectrophotometry [1]. Five commercially available tea products, including green tea, bergamot-flavored black tea, fruit tea and moringa tea leaves were analyzed in both raw and brewed forms. Tea extracts were prepared with 80% ethanol using ultrasonication-assisted extraction followed by centrifugation [2]. Antioxidant activity was determined by monitoring the decrease in DPPH absorbance at 515.5 nm after 30 min incubation and expressed as ascorbic acid equivalents (AAE).

The calibration curve obtained with ascorbic acid standards showed excellent linearity. The IC_{50} value of ascorbic acid (concentration at which the antioxidant neutralizes 50% of the DPPH radicals) was determined to be low, indicating the excellent ability of the antioxidant to scavenge radicals. Green tea and bergamot-flavored black tea [2] exhibited the highest antioxidant capacities, with DPPH scavenging values above 91%. Fruit tea also demonstrated high antioxidant activity likely due to the presence of vitamin C and phenolic compounds from fruit ingredients. In contrast, moringa tea [3] leaves showed lower antioxidant capacities explained by its composition. Brewing decreased antioxidant activity in all cases, indicating partial degradation or incomplete extraction of antioxidant compounds during infusion preparation. Extraction efficiencies ranged between approximately 20–80%, depending on tea composition and brewing conditions recommended by manufacturers.

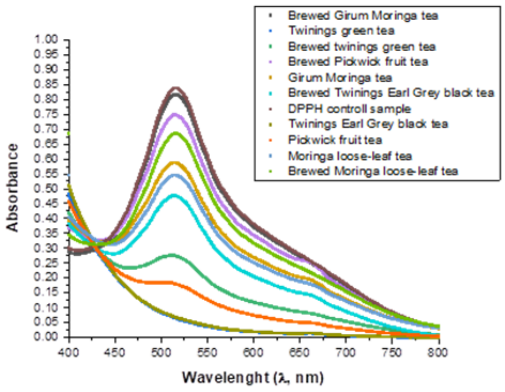

Figure 1. Visible spectra of analyzed tea samples before and after brewing.

The observed differences among tea types were consistent with their expected polyphenol content and with literature data, highlighting that green and bergamot-flavoured black teas as significant dietary sources of antioxidants.

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ASSESSMENT OF TOXIC ELEMENTS IN ONLINE-MARKET COCOA POWDERS

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Europe represents only 6% of the world's population, yet it consumes approximately half of the global chocolate production. As cocoa is not cultivated within Europe, the European Union relies entirely on imports of cocoa beans and cocoa-based products [1]. The growing availability of cocoa powders through online marketplaces highlights the need for continuous monitoring of potentially toxic elements in these commodities. In this study, toxic and potentially toxic elements—aluminium, arsenic, barium, cadmium (Cd), mercury and lead (Pb)—were quantified in cocoa powders purchased through online channels. These products, often marketed as premium or specialty cocoa (including Trinitario, Criollo and Forastero types), and partly originating from ecological farming, may not consistently undergo the same regulatory scrutiny as conventionally distributed brands, making them an important target for analytical evaluation.

Twelve cocoa powder samples from major cocoa-exporting countries (Colombia, Ecuador, Peru, Ghana and Indonesia) were analysed. Samples were subjected to microwave-assisted acid digestion, followed by inductively coupled plasma mass spectrometry (ICP-MS). Among the investigated elements, only Cd has a harmonised health-based limit value in the European Union for cocoa products (0.6 mg/kg) [2], while Pb has a defined limit value in Chinese regulations (0.5 mg/kg) [3]. No unified international legislative framework exists for the remaining elements, underscoring the relevance of analytical surveillance.

The results revealed that 25% of the samples exceeded the EU Cd concentration limit, with one Ghanaian sample reaching 0.64 mg/kg. For Pb, 50% of the samples surpassed the Chinese limit value, indicating potential consumer-exposure concerns. To complement concentration-based evaluation, Estimated Daily Intake (EDI) and Target Hazard Quotient (THQ) calculations will be performed for toddlers, children and adults using realistic cocoa-consumption scenarios. These risk-assessment metrics will provide a more comprehensive view of potential health risks associated with regular cocoa consumption.

Overall, our study highlights the analytical strength and sensitivity of ICP-MS for food-contaminant monitoring and emphasises the importance of continuous surveillance of widely consumed products such as cocoa - particularly those sourced from ecological farming and distributed through online platforms where regulatory oversight may vary. The results contribute to ongoing discussions on harmonised international safety limits and support the need for evidence-based consumer-protection strategies.

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TOXIC ELEMENT PROFILING OF FAST-BEAUTY LIPSTICKS

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Lipsticks are applied directly to the lips, where incidental ingestion and prolonged contact with the oral mucosa may expose consumers to potentially toxic elements. This is particularly relevant for low-cost cosmetics purchased through ultra-fast fashion online platforms, which are widely accessible while offering limited information on elemental impurities associated with pigments, raw materials or manufacturing processes. As products imported from outside the European Union may be subject to different regulatory and market surveillance frameworks than locally distributed cosmetics, their analytical screening can provide useful information for consumer safety and risk awareness.

In this study, nine lipstick samples were investigated, including seven products ordered from an ultra-fast fashion website based on user popularity and two budget-category lipsticks purchased from local drugstores. The samples were homogenized by melting to allow representative subsampling, followed by microwave-assisted acid digestion. After centrifugation and dilution, the digests were analyzed by inductively coupled plasma mass spectrometry. The elements investigated included Al, Cr, Co, Ni, As, Cd, Sn, Hg and Pb.

The determined elemental concentrations showed wide variation among the lipstick samples. Aluminium was present at the highest concentrations, ranging from 0.76 to 8.6 mg/g, followed by Sn (0.3–317 μg/g), Ni (2.34–77.2 μg/g), Cr (1.73–5.42 μg/g), Co (0.074–5.32 μg/g), Pb (0.003–2.07 μg/g), As (0.004–0.49 μg/g), Cd (0.001–0.070 μg/g). Mercury was detected only in one sample at the 0.007 μg/g concentration level. The concentrations of potentially toxic elements determined in the nine lipstick samples were compared against the strictest limits available in the compiled international cosmetic regulations. Lead exceeded the applicable limit in 11.1% of the samples (strictest limit considered: 2 μg/g, Germany). Nickel also exceeded the applicable limit in 11.1% of the samples (strictest limit considered: 10 μg/g, Germany/Korea) in the same sample. For Cd, Hg and As, none of the samples exceeded the strictest available limits. No limit-based evaluation was performed for Al, Cr, Co and Sn, as no directly comparable regulatory limits for these elements were included in the compiled cosmetic limit table.

The detection of potentially toxic elements in products intended for direct lip application underlines the importance of routine analytical control of low-cost cosmetics obtained from international online marketplaces. The study demonstrates that ICP-MS is a suitable technique for multi-element profiling of lipstick samples and may contribute to the identification of products that require further safety evaluation.

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STATISTICAL ANALYSIS OF REAL-TIME CONCENTRATION OF AIR POLLUTANTS IN VEGAN AND VEGETARIAN COMMERCIAL KITCHENS

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Indoor air quality is an important public health concern, as individuals spend approximately 87% of their time indoors [1]. Cooking activities are major sources of indoor air pollution, emitting particulate matter (PM), aldehydes, and volatile organic compounds that may adversely affect human health [2, 3]. Real-time monitoring of indoor air pollutants captures temporal variability and short-term emission events associated with cooking activities. While considerable research has examined cooking-related indoor air pollution, commercial kitchens serving vegan and vegetarian dishes remain largely understudied. These kitchens frequently use vegetable oils high in polyunsaturated fatty acids, and their thermal degradation produces cooking oil fumes rich in aldehydes and other pollutants. [4]. Previous studies have reported considerable emissions of PM, polycyclic aromatic hydrocarbons, volatile organic carbons (VOCs), secondary organic aerosols, and benzene, toluene, ethylbenzene, and xylenes from plant-based cooking processes [5, 6].

In this study, we collected real-time indoor air pollutant concentrations of ultrafine particles (UFPs), CO_2, O_3, NO_2, total VOCs, and formaldehyde using continuous online monitoring at 1-minute resolution over 4–8 hours across 11 vegan, vegetarian, and traditional restaurants during one warm and one cold seasons. Several portable instruments and sensors were used, including non-dispersive infrared detection for CO_2, UV absorption at 254 nm for O_3, and a photoionization detector for TVOCs. Other sensors such as electrochemical sensors for NO_2 and formaldehyde, as well as a condensation particle counter for UFPs were also employed. Because seasonal changes and variations in kitchen operations can influence pollutant levels and exposure, thorough statistical analysis of the real-time data sets were required. Quantifying these differences provides insights into the factors shaping indoor pollutant dynamics in commercial kitchens. To identify statistically significant differences in pollutant concentrations between kitchen types and seasons, we applied quantitative statistical evaluation methods, including distribution visualization through box plots, normality testing with the Kolmogorov–Smirnov test, group comparison using the Mann–Whitney U test, and effect-size estimation using Cohen's d to determine the magnitude of statistically significant differences.

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INTEGRATED ATOMIC SPECTROMETRIC METHODS FOR MULTI-MATRIX ELEMENTAL ASSESSMENT OF THE SOIL–PLANT–ANIMAL CONTINUUM

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Reliable assessment of mineral status in grazing livestock requires the integrated evaluation of environmental and biological matrices because elemental metabolism is influenced by soil properties, forage composition, feeding practices and animal physiology. The diversity of sample types and the wide concentration ranges of essential and potentially toxic elements often require the complementary application of different atomic spectrometric techniques.

An integrated analytical workflow has been established at the University of Veterinary Medicine Budapest for routine multi-element analysis of environmental and biological samples relevant to veterinary diagnostics and mineral nutrition studies. The workflow combines ICP-OES, ICP-MS and graphite furnace atomic absorption spectrometry (GFAAS) with matrix-specific sample preparation, including microwave-assisted acid digestion and direct dilution. The methodology has been applied to soil, forage, drinking water, blood plasma, whole blood, urine, hair, faeces and animal tissues.

The workflow is demonstrated through a seasonal monitoring study on an organic beef cattle farm in Hungary. Simultaneous analysis of environmental and biological matrices enabled the investigation of elemental transfer across the soil–plant–animal continuum. Particular attention was paid to selenium, copper, zinc, iron, cobalt, molybdenum and aluminium because of their nutritional importance and known antagonistic interactions. The study revealed limited selenium transfer from soil to forage despite adequate soil selenium concentrations and highlighted the importance of considering Fe–Mo–S interactions when interpreting copper status. Seasonal differences between plasma and hair further demonstrated the complementary value of these matrices for assessing mineral status.

The proposed workflow illustrates how complementary atomic spectrometric techniques can be integrated into a practical strategy for multi-matrix elemental assessment in veterinary diagnostics and may also support agricultural, environmental and biomonitoring studies.

ADSORPTION OF HEAVY METAL IONS IN MICROPLASTIC-CONTAINING WATERS

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Microplastics are persistent environmental pollutants that, due to their small size and surface properties, can interact with various contaminants, including heavy metal ions. Therefore, they may act not only as pollutants themselves, but also as potential carrier surfaces [1,2].

The aim of our work was to investigate how cold plasma treatment, used as an imitation of natural ageing processes, affects the surface of three common polymer pollutants, polyethylene (PE), polypropylene (PP) and polyethylene terephthalate (PET), as well as their adsorption behaviour toward Cd(II), Cr(VI), Cu(II), Pb(II) and Zn(II) ions.

The polymers were ground by cryogenic milling and then investigated in pristine (P) and aged (A) forms. The adsorption experiments were carried out in deionized water, and the remaining metal ion concentrations were determined by ICP-OES. Surface changes were characterized by SEM, ATR-FTIR, XPS, DSC, particle size distribution measurements and specific surface area analysis.

Based on the results, cold plasma treatment mainly caused surface chemical modifications, XPS measurements showed an increase in oxygen content and in the O/C ratio, while the bulk thermal properties remained essentially unchanged.

In the adsorption experiments, Pb(II) showed the highest adsorption, while Cr(VI) showed the lowest. Plasma treatment did not result in a general increase in adsorption, suggesting that metal ion binding is determined not only by surface oxidation and polarity, but also by the polymer type, the chemical and physical state of the surface, and the chemical form of the metal ion.

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DETECTION OF HALOGENATED PESTICIDES ON TOMATO FRUITS USING LASER-INDUCED PLASMA SPECTROSCOPY AND MACHINE LEARNING ALGORITHMS

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Nowadays, there is a growing demand for simple, fast, non-destructive and cost-effective analysis of agricultural and food products. Laser-induced breakdown spectroscopy (LIBS) is gaining popularity in many industrial areas, including agriculture and the food industry, due to its many advantageous features (e.g. fast, multi-element method, minimal sample preparation and sample requirements, field applicability, "fingerprint-like" information-rich spectra, etc.). Literature data show that evaluating LIBS spectra with multivariate statistical methods is an effective approach for classifying food samples. The information obtained in this way can be used for quality control, adulteration detection, and contamination detection [1,2].

The aim of our work was to investigate the feasibility of qualitative discrimination analysis of halogenated pesticides on the surface of tomato fruits based on their LIBS spectra. We worked with five pesticides (acetamiprid, chlorpyrifos-ethyl, lambda-cyhalothrin, tebuconazole and tefluthrin) and tested the effectiveness of several machine learning methods (linear discriminant analysis (LDA), classification tree (CT), random forest (RF)) [3]. Several data reduction and variable selection methods were also tested. For the analysis of pesticides, a small, closed cylindrical ablation cell was also developed. They were applied to the skin of tomato fruits in concentrations similar to their spraying concentration in agricultural applications (0.01-1 m/v%). We tested the performance of the methpd both with and withut sampling.

Acknowledgements
The authors gratefully acknowledge the financial support received from the National Research, Development and Innovation Office (NKFIH) of Hungary through K146733, TKP2021-NVA-19 and GINOP-2.3.3-15-2016-00040.

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DEVELOPMENT OF A DIRECT SAMPLING GFAAS METHOD FOR SIMULTANEOUS DETERMINATION OF CADMIUM AND LEAD IN FRUIT JUICES

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Simultaneous determination of Cd and Pb in complex beverages by graphite furnace atomic absorption spectrometry (GFAAS) is analytically challenging, due to the different thermal behavior of the analytes, which requires compromise furnace conditions, while minimizing matrix interference. For this purpose, a direct-sampling multi-element GFAAS method was developed using a PerkinElmer SIMAA-6000 spectrometer equipped with a transversely heated graphite atomizer fitted with an end-capped graphite tube and an integrated platform (IGP). The analytical lines of Cd I 228.8 nm and Pb I 217.0 nm were selected for the analysis.

The graphite furnace heating program, the amount of oxidizing agent, and the chemical modifier composition were optimized. A 5 µL aliquot of oxidizing agent consisting of 10% (v/v) HNO_3 and 60% (v/v) H_2O_2, with 5 µL of 1 g/L Pd and 5 µL of 0.6 g/L $Mg(NO_3)_2$ modifier was directly injected into the pre-heated IGP (70 ˚C) along with 10 µL of fruit juice sample. The Optimum pyrolysis and atomization temperatures were 600 ˚C and 1600 ˚C, respectively. The experimental characteristic mass was 1.2 pg Cd and 15.1 pg Pb. The detection limit was 0.1 µg/L for Cd and 1.2 µg/L for Pb, both well below the European Food Safety Authority regulatory limits. Mean recoveries obtained from 32 spiked fruit juice samples were 100.9% for Cd and 110% for Pb, with mean RSDs of 2.7% and 2.2%. Cd and Pb concentrations in fruit juice samples ranged from non-detectable to 7.3 µg/L and 18.1 µg/L, respectively.

The method greenness assessment showed a moderate-to-good environmental profile, with an AGREE score of 0.65. Product contamination assessment, single pollution index, and health risk assessments (tolerable weekly intake for Cd and margin of exposure for Pb) showed that the measured samples are within safety limits. The method enables the rapid, simultaneous determination of Cd and Pb in fruit juice without sample pretreatment, thereby reducing reagent consumption, analysis time, and the risk of contamination.

SIMULTANEOUS DETERMINATION OF CHROMIUM AND BERYLLIUM IN FRUIT JUICES BY DIRECT SAMPLING GFAAS

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Conventional GFAAS determination of trace elements in fruit juices generally relies on acid digestion, which is time-consuming, requires relatively large volumes of reagents, and generates considerable chemical waste. This study aimed to develop a direct-sampling GFAAS method for the simultaneous determination of Cr and Be in fruit juices without sample pretreatment. A SIMAA-6000 spectrometer equipped with a transversely heated graphite atomizer (THGA) fitted with an end-capped graphite tube and an integrated graphite platform (IGP) was employed. The sample introduction and graphite furnace heating program were optimized using apple juice samples with a sugar content of 11%. The volume of a mixture of H_2O_2 (60%) and HNO_3 (10%) as an oxidizing agent was optimized using a 3^2 factorial experimental design with a general linear model analysis. The optimal pyrolysis and atomization temperatures were 1500 ˚C and 2300 ˚C, respectively. External calibration exhibited good linearity for both analytes (R^2=0.9995 for Cr and 0.9951 for Be), up to 32 µg/L for Cr and 8 µg/L for Be. The experimental characteristic mass was 9.6 pg Cr and 2.7 pg Be. The detection limits were 0.1 µg/L for Cr and 0.06 µg/L for Be, both well below the US EPA regulatory limits for drinking water: Cr: 100 µg/L; Be: 4 µg/L. Optimized sample introduction was performed using a 10 µL aliquot of the fruit juice sample dispensed onto the IGP preheated to 70 °C, along with 5 µL of oxidizing agent, 5 µL of 3 g/L $Mg(NO_3)_2$, and 10 µL of ultrapure water as a diluent.

Standard addition calibration provided good recovery for Cr (97%), while further optimization was required for Be due to matrix-dependent signal enhancement. The developed method was applied to 27 commercial fruit juice samples, of which Cr and Be concentrations ranged from non-detectable to 7.6 µg/L and 1.9 µg/L, respectively.

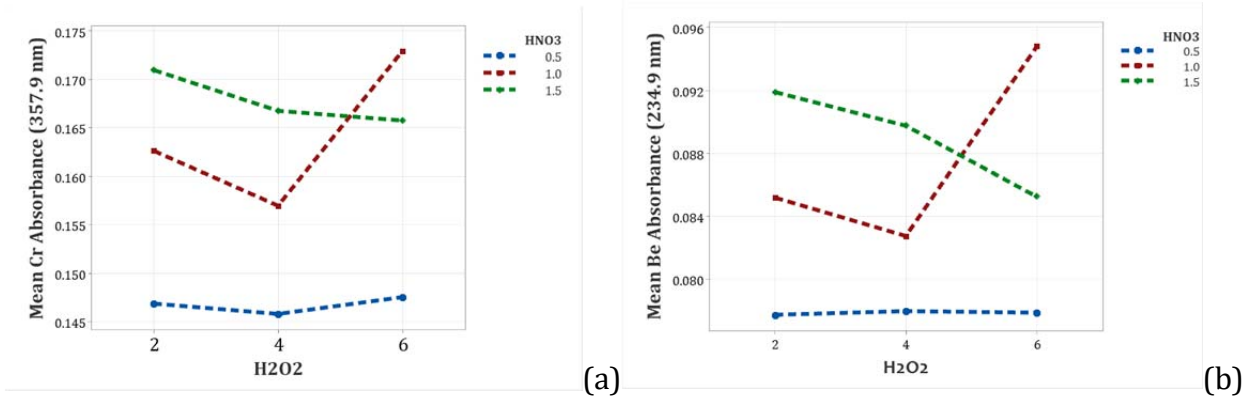

Figure 1. Effects of HNO_3 and H_2O_2 concentrations on the integrated absorbance of Cr (a) and Be (b).

DIRECT ANALYSIS OF SIZE FRACTIONATED AIRBORNE PARTICLES WITH TOTAL REFLECTION X-RAY FLUORESCENCE SPECTROMETRY

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Airborne particular matter (PM) or aerosols are ubiquitous in ambient conditions and a topic for research investigating the origin and health effects of these substances. Aerosols are classified based on their size which determines the capability of deep penetration into the lungs. The separation and collection of these size-fractions is usually performed by filtration or through impaction on a substrate in an impactor [1,2]. In this research, a specially designed impactor for the direct analysis on quartz glass reflectors for Total Reflection X-Ray Fluorescence (TXRF) Spectrometry is used.

TXRF is a powerful method for the quantitative and qualitative analysis of trace-elements in the nano- or picogram regime. It commonly provides *quasi* matrix-free results with short measuring times and cost-efficient sample preparations [2].

An overloading of the sample carrier for TXRF can happen quickly depending on the ambient conditions for the aerosol collection. An optimization of the collection time is necessary depending on the concentrations of airborne particles and might require only a few minutes or up to multiple hours. This work contains the first results of aerosol collections and the direct analyses in different environments to show the influences of the collection duration and location on the traceable composition of the samples.

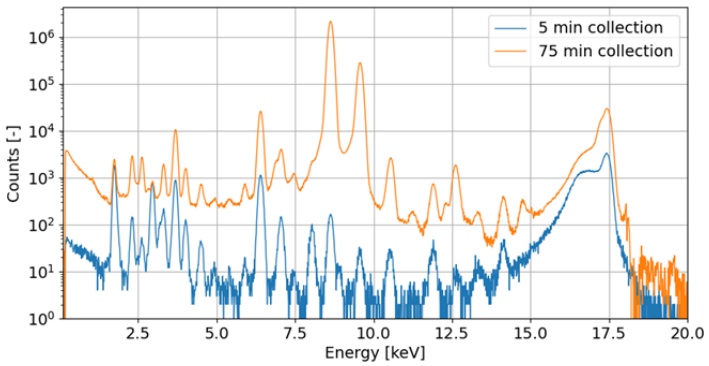

Figure 1. Comparison of two spectra for the $PM_{0.15}$ fraction collected for 5 and 75 minutes.

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AGING THE TIMELESS POLLUTANT: THE ANALYSIS OF ARTIFICIALLY AGED PET SAMPLES USING POSITRON ANNIHILATION LIFETIME SPECTROSCOPY

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Plastics from coastal litter end up in rivers, placing a significant burden on the environment where it stays for a long time, accumulating ever more rapidly. In the long term, this poses a threat to human and animal health, which is why recycling is important. The recyclability of plastic is highly dependent on the degradation it suffered while in the environment.

In this work, positron annihilation lifetime spectroscopy (PALS) was used to investigate PET bottle samples artificially aged in a Xenon chamber and recovered riverine samples. Measurements were performed using a ^{22}Na positron source and scintillation detectors. The data was plotted to visualize the results. The results show a decrease in positronium-intensity with increasing ageing time, indicating changes in the number and size of free volume holes in the PET structure. The observed trend is consistent with previous studies [1]. The method allows for solvent free green analytics and the results enabled the comparison of PET samples at different ageing stages and allowed the characterization of the extent of degradation.

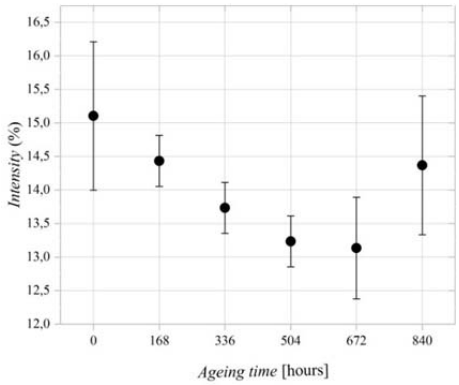

Figure 1. Change of positronium intensity during artificial ageing of PET.

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THE USE OF BACTERIAL CELLULOSE IN THE FIELD OF ANTI-COUNTERFEITING USING A FLUORESCENT ADDITIVE

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Counterfeiting remains a persistent global challenge, driving continued interest in advanced materials with difficult-to-replicate security features.

Cellulose nanocrystals, derived from plant cellulose, are already used in anti-counterfeiting technology such as security labels. The production and isolation of cellulose nanocrystals require aggressive chemical treatments to remove impurities and other components of plant cellulose like lignin or hemicellulose [1]. On the other hand, bacterial cellulose (BC) consists of only cellulose without lignin or hemicellulose. Thus, BC presents a great alternative due to its very high chemical purity and mechanical strength. Nowadays, BC is already used with excellent efficiency in wound healing applications and packing technology [2,3]. These exceptional properties of BC allow its applicability in fine printed or embossed security features completed with e.g. fluorescent additives.

BC was subjected to acid dissolution using sulfuric acid (H_2SO_4) to form a clear solution. The dissolved BC was functionalized with fluorescein as a fluorescent additive to impart optically detectable security features. The resulting fluorescein-BC system was measured using UV-Vis spectrometry to evaluate its absorption and emission behavior. Through these measurements, the successful incorporation of the additive can be confirmed and its potential applications for anti-counterfeiting can also be attested.

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THE HIDDEN LANGUAGE OF PROTEINS IN PSORIASIS: A MASS SPECTROMETRY PERSPECTIVE

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Proteomics is one of the key disciplines of modern biomedical sciences, focusing on the comprehensive analysis of proteins, including their abundance, structure, post-translational modifications, and mutual interactions in cells and tissues. Unlike genomic and transcriptomic studies, proteomics captures the functional landscape of biological processes, as proteins are the direct effectors of cellular and tissue responses. The dynamic development of high-resolution mass spectrometry and bioinformatic tools has enabled the simultaneous identification and quantitative analysis of thousands of proteins in complex biological samples. As a result, proteomics has become an important tool in studying disease pathogenesis, searching for biomarkers, and advancing precision medicine.

This approach has gained particular importance in the investigation of inflammatory skin diseases, including psoriasis, which is a chronic immune-mediated dermatosis with a complex molecular background. Proteomic analyses have demonstrated that psoriatic skin exhibits a distinctly altered protein profile compared with both healthy skin and clinically unaffected skin. These changes involve proteins associated with inflammatory response, activation of innate immunity, keratinocyte differentiation, epidermal remodeling, and regulation of the IL-17 and IL-36 pathways. The results of these studies indicate that proteomics not only deepens our understanding of the pathogenic mechanisms underlying psoriasis, but also creates real opportunities for the identification of diagnostic, prognostic, and predictive biomarkers that may, in the future, support the selection of targeted therapies and the development of personalized treatment strategies.

Acknowledgement
Research in this area is conducted in collaboration with the Military Institute of Medicine – National Research Institute (WIM-PIB) in Warsaw, which strengthens its translational dimension and highlights the importance of an interdisciplinary approach combining basic science with clinical practice.

SENSITIVE DETERMINATION OF GERMANIUM USING HYDRIDE GENERATION, MINIATURE PLASMA AND HIGH-RESOLUTION MASS SPECTROMETRY WITH ORBITRAP ANALYZER

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Chemical hydride generation (HG) is a powerful technique for producing volatile species of elements from groups 14–16 of the periodic table, enabling efficient matrix-free sample introduction. Among the hydride forming elements, Ge is known to be difficult to atomize in heated quartz tube and diffusion flame atomizers, as well as in dielectric barrier discharges (DBDs). This significantly impairs the analytical performance of methods based on atomic absorption or fluorescence spectrometry. ICP-MS coupled with HG is a feasible way of ultrasensitive Ge determination and speciation analysis, including isotope ratio analysis.

High-resolution mass spectrometry using an Orbitrap mass analyzer (HRMS) provides high mass accuracy and resolving power. In combination with an ambient ionization technique, direct analysis in real time (DART), it was recently used in mechanistic studies of HG [1] or volatile species identification [2,3]. However, no attempts have been made to achieve sensitive HRMS determination of elements following their HG.

In the preliminary experiments, HG of Ge was coupled with DART-HRMS to investigate the parameters that influence Ge ion transmission, fragmentation and detection. GeH_4 was generated by the reaction of Ge^{4+} with $NaBH_4$ in a TRIS buffer medium. Then, it was ionized in the DART at 250°C using N_2 as a discharge gas. Several HRMS parameters were examined to achieve the highest signal-to-noise ratio (SNR) for total Ge determination. Significant effects on SNR were found from RF lens voltage and the collision-induced dissociation approaches (in-source fragmentation and higher-energy collision dissociation). A much higher SNR was obtained in negative ion mode, where several $GeO_x(H_y)^-$ ions, where x= 2–4 and y= 0–3, were detected. The applied fragmentation approaches "simplified" the spectra, primarily detecting GeO_2^-. To improve SNR, HRMS acquisition parameters were also examined, including the m/z measurement range, ion accumulation time in the C-trap, and number of microscans. Preliminary tests indicate that the LOD may be in the ng/L range.

This ongoing work focuses on the development and optimization of a laboratory DBD ionization source to further improve ionization efficiency and analytical robustness. Two DBD designs will be demonstrated: *a)* a tubular design based on a quartz tube with two brass outside electrodes, creating a plasma jet; and *b)* a cylindrical design with an outer brass electrode and an inner aluminum rod electrode within a heat-sealed quartz capillary. Analytical performances of both designs will be compared to that obtained using DART.

Acknowledgements
The research was supported by the Czech Science Foundation (project 26-22432S) and the Inst. of Anal. Chem. of the Czech Academy of Sciences (Inst. Res. Plan No. RVO: 68081715).

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ELEMENTAL COMPOSITION AND BIO-BASED CONTENT OF POLYMERS USING ICP-OES AND ^{14}C TECHNIQUES

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Plastics are one of today's dominant factors, widely used in many areas of industry and life over the years thanks to their versatility and relatively low production costs. More than a third of the world's plastic production is used for packaging that comes into contact with food and the human body. Environmental concerns and the limited availability of fossil resources mean that plastics from renewable sources are becoming increasingly important. Our study presents a rather new perspective on the analysis of polymers using accelerator mass spectrometry radioactivity (^{14}C) and inductively coupled plasma optical emission spectrometry techniques. In our research, different types of polymer samples were analysed, including raw materials, commercially available finished products and selected materials from recycling plants. Elemental analysis was used to determine the amounts of selected elements (Ag, Al, B, Ba, Bi, Ca, Cd, Co, Cu, Cr, Fe, K, Li, Mg, Mn, Na, Ni, P, Pb, Pd, S, Sb, Sn, Sr, Ti, Zn).

The measured concentration values give a good indication of the quantitative relationships of the additives added during the manufacturing processes and the importance of Ca. When the concentrations of lead and cadmium in the samples were compared with the limit values of the EU legislation, it was found that only one bin liner with a lead concentration of 294 $mg \cdot kg^{-1}$ exceeded the limit value of 60 $mg \cdot kg^{-1}$. The bio-based carbon content of each fossil and bio-based polymer tested by our ^{14}C measurements was within the expected quantitative ranges. In the case of the PLA-based samples, we observed products that differed from the expected value and were found to be a mixture. By combining the two analyses, it was concluded that despite the lack of a strong relationship, a much more comprehensive picture of the polymers can be obtained by combining the two measurement techniques.

FEASIBILITY STUDY OF COUPLING PHOTOCHEMICAL VAPOR GENERATION AND HIGH RESOLUTION MASS SPECTROMETRY WITH ORBITRAP ANALYZER FOR TUNGSTEN ULTRA-TRACE DETERMINATION

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Photochemical vapor generation (PVG) is a sample introduction technique that converts analytes into volatile species under UV irradiation, improving matrix separation and transport efficiency [1]. In our previous work, efficient PVG of W was achieved from 40% (v/v) formic acid in the presence of Cd^{2+} as a mediator. Coupled with ICP-MS detection, this approach enabled the development of an ultrasensitive method for W determination [2]. High-resolution mass spectrometry (HRMS) with an Orbitrap mass analyzer provides high mass accuracy and resolving power. In combination with direct analysis in real time (DART), it was recently used to characterize various volatile species generated by PVG [3]. In this context, DART-HRMS was also valuable for identifying a myriad of ions produced in the DART from volatile $W(CO)_6$. This work used PVG to optimize parameters influencing W ion transmission and fragmentation for sensitive determination of W using DART-HRMS.

Instrumental conditions were investigated using W ions generated in the DART to "simplify" the spectra and detect only bare M^+ or $MO_xH_y^+$ ions in positive ion mode, and $MO_xH_y^-$ ions in negative ion mode. The examined conditions included RF lens voltage and collision-induced dissociation approaches (in-source fragmentation and higher-energy collision dissociation, HCD) to achieve the highest signal-to-noise ratio. Negative ion mode gave significantly higher SNR. Excessive fragmentation reduced or eliminated ions containing CO groups, while higher RF lens voltages enhanced the signal of the major W oxide species. The optimal HRMS parameters selected for sensitive W detection were 80 V for in-source fragmentation and an RF lens voltage setting of 150%. This resulted in the detection of primarily O_3W^-, with the main isotopologues detected between m/z 229.93 and 233.94. To improve SNR, HRMS acquisition parameters were also examined, including the m/z measurement range, ion accumulation time in the C-trap, and number of microscans. Calibration in the range of 0–250 $ng \cdot L^{-1}$ W showed excellent linearity (R^2 = 0.9999). The limit of detection was approximately 3 $ng \cdot L^{-1}$, which is comparable to that of ICP-MS [2].

Future work will focus on the development and optimization of a laboratory-made dielectric barrier discharge (DBD) ionization source to further improve ionization efficiency and analytical robustness. Overall, this preliminary study demonstrates the potential of combining Orbitrap HRMS with PVG for ultra-trace W determination and provides a foundation for future developments.

Acknowledgement
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OPTIMIZATION OF PHOTOCHEMICAL VAPOR GENERATION OF FLUORINE COUPLED WITH INDIRECT DETECTION BY ICP-MS/MS

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Fluorine is an environmentally relevant element because of its involvement in persistent and toxic organofluorine compounds, but its trace-level determination remains analytically challenging. Although ICP-MS is widely used for trace and ultratrace elemental analysis, direct determination of F using Ar-based plasma is inefficient due to its high first ionization potential and severe polyatomic interferences at m/z 19. Triple-quadrupole ICP-MS/MS can partially overcome these limitations by monitoring plasma-formed metal-fluoride ions, especially $[^{138}Ba^{19}F]^+$, enabling sub-ppm determination of F [1]. However, conventional solution nebulization still limits introduction efficiency and matrix tolerance. Photochemical vapor generation (PVG), which converts analytes in solution into volatile species, is a promising alternative for improving introduction efficiency and reducing matrix transport to the plasma. For F, a previous study using GC-MS demonstrated the photochemical formation of fluoromethane (CH_3F) from dilute acetic acid with Cu^{2+} as a mediator, but the yield remained low (<1%) [2]. Moreover, it was not possible to perform a detailed optimization of the PVG conditions because GC-MS was not directly connected to PVG. This motivated us to combine PVG with indirect F detection by ICP-MS/MS.

The results of this ongoing study will be presented. First, indirect F detection by ICP-MS/MS was optimized using conventional solution nebulization of F and Ba^{2+}, improving the signal-to-background ratio (SBR) of plasma-formed $[^{138}Ba^{19}F]^+$ ca. 5-fold. The ICP-MS/MS with the optimized BaF^+ detection was then coupled to a flow-injection (FI) PVG system based on a low-pressure Hg lamp and thin-film flow-through photoreactor, enabling online monitoring of transient BaF^+ signals for systematic optimization of PVG conditions.

The acid medium was one of the most important PVG conditions that controlled the BaF^+ response and thus PVG efficiency. Among formic, acetic, and propionic acids, and their mixtures, propionic acid provided the highest PVG efficiency; the response increased markedly from 0.5% to 5% (v/v) and then reached a plateau up to 40% (v/v). The effect of various metal ions mediators was also examined. Cu^{2+} remained the most efficient mediator for PVG of F, while combinations of Cu^{2+} with Mn^{2+} or Fe^{2+} resulted in only modest additional enhancement. Other tested elements, including Pt, Pd, Ni, Co, Cd, and Zn, did not significantly improve the response. The results also indicate that irradiation time is a key parameter. Unfortunately, operating the thin-film flow-through photoreactor in flow mode with long irradiation times (>90 s) is not feasible. Therefore, alternative operation modes and photoreactor geometries, such as stop-flow and coiled tubing reactors, are currently being evaluated to extend the effective irradiation time and further improve the PVG efficiency.

Acknowledgements
This work received support from the Grant Agency of Charles University (GAUK, project 616225) and the Czech Academy of Sciences (Institutional Research Plan RVO: 68081715).

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GRAPHITE FURNACE ATOMIC ABSORPTION SPECTROMETRIC ANALYSIS OF SOME TRACE ELEMENTS IN LITHIUM NIOBATE OPTICAL CRYSTALS

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Lithium niobate ($LiNbO_3$) single crystals are characterized by excellent optical properties, including real-time holographic imaging [1]. Dopants (e.g., Bi, Mg [2]) and contaminant elements (e.g., Fe, K) built into the host material during crystal growth can modify optical and mechanical properties, deteriorating and/or increasing the crystal quality. Knowing their exact concentrations in the host material is important for support of fundamental crystal research and industrial applications.

High-resolution continuum source graphite furnace atomic absorption spectrometry (HR-CS-GFAAS) is an effective tool to investigate the trace elemental content of such materials, exhibiting the direct analysis of powdered solid samples [3, 4]. Nevertheless, the calibration of solid sampling methods is difficult due to the lack of solid standards with accurately known composition. Apparently, solution standard-based calibration is usually applied for that purpose. In this study, HR-CS-GFAAS methods were examined to quantify the trace elements (e.g., Bi, K, Fe) in $LiNbO_3$ samples. The Welz's pyrolysis and atomization curves were recorded for solid samples and solution standards, showing the optimal (compromise) pyrolysis and atomization temperatures at 700 °C and 2000 °C, respectively. Conventional standard addition and the three-point estimation standard addition methods were examined. The limit of detection of the solid sampling method was 0.1 µg/g for K, using a less sensitive line of K I 404.414 nm. The accuracy of the methods was verified against solution introduction HR-CS-AAS using microwave-assisted sample digestion.

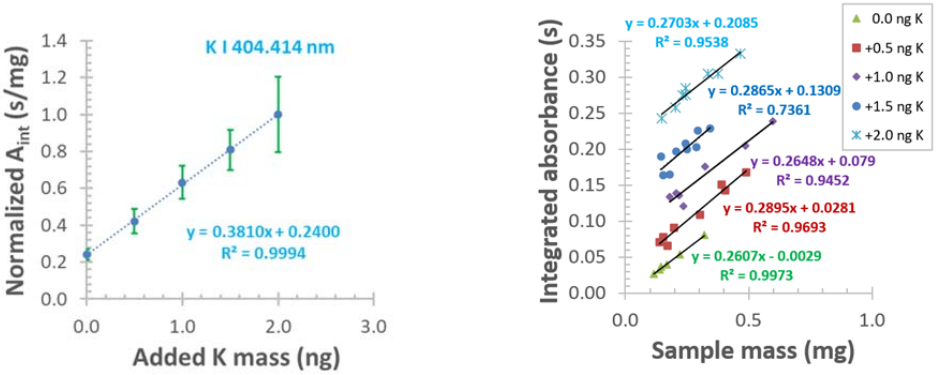

Figure 1. Solid sampling HR-CS-GFAAS standard addition curves of K determined in lithium niobate.

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ULTRATRACE DETERMINATION OF TRIMETHYLGERMANIUM (TMGe) BY HG-CT-ICP-MS/MS

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Germanium (Ge) is a technology-critical element widely used in electronics, fiber optics, infrared optics, and polymerization catalysts. In natural waters, it occurs as inorganic germanium (iGe) and as methylated species such as monomethylgermanium (MGe) and dimethylgermanium (DMGe). Although the sources and biogeochemical behavior of iGe are relatively well understood, the origin and environmental fate of methylated Ge species remain poorly known [1]. Identifying potential anthropogenic sources is therefore essential for advancing our understanding of Ge speciation in aquatic environments.

Due to the chemical similarity between germanium and silicon, silicone-based products were investigated as potential sources of methylated germanium species. A HG-CT-ICP-MS/MS [2] method, initially developed and validated for the determination of (sub)ng L^{-1} concentrations of iGe, MGe and DMGe in natural waters, was updated to include trimethylgermanium (TMGe). TMGe standards were mineralized by microwave-assisted digestion in concentrated HNO_3 and quantified against an external inorganic germanium (iGe) calibration. The method was subsequently applied to aqueous extracts of five silicone-based materials: oils, greases, and caulk.

The method achieved a limit of detection (LOD) of 0.024 ng L^{-1} and a limit of quantification (LOQ) of 0.080 ng L^{-1}. High TMGe concentrations were consistently observed across all silicone samples, often as the dominant Ge species. These findings suggest that consumer and industrial silicone-based materials could be an anthropogenic source of germanium methylated species in environmental samples.

Acknowledgements
This study was financed by the São Paulo Research Foundation (FAPESP), Brazil. Process Number (2025/14415-5, 2023/03197-1), the Czech Science Foundation (26-22432S) and institutional support of the Czech Academy of Sciences (RVO: 68081715).

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IMAGING FLOW-ENHANCED SPATIOTEMPORAL pH OSCILLATIONS IN A MICROFLUIDIC REACTOR

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Flow-based reaction systems represent an effective means of examining non-equilibrium chemical dynamics. In this work, spatiotemporal pH oscillations were investigated in a microfluidic reactor under laminar-flow conditions. The work focuses on how flow influences the interaction between reaction kinetics and diffusion, leading to oscillatory behavior.

Oscillations were studied in flow systems using reactions involving bromate and sulfite, as well as those involving bromate, sulfite, and ferrocyanide. Experimental observations show that oscillatory pattern formation occurs at a finite distance from the inlet rather than directly at the boundary. Because of the flow, there are continuous supplies of fresh reactants and changes in local residence time, which promote autocatalytic feedback and simultaneously enable delayed inhibitory pathways.

The experimental results were interpreted using reaction–diffusion–advection modeling. Numerical simulations reproduced the major features, which included observed oscillations, and showed that proton diffusion contributes to oscillation stability and broadens the stabilized oscillatory regime.

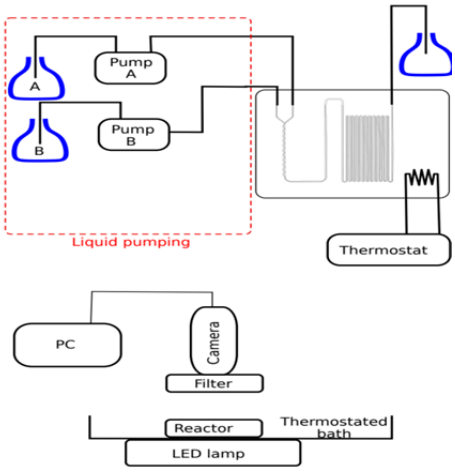

Figure 1. Experimental setup for imaging flow-enhanced spatiotemporal pH oscillations.

These findings demonstrate that flow is not only a transport mechanism but also a dynamic control parameter that can enhance and stabilize spatiotemporal pH oscillations in microfluidic environments.

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DEVELOPMENT OF A NEW HR-CS ETAAS METHOD FOR Eu DETERMINATION IN LED PHOSPHORS USING PERMANENT GRAPHITE TUBE MODIFIERS

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Europium belongs to the rare earth elements (REEs), a group of technologically critical elements used in phosphors, magnets, lasers, batteries, and high-temperature superconductors. Eu is one of the most critical REEs due to its low natural abundance among the REEs, and consequently its limited global supply, as well as its key role as a red- and blue-emitting activator in phosphor materials [1]. Phosphors are essential components of light-emitting diodes (LED). LED lighting is a rapidly growing segment of the lighting industry, with the market valued at USD 104.9 billion in 2025 and projected to grow to USD 145 billion by 2031 [2]. Simultaneously, the disposal of end-of-life LED lighting products is also increasing. The scale of this phenomenon can be illustrated by data from France, where the percentage of collected lamps consisting of LED lighting products, particularly lamps and tubes, increased from 2% to 10% between 2019 and 2023 [3]. These trends indicate the rapid expansion of LED lighting technologies and an increasing share of LED products in end-of-life electronic waste, highlighting the need for efficient recovery strategies as well as rapid, cost-effective, and accurate analytical methods for the determination of Eu in such matrices.

This work presents a new high-resolution continuum source electrothermal atomic absorption spectrometry (HR-CS ETAAS) method for the determination of Eu in LED phosphor materials. Due to the Eu forming stable carbides when upon contact with graphite at high temperatures, Zr, La, Hf, Ta, Y and Ir, thermally deposited on the platform graphite tube, were investigated for their suitability as permanent chemical modifiers. Based on the results obtained, the characteristics of the developed analytical method are reported, namely the limit of detection, limit of quantification, precision, and trueness. The method was used for the determination of Eu in leached LED phosphor samples. The method offers a simple, cost-effective, and selective alternative to ICP-based techniques for Eu determination in LED phosphors matrices.

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A MODULAR MICROFLUIDIC PLATFORM FOR SAMPLE PREPARATION IN SINGLE PARTICLE ICP-MS ANALYSIS

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Single-particle ICP-MS (spICP-MS) has gained significant popularity over the past decade due to its versatility and recent advances in instrumentation and methodology, making it a powerful technique for the characterization of suspended particulate species. Microfluidic devices are widely employed in many fields such as biology, life sciences, and chromatography. They offer versatile and customizable platforms that are particularly well suited for hyphenated analytical techniques. Microfluidic devices have proven to be valuable interfaces for ICP-MS, enabling versatile sample handling and expanding the capabilities of ICP-MS across a variety of applications. [1,2].

The aim of this study was to develop a modular microfluidic platform integrating an easily replaceable microfluidic chip with microelectronic components, including microvalves, piezoelectric pumps, and flow meters, to enable programmed or automated sample preparation for spICP-MS analysis. The platform was designed such that its functionality is defined by the microfluidic chip mounted on it, while its modular architecture allows multiple platforms to be coupled to perform multistep sample preparation workflows. The platforms were designed in AutoCAD 2026, and they were fabricated using a vat photopolimerisation (VVP)- based 3D printer.

In this study, we present the design of the microfluidic platform and demonstrate its programmed operation through several common sample preparation tasks, including the injection of small sample volumes (10–50 μL), automated serial dilution of nanoparticle suspensions with unknown concentrations, and complete instrument calibration from a single standard solution. The results highlight the versatility and potential of the proposed platform to streamline routine spICP-MS sample preparation, reducing sample consumption, analysis time, and manual intervention.

Acknowledgement
This work was partially funded by the National Research, Development and Innovation Office (NKFIH) of Hungary through projects OTKA K 146733. The authors also thankfully acknowledge the support received from the Austrian Research Promotion Agency (FFG) in the frame of the Important Project of Common European Interest (IPCEI) on Microelectronics and Communication Technologies.

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ASSESSMENT OF THE SUITABILITY OF 3D-PRINTED POROUS POLYMER SUBSTRATES FOR USE IN LIQUID MICROSAMPLE ANALYSIS BY LASER INDUCED BREAKDOWN SPECTROSCOPY

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Laser-induced breakdown spectroscopy (LIBS) is a versatile trace analytical atomic spectroscopy technique, with several compelling and practical attributes that make it attractive to various fields. LIBS is performing well so far in solid sample analysis while its practical applicability in buck liquid/solution sample analysis is significantly hindered by several limitations such as high liquid breakdown threshold, liquid incompressibility, liquid splashing during interaction with laser energy and large thermal coefficient of water. These challenges generally affect the LIBS signal formation, signal reproducibility and even lead to high limit of detection [1-3]. Despite several attempts documented in the literature to address these problems, LIBS analysis of liquid microsample still need additional efforts to establish a better approach that can reliably yield reproducible and better results.

In this study, we present a novel approach of using 3D-printed solid porous polymer substrates to enhance LIBS performance in liquid sample analysis through liquid-solid conversion. Solid porous polymer substrates with various pore sizes and shapes were designed and fabricated in our lab from commercially available standard resins using vat photopolymerization (VPP) 3D-printing technology. The chemical suitability of above base polymer materials was directly tested with LIBS and they were found to be sufficient pure for trace elemental analysis [4]. The surfaces of the 3D-printed porous substrates were found to be hydrophilic that allowed for homogeneous liquid sample distribution. We performed detailed optimization of the LIBS experimental parameters to assess their impact on analytical performance. Our findings will be presented in our presentation. This proposed liquid-to-solid conversion approach via 3D printed solid porous polymer substrates is inexpensive and it also offers further possibilties for signal enhancement methodologies.

Acknowledgements
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DISCRIMINATION OF AEROSOLIZED CONTAMINANTS ORIGINATING FROM BURNING PLASTICS USING LIBS AND MACHINE LEARNING

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Coal and wood are regularly used as traditional combustible fuels for domestic purposes. However, there is a concern that people sometimes burn these materials by mixing them with plastic waste, other household waste, or even replacing them entirely with combustible plastic alone. These practices tend to produce complex mixtures of toxic airborne pollutants that pose significant environmental health risks. Identification and detection of whether plastics or other household waste have been added during burning is particularly difficult once the only evidence left behind is aerosol particles rather than solid residues, making this a significant analytical challenge.

In this study, we investigated the applicability of laser-induced breakdown spectroscopy (LIBS) to address this challenge by analysing aerosols collected from burning processes to reveal whether plastics were also added to conventional fuels. Controlled burning experiments using five common plastics, including polyethylene (PE), polypropylene (PP), polystyrene (PS), polyethylene terephthalate (PET), and polyvinyl chloride (PVC), and several wood and coal types were performed in a laboratory-scale combustion chamber, and aerosol particles originating from the burning products were sampled directly from the lower and upper sections of the chimney for LIBS analysis. Conditions of the LIBS measurements were optimised, and seventy spectra were collected and correlated against the mean spectrum to remove outliers. Fifty spectra that gave above 0.9 correlation coefficient for each sample were evaluated using several machine learning and clustering techniques such as principal component analysis (PCA), Linear discriminant analysis (LDA), classification tree (CT) and random forest (RF). Several classification scenarios were examined, ranging from binary discrimination of plastics versus legitimate fuel (coal, wood vs. plastics) to the more demanding identification of individual fuel and plastic types, as well as a combined model including all fuel classes. We found that classification can be performed with good accuracy in many of the cases. However, RF consistently delivered the most accurate and robust classification, reaching overall accuracies between 90-98%. It was also observed that data from aerosol particles originating from the upper section of the chimney gave much better discrimination performance than those from the lower section. These results demonstrate that LIBS combined with chemometric analysis of chimney aerosol residues is a promising tool for the detection of illegitimate burnt plastic in co-combustion with conventional solid fuels from aerosol samples alone.

Acknowledgements
This work was funded by the National Research, Development and Innovation Office (NKFIH) of Hungary through projects OTKA K 146733 and 2024-1.2.3-HU-RIZONT-2024-00032.

A FAST PULSED UV RAMAN MICROSCOPE FOR MICROPLASTIC IMAGING

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Today's omnipresence of microplastic particles poses an imminent threat to the environment and health. Consequently, many analytical techniques have been suggested for their detection and identification regarding size and chemical composition. Among these, Raman microspectroscopy combines chemical identification of polymers with micrometer spatial resolution, but its conventional visible-light excitation requires long integration times, impractical for mapping experiments with sufficient throughput. Extensive and high-resolution mapping can thus extend measurement times to several days.

We present a highly accelerated UV Raman microscope based on the 355 nm output of a DPSS laser for excitation to overcome long measurement times and to take advantage of the benefits UV excitation offers. UV light exhibits enhanced Raman scattering which makes drastically shorter integration times viable, leading to an overall reduction in measurement times. Furthermore, UV Raman can be conducted in ambient light as well, thus simplifying integration into processes and workflows. Additionally, UV light allows for tighter focusing and therefore good spatial resolution can be realized even with cost-effective optics, allowing for a rapid and low-cost setup.

The presented microscope was able to extensively map dispersed microplastic particles on a 256 mm² surface in under eight hours. The analyzed microplastics consisted of four cryo-milled end of life polymer products distributed across a silicon wafer. An integration time of only 100 ms led to the collection of more than 140,000 spectra in this period allowing for the identification and mapping of microplastics. For the unambiguous identification of polymers with sufficient discrimination within the resulting large dataset unsupervised classification algorithms were successfully employed. As a result, combining fast UV Raman and unsupervised classification schemes, mapping and classification can be achieved within a single working day.

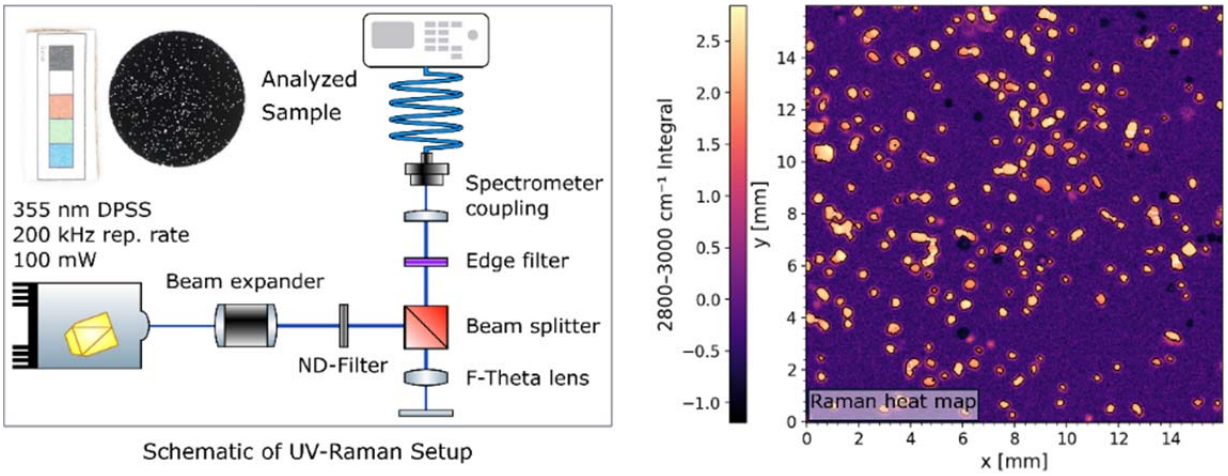

Figure 1. Schematic of the instrument (left) and a recorded Raman heat map of microplastics (right).

IMPROVING SPATIAL RESOLUTION OF LASER-INDUCED BREAKDOWN SPECTROSCOPY FOR MINERALIZED BIOLOGICAL STRUCTURES

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Bones and teeth are examples of hard tissues – mineralized biological structures that support the body, shield vital organs, and withstand mechanical stress. These tissues develop through a process called biomineralization, which involves cellular activity, the assembly of an extracellular matrix, and its progressive mineralization. A defining characteristic shared across hard tissues is a mineral phase built upon hydroxyapatite, the principal inorganic constituent found in both bones and teeth.

The current standard lateral resolution for hard tissues for Laser-induced Breakdown Spectroscopy (LIBS) stands at 30 μm [1]. Our group has previously demonstrated a spot size of 20 μm on human teeth affected by ankylosis [2], and we aim to reduce the spot size even further. Achieving continued reductions in spot size represents a notable technological advancement and extends the limits of what is currently possible in microimaging of hard tissues using the LIBS method.

To improve spatial resolution, modifications to the laser focusing optics are required, as spot size is a key determining factor. The laser beam is expanded using a beam expander, followed by focusing through a diffraction-limited aspheric lens. The current setup employs a nanosecond Nd:YAG laser, which will be replaced by a picosecond Nd:YAG laser (QS Lasers MPL2210) in the LIBS configuration. The use of shorter pulse durations reduces the thermally affected volume generated by each laser pulse, thereby minimizing the evaporated area and ultimately enhancing spatial resolution. [3]

Acknowledgements
The authors gratefully acknowledge financial support from the Faculty of Mechanical Engineering and Central European Institute of Technology, Brno University of Technology (CEITEC VUT/FSI-J-26-9058).

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THE IMPORTANCE OF SCIENTIFIC TERMINOLOGY AND CONCEPTS: TXRF NEW STANDARD ISO 18115-4

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Total Reflection X-ray Fluorescence (TXRF) presents appealing capabilities, as it enables a simultaneous multi-elemental analysis of a sample which can be of qualitative, quantitative or screening character. The ease-of-use along with access to dedicated commercial instruments means that TXRF is a technique that can be employed by a broad range of people from very different backgrounds and from diverse fields for very different surface chemical analyses. Those conducting TXRF can be materials scientists, chemists, physicists, or biologists with those making use of the data and results extending beyond this group into other disciplines.

The wide range of disciplines, expertise, and skill levels have led to divergence of meanings being attributed to specific terms and/or, different terms being used to describe the same concept, approach, or analysis. To avoid the consequent misunderstandings between communities and to facilitate the clear exchange of information, as well as to provide basis for a TXRF normative framework, it is essential to clarify the concepts needed when undertaking a TXRF analysis. A TXRF chemical measurement process, when considered holistically, combines knowledge in instrumentation, physics, analytical chemistry (sampling, sample preparation and handling), metrology, quality management, software and data analysis. This is motivated further by the need for correct reporting of metadata with the move to open access and FAIR (Findable, Accessible, Interoperable and Reusable) data repositories, and by the advent of artificial intelligence for the treatment and exploitation of the data.

Thus, it is critical that the terms relating to all aspects of a TXRF experiment are established, their concepts clarified and their validity ensured across all scientific disciplines. This is the purpose and justification for the development of this new ISO standard [1]. The ISO 18115 standard defines, and gives references for terms for surface chemical analysis, and is composed by several parts. ISO 18115-4 “Terms used in Total Reflection X-ray Fluorescence” will extend the standard, and will help in ensuring consistency, precision, and efficiency in TXRF analysis, and in fostering exchanges within scientific communities.

This presentation will highlight the rationales behind the ISO 18115-4 standard, and demonstrates that the terminology for TXRF is not fully autonomous and only based on terms sourced in physics, but is a consequence of the existence of intra-, inter-, multi- and trans-disciplinary relations. It will also discuss how this terminology standard is reflecting and supporting the contents of the VAMAS pre-normative activity [2] aiming at describing the TXRF chemical measurement process, via the elaboration of procedures and validation steps. Finally, this standard is also applicable in most uses of X-ray Fluorescence Analysis.

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METHODOLOGICAL ADVANCES IN MICROPLASTIC ANALYSIS OF AGRICULTURAL SOILS: PRELIMINARY RESULTS USING SAMPLE PREPARATION, AUTOMATED IMAGE ANALYSIS, AND RAMAN SPECTROSCOPY

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High-resolution analytical methods have enabled the rapid and objective characterization of a large number of particles based on size, shape, and material properties. The size, shape, and material properties of particles were examined using the Malvern Morphologi G3ID-SE automated image analysis system. Quantitative shape analysis was conducted based on four shape factors, while integrated Raman spectroscopy facilitated the identification of individual microplastics. This method was previously tested on various environmental samples, including microplastic particles from treated wastewater, surface waters, and atmospheric dust. Prior to analyzing soils intended for agricultural use, model experiments were conducted to optimize the sample preparation protocol. Recovery experiments were performed on two soil types with differing physical properties and organic carbon content, utilizing specified quantities, sizes, and types of microplastics. Sample preparation involved processing soil samples of varying weights. To reduce organic matter content, H_2O_2 treatment was applied, followed by density separation using a $ZnCl_2$ solution, after which the supernatant was dispersed onto filter paper. The identification of particles was supported by the creation of a reference database containing Raman spectra of 12 polymer types. Integrated Raman spectroscopy was determined to be suitable for assessing polymer composition, while automated image analysis enabled the distinction of microplastics from the filter paper background and soil-derived particles based on optical characteristics. The filter paper-based measurement protocol developed was found to be suitable for the automated counting, size and shape characterization, and polymer identification of microplastics. The combination of optical and spectroscopic methods offers a reliable tool for characterizing the microplastic content of soils.

Acknowledgements
The research was conducted as part of the STARTING-152507 project, funded by the NKFI Fund.

COMPARATIVE ELEMENTAL ANALYSIS OF EIGHTEENTH-CENTURY INKS IN HISTORICAL HANDWRITTEN DOCUMENTS BY X-RAY FLUORESCENCE SPECTROMETRY

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Iron-gall ink, prepared from tannin extracts, iron salts, and gum arabic, was widely used in Europe from antiquity until the 20th century. Variations in recipes, raw material sources, and salt impurities result in significant differences in elemental composition, which may be used to distinguish between inks. Hahn's fingerprinting approach, based on non-destructive X-ray fluorescence spectrometry (XRF), uses elemental ratios such as Cu/Fe, Zn/Fe, and Mn/Fe to differentiate between iron-gall inks [1].

This study examined three handwritten copies of the Constitution of 3 May 1791 preserved in the Central Archives of Historical Records (AGAD, Warsaw). Visual inspection suggested the presence of iron-gall ink in the main text, corrections, and deputies' signatures. The aim was to assess elemental variability across different written sections and to investigate possible relationships between the chemical composition of the main text, annotations, and signatures. Due to the exceptional historical value of the manuscripts, only non-destructive methods could be applied [2].

Measurement conditions were optimized by testing acquisition times from 30 to 300 s and several radiation shields (Rh, Pd, Si, Al, Au, acrylic, graphite) to minimize signal contribution from underlying pages. An acquisition time of 210 s and a rhodium shield were selected as optimal. Detection and quantification limits for selected elements were established using a model ink solution and its serial dilutions. The manuscripts were analyzed in situ at AGAD using a portable Bruker ELIO XRF spectrometer.

The results were evaluated to determine the elemental composition of inks in all measured areas. In addition, machine-learning-based dimensionality reduction methods were applied to compare chemical signatures of different writings. The approach enabled discrimination between iron-gall and plant-based inks and indicated that some corrections may be chemically associated with deputies' signatures.

Acknowledgements
Research supported by the National Science Centre, Poland, under the project "Spectral Analysis of Legacy Inks using machiNe leArning: ALiNA" (No. UMO-2021/41/B/ST4/02860).

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FROM INSTABILITY TO RELIABILITY: OXIDATIVE MODIFICATION OF COPPER SERS SUBSTRATES

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Copper (Cu) substrates represent a promising, cost-effective alternative to noble metals for Surface-Enhanced Raman Scattering (SERS) technique. While Cu offers enhancement factors comparable to gold or silver, its widespread application in analytical practice is currently hindered by its high reactivity and susceptibility to oxidation [1]. However, controlled oxidation can also induce a passivation layer that preserves surface integrity and enhances long-term stability.

This study investigates strategies to modify and stabilize Cu surfaces to achieve higher signal enhancement, improved temporal stability, and reproducible analytical results. We employ two complementary approaches: (i) an *in-situ* electrochemical method on Pt/Cu targets [2], utilizing EC-SERS to correlate surface speciation with enhancement performance in real-time; and (ii) controlled aging of Al/Cu [3] substrates under defined environmental conditions to assess batch reproducibility and long-term stability. Riboflavin (Rf) serves as the primary Raman probe for evaluating substrate performance. Our preliminary findings aim to establish a robust protocol for transforming reactive Cu surfaces into reliable SERS platforms for broader analytical applications.

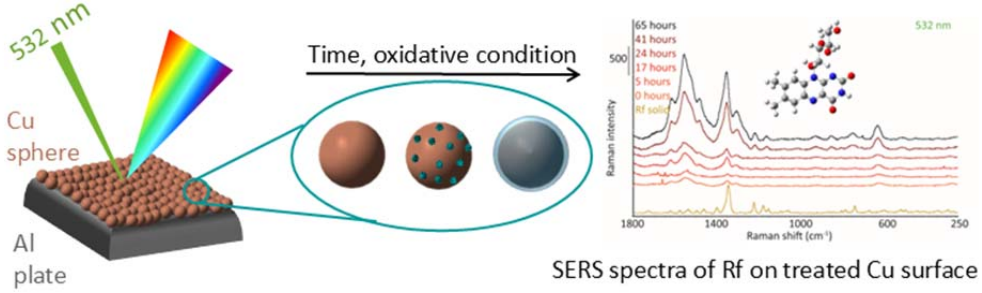

Figure 1. Schematic illustration of the study.

Acknowledgements
This work was financially supported by the Czech Science Foundation (Project No. 23-07610O).

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DEVELOPMENT OF (LA)-ICP-MS ANALYTICAL METHODOLOGY FOR ELEMENTAL ANALYSIS OF HISTORICAL SILVER COINS AND ASSESSMENT OF ISOTOPE ANALYSIS POSSIBILITIES

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Building upon previous research on the chemical analysis of historical silver coins, the presented work focuses on the development and optimization of advanced analytical methodologies based on ICP-MS, including laser ablation (LA-ICP-MS). Particular emphasis is placed on improving the accuracy and precision of elemental analysis through the preparation and validation of in-house matrix-matched reference materials. These standards closely resemble the complex composition of historical silver alloys, thereby reducing matrix effects and improving data reliability.

In parallel, solution-based ICP-MS is utilized to assess the potential of lead isotope analysis for determining the geographical origin of the silver ore. To support this liquid-sample approach, electrogravimetric separation of the silver matrix is being optimized. This process is crucial for preventing silver deposition within the instrument interface, thereby ensuring the stability required for isotopic measurements.

By combining elemental fingerprinting with the preliminary assessment of isotopic ratios, this research aims to provide a more reliable interpretation of compositional data and contributes to the understanding of metallurgical practices and raw material sourcing in historical coinage. The proposed methodologies are critically evaluated with respect to their applicability in micro-destructive and non-destructive archaeological research.

Acknowledgments
This research was supported by the Grant Agency of Masaryk University project No. MUNI/C/0129/2026.

RAPID IMS-MS ANALYSIS OF THERMAL DEGRADATION IN BIODEGRADABLE POLYMERS

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Ion mobility spectrometry (IMS) was applied to monitor the thermal degradation of biodegradable polymers, namely polyhydroxybutyrate (PHB), polybutylene adipate terephthalate (PBAT), and polylactic acid (PLA). These materials are increasingly used as environmentally friendly alternatives to conventional plastics; however, their lower thermal stability requires detailed investigation. In this work, IMS in combination with time-of-flight mass spectrometry (TOF-MS) was used for rapid qualitative analysis of degradation products and determination of degradation onset temperatures.

Polymer samples were analysed by headspace IMS in the temperature range of 25–100 °C. The obtained results revealed differences in thermal stability among the studied polymers. In the case of PBAT, degradation products were detected already at 25 °C. Mass spectrometric analysis identified the dominant species as protonated 1,4-butanediol and its water clusters, which is consistent with the chemical structure of PBAT. For PHB, the onset of thermal degradation was observed at 40 °C, where several ion peaks appeared in the IMS spectra. These peaks were attributed to crotonic acid, a known degradation product of PHB. PLA exhibited the highest thermal stability, with the first degradation products detected at 80 °C. The main product was identified as protonated lactic acid with attached water molecules.

The results demonstrate that IMS enables fast and sensitive detection of volatile degradation products and allows determination of degradation onset temperatures. Compared to conventional analytical techniques, IMS provides significantly shorter analysis time while maintaining reliable identification when combined with MS. The method shows potential for rapid screening of biodegradable polymers and can be extended to the analysis of conventional plastics.

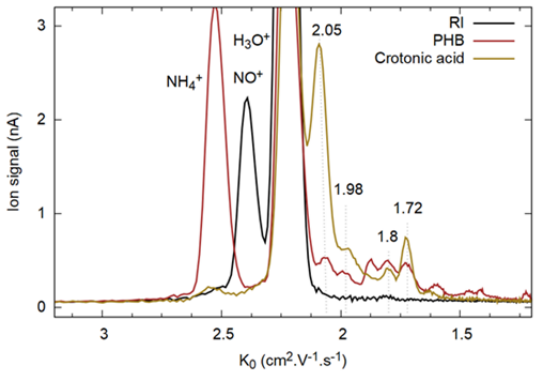

Figure 1. IMS spectra of PHB at a heating temperature of 100 °C and crotonic acid at room temperature.

Acknowledgments
This work was supported by the Slovak Research and Development Agency APVV-22-0133, APVV-23-0522, and the Slovak Grant Agency for Science (contract no. VEGA 1/0553/22).

LASER-BASED DETECTION AND IMAGING OF MICROPLASTICS IN CAVE SEDIMENT MATRICES

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Microplastics represent a serious environmental contamination issue, as their presence has been demonstrated not only in surface ecosystems but also in subsurface environments. Cave sediments and cave waters may serve as sensitive indicators of anthropogenic impact on the landscape. However, the analysis of microplastics in cave matrices remains limited and requires suitable methods for heterogeneous mineral-rich samples. This work focuses on the comparison of laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) and laser-induced breakdown spectroscopy (LIBS) for the detection and spatially resolved analysis of microplastics in clay-based matrices simulating cave sediments.

Both methods are based on laser-matter interaction, but they differ in ablation conditions, detection principles and analytical information obtained. For LA-ICP-MS, a pulsed Nd:YAG laser operating at 213 nm was used. In the case of LIBS, two pulsed Nd:YAG laser sources with wavelengths of 266 nm and 1064 nm were employed. Pressed pellets containing ferrosilicate clay with the addition of polypropylene (PP) and polyethylene terephthalate (PET) particles were prepared as model samples. Blank pellets without microplastics were used to distinguish signals originating from the clay matrix from those associated with plastic particles.

LIBS enabled the detection of plastic particles mainly through carbon emission lines, together with additional emission signals related to the polymer composition. In LA-ICP-MS, direct carbon determination is limited. Therefore, PET particles containing antimony were used as a suitable model system, with Sb serving as an elemental marker of the plastic phase. The LA-ICP-MS measurements showed that Sb can be detected in PET-containing pellets and clearly distinguished from blank clay pellets, confirming that the Sb signal originates from the plastic particles rather than from the ferrosilicate matrix.

The results demonstrate that both LIBS and LA-ICP-MS are suitable for microplastic detection in sediment-like mineral matrices, but they provide different and complementary analytical information. LIBS enables the detection of major elements characteristic of plastics, particularly carbon, and can therefore be used for direct recognition of plastic particles in the mineral matrix. In contrast, LA-ICP-MS is especially suitable for detecting elemental additives and dopants incorporated into plastics for technological purposes. These marker elements, such as Sb in PET, can be used not only to identify plastic particles in the sediment matrix, but also to distinguish between different plastic types according to their additive composition. Together, these techniques may provide a promising approach for chemical mapping and classification of microplastics in complex sediment matrices, including cave sediments.

INVESTIGATION OF THE PHOTOCHEMICAL TRANSFORMATION OF SUBSTITUTED BENZOQUINONE AND ANTHRAQUINONE DERIVATIVES AND LC–MS/MS-BASED IDENTIFICATION OF REACTION PRODUCTS

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Substituted quinones are vital in biological redox processes and solar energy applications [1], yet their environmental fate and photolytic transformation pathways require comprehensive characterization. This study investigates the photostability and degradation mechanisms of structurally diverse quinones, specifically substituted 1,4-benzoquinones (namely: 2-chloro-, 2,5-dichloro-, 2,6-dichloro-, and 2,6-dimethyl-1,4-benzoquinone) and sodium anthraquinone-2-sulfonate, under UV (365 nm) and white light irradiation.

By integrating LC–UV kinetic tracking with advanced Matrix Rank Analysis (MRA) of spectrophotometric data, we identified the presence of multiple light-absorbing species during photolysis [2,3]. Furthermore, LC–MS/MS was utilized to track the stepwise formation and disappearance of complex intermediate mixtures. Our findings highlight a stark contrast in photoreactivity: benzoquinones degrade rapidly into hydroxylated derivatives and hydroquinones [4], while the extended aromatic conjugation of the anthraquinone derivative confers significantly enhanced photostability. Notably, product distributions formed during illumination differed markedly from those formed during dark storage.

This research demonstrates that purely kinetic measurements fall short in capturing the complexity of quinone photochemistry. Advanced product-specific LC–MS/MS profiling is essential to fully elucidate reaction mechanisms, assess environmental persistence, and evaluate the toxicological profiles of photochemically generated derivatives.

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MÖSSBAUER AND XRD INVESTIGATIONS OF Eu-DOPED GOETHITES FOR NOVEL BATTERY ELECTRODES

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^{57}Fe and ^{151}Eu Mössbauer spectroscopy, combined with powder X-ray diffraction, was applied to the phase and local-structure analysis of Eu-doped goethite nanocomposites with nominal composition $Eu_xFe_{100-x}OOH$, where x = 0, 10, and 30 mol%. The samples were synthesized by a hydrothermal route using $Fe(NO_3)_3$ together with either Eu_2O_3 or $Eu(NO_3)_3$ as europium-containing precursors. Both the as-prepared and heat-treated (300 °C for 30 min) states were investigated with respect to their possible application as anode materials in Na-ion batteries and as photocatalysts for water purification. The main objective was to study the difference in the phase composition of the samples prepared from Eu_2O_3 and $Eu(NO_3)_3$.

The ^{57}Fe Mössbauer and XRD results confirmed the formation of goethite during hydrothermal synthesis. The phase composition of the Eu-containing components was found to depend on the chemical nature of the europium precursor. XRD analysis indicated $Eu(OH)_3$ as the dominant crystalline Eu-related phase in all the investigated samples, while a significant amorphous contribution was also observed.

The combined ^{57}Fe Mössbauer- and XRD results revealed that the thermal treatment resulted in the complete transformation of goethite into hematite in the composite synthesized from Eu_2O_3, whereas only partial transformation occurred in the $Eu(NO_3)_3$-derived composite.

Furthermore, the results showed that a fraction of the goethite phase in the Eu_2O_3-derived sample exhibits paramagnetic behavior, while the goethite formed from $Eu(NO_3)_3$ precursor remains fully antiferromagnetic. This demonstrates that the Eu precursor has a pronounced influence on both the phase composition and the thermal transformation behavior of the composites. An anomalous change of the goethite-related XRD reflections was also observed for the $Eu_{10}Fe_{90}OOH$ composite prepared from Eu_2O_3 as compared to the undoped sample. This effect can be attributed to Eu incorporation into the goethite structure.

The ^{151}Eu Mössbauer spectra of the 10 mol% Eu-containing samples showed distinct changes in the average hyperfine parameters between the as-prepared and heat-treated states in both precursor systems. These changes are also interpreted as evidence for partial Eu incorporation into the goethite phase.

ISOTOPE DILUTION-ASSISTED LC-HRMS FINGERPRINTING OF SELENIZED YEAST

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Selenized yeast is widely used selenium-enriched product in food industry. Selenomethionine is the key selenometabolite for the food industry; however, microorganisms also metabolize selenium into other forms, resulting in the formation of the selenometabolome [1, 2]. The composition of this selenometabolome may vary depending on the yeast manufacturer. The distribution of selenometabolites may therefore provide a sample-specific fingerprint reflecting the production process and manufacturer. In this work, isotope dilution was employed for the classification of selenized yeast extracts by liquid chromatography coupled to high-resolution mass spectrometry (LC-HRMS). The approach is based on the addition of a certified reference material enriched in ^{82}Se (SEEY-1 provided by National Research Council Canada) enables to artificially change natural isotope abundances of selenometabolites in yeast samples [3].

This approach meets several limitations, first of which is the significance difference between selenium contents in commercial selenized yeast, containing for e.g. 2000 ppm of total Se, and the isotopically enriched certified reference material, containing approximately 300 ppm Se. Too low a spike contribution results in only a weak change in the ^{82}Se signal, while too high dilutes the real sample and introduces additional background. Non-selenium-containing compounds dominates the mass spectrum and suppress analite ionization, making chromatographic separation essential. Additional clean-up or fractionation, for example by solid-phase extraction, may further improve detection and reduce matrix contribution. Another limitation is the occurrence of isobaric interferences. HRMS allows to separate closely spaced ion signals and to increase confidence in the recognition of selenium-related isotope patterns. The proposed isotope dilution-assisted LC-HRMS workflow provides a basis for more selective fingerprinting of selenized yeast and may allow the classification of yeast according to their manufacturer.

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COMPREHENSIVE INVESTIGATION OF THE CARBONATION REACTION OF LIME PASTES PRODUCED BY MODERN AND TRADITIONAL TECHNOLOGIES

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Lime represents one of the oldest materials used by humankind over centuries as a binder in mortars for brickwork, stonework, rendering and plastering. Nowadays, lime technologies are again in the focus of researchers not only for the conservation of cultural heritage objects, but also for their sustainability. Lime is produced by a burning process (using significantly lower temperatures in contrast with cement clinkers) from limestone rocks, which are largely composed of calcium carbonate ($CaCO_3$). During lime hardening, the carbonation reaction gradually transforms lime into newly formed $CaCO_3$ due to uptake of atmospheric carbon dioxide. Overall, carbonation is a multistep process, highly depending on the environmental conditions and may result in the formation of various $CaCO_3$ polymorphs, including hydrated and anhydrous phases.

This contribution focuses on a comprehensive investigation of the carbonation reaction in three types of lime-based materials. Two of them are commercially available lime hydrates. The third is the lime paste produced using traditional lime kiln construction in accordance with historical methods. The carbonation was studied in samples aged for up to 24 weeks and stored at a constant temperature (20 ± 1°C) and relative humidity (65 ± 5%). The combination of instrumental techniques, including micro-Raman spectroscopy, X-ray powder diffraction, thermogravimetric analysis, and scanning electron microscopy, was used to reveal the formation of new phases and microstructural rearrangements. The analysis enabled the kinetic description of the gradual transformation of portlandite into $CaCO_3$, the plotting of phase distribution maps, and the identification of an amorphous $CaCO_3$ precursor. The obtained results may help to gain deeper insight into lime carbonation, a crucial process of its hardening.

Acknowledgements
The authors gratefully acknowledge the support provided by the Czech Academy of Sciences, namely Institute of Theoretical and Applied Mechanics - RVO 68378297, Czech Academy of Sciences Strategy AV21 scheme as part of "The Power of Objects: Materiality between Past and Future" grant at the Institute of Theoretical and Applied Mechanics

BIOCOMPATIBLE COMPOSITE PROTECTIVE THIN LAYER BASED ON CELLULOSE MATRIX REINFORCING WITH SILICA CRYOGEL

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This study explores the synthesis and characterization of composite materials, focusing on the integration of silica cryogel and cellulose. The aim is to develop environmentally friendly, biodegradable thermal insulation thin continuous layers with optimized physical properties, like thermal conductivity adhesion on diverse surfaces, connection between the components of the composite. The continuous matrix phase of the composite is composed of cellulose fibers, known for their high thermal insulation capabilities, biodegradability, and abundant availability. Silica cryogel, selected for its excellent resistance to heat and chemical impacts, serves as the reinforcing phase.

To improve the matrix-reinforcement phase connection, different additives were utilized, including a solvent mixture of NaOH and carbamide, and hydroxyethyl cellulose (HEC).

Characterization of the composite materials involved advanced techniques. Scanning electron microscopy (SEM) provided insights into the structure, morphology, and homogeneity, revealing the average pore size and overall porosity. Infrared spectroscopy (FT-IR) was used to identify bond structures and interactions between the composite components, providing a detailed understanding of the material's chemical composition.

The study puts a focus on the physical and chemical properties that arise from the interaction of silica cryogel and cellulose. The results demonstrate that the synthesized composites exhibit excellent thermal insulation and mechanical properties, highlighting their potential application in various industrial fields where thermal management and environmental sustainability are essential.

The final products were also subjected to thermal conductivity measurements, confirming their efficiency as insulating materials. The measured heat conductivity of 0.042 W/mK value of our composite is comparable to that of the commonly used mineral wool (Rockwool’s product).

Adhesional measurements revealed strong bonding to diverse substrates, including metal, ceramic and glass, demonstrating the composite's practical applicability in various settings.

The integration of natural cellulose with synthetic silica cryogel represents a significant advancement in the development of sustainable materials, offering a promising solution for reducing the environmental footprint of thermal insulation products.

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FTIR ANALYSIS AND MICRO-RAMAN MAPPING OF ORGANOSILANE-BASED ADDITIVES IN GEOPOLYMERS

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Geopolymers represent a sustainable alternative to cementitious binders, but their porous structure can negatively affect their performance, especially in moisture-exposed environments. The development of composite systems incorporating organosilane-based additives aims to improve hydrophobicity and thereby the durability of the material. The effectiveness of such modifications depends not only on the chemical structure of the organosilane used, but also on its incorporation and distribution within the geopolymer.

This study investigates metakaolin-based geopolymers modified with three types of organosilane additives with different functional groups. The additives were incorporated into the geopolymer matrix using two mixing techniques, which influence their interaction with the alkaline activating solution.

Fourier-transform infrared (FTIR) spectroscopy was employed to evaluate possible chemical changes and to identify characteristic vibrational bands originating from the inorganic geopolymer matrix and the organic additives. The chemical mapping of the spatial distribution of the additives was performed by micro-Raman spectroscopy. The surfaces of the cross-sections were measured, and the resulting maps were obtained through multivariate curve resolution.

The visualization of organosilane additives in the geopolymer matrix provides information on how both the mixing techniques and the molecular structure of the silanes affect their distribution, homogeneity, or segregation within the matrix. Understanding these spatial arrangements contributes to the optimization of hybrid geopolymer formulations, as the homogeneity of the organosilane additive distribution directly influences the hydrophobicity of the resulting composite.

Acknowledgements
The authors gratefully acknowledge the support provided by the Czech Academy of Sciences, namely Institute of Theoretical and Applied Mechanics - RVO 68378297, Czech Academy of Sciences Strategy AV21 scheme as part of "The Power of Objects: Materiality between Past and Future" grant at the Institute of Theoretical and Applied Mechanics.

STRUCTURE AND THERMAL DECOMPOSITION STUDIES OF DIFFERENT [HEXAKIS(UREA-O)IRON(III)] COMPLEXES

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The aim of our work is the preparation and structural characterization of various transition metal complexes having different kinds of (reducing) ligands (*e.g.* urea) and oxidizing anions (MnO_4^-, $C_2O_7^{2-}$, $S_2O_8^{2-}$ etc.) and can be used as precursor materials for the preparation of transition-metal oxide catalysts in a cost- and energy-efficient way [1-4].

In this work $[Fe(urea\text{-}O)_6](ClO_4)_3$ was synthesized and its structure was studied via powder- and single-crystal X-ray diffraction and various spectroscopic (Mössbauer, IR, Raman) methods. In the complex extended hydrogen bond networks formed by N-H and Cl-O functionalities verified by single crystal X-ray diffraction and spectroscopic methods as well. In addition to the structural studies, thermal characterization of the complex was also performed using TG-MS and DSC methods. These measurements revealed the presence of solid-phase quasi-intramolecular redox reaction (SPQIR) between the oxidizing anion and reducing ligand already below 200 °C. Based on the thermal studies we performed the isothermal heat treatment of the complex at different temperatures under oxidative and inert atmospheres. The decomposition products were studied by powder X-ray diffraction, IR and Mössbauer spectroscopy (MB). With the help of MB, different non-equilibrium state iron(II) and (III) chemical environments were identified and already at low temperatures (245 °C) crystalline iron oxides with mixed oxidation state are resulted by the SPQIR reactions. The parameters of the decomposition products (*e.g.,* ratio of the oxidized – reduced phase) were found to be tuneable by changing the decomposition temperature and the atmosphere.

During our work we also synthetized $[Fe(urea\text{-}O)_6](ClO_4)_x(MnO_4)_y$ via different routes. The products were studied by ICP-OES, powder X-ray diffraction, IR and Mössbauer spectroscopy. We showed that the position and relative intensity of the infrared bands of the anions correlate with the ratio of permanganate to perchlorate ions. Therefore, IR spectroscopy could be used as an alternative method for easily tracking the composition of these mixed-anion complexes.

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HYPOTHESIZED METASOMATIC ALTERATION OF OLIVINE MINERALS IN CARBONACEOUS CHONDRITE METEORITES

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Olivine $(Mg, Fe)_2\ SiO_4$ mineral is a highly sensitive geochemical indicator capable of preserving structural and chemical signatures of early solar system processes on asteroid parent bodies [1]. This study presents a combined analytical and statistical approach to characterize the relationship between elemental composition, structural irregularities, and lattice strain in CV3 carbonaceous chondrites (*K□S* 1/*T*, *NWA* 5491, and *NWA* 2086), what is the BSc thesis of the first author.

Our methodology pairs micro-scale SEM-EDX and FTIR-ATR laboratory measurements of meteorite samples. High-resolution compositional profiles across individual olivine grains were correlated with corresponding infrared spectra, focusing on the asymmetric stretching vibration (ν_3) band of silicate tetrahedra (810–860 cm^{-1}). Data processing was performed in MATLAB, utilizing local linear baseline correction to precisely extract full width at half maximum (*FWHM*) values.

The statistical and spectral results reveal distinct variations in how chemistry and crystal structure correlate across different samples and grains inside. In the *K□S* 1/*T* and *NWA* 5491 samples, a statistically significant Pearson correlation was found between the forsterite content (*Fo* %) and *FWHM*. Progressing from rim to core in olivine crystals, a drastic magnesium enrichment (*ΔFo* up to 40–70%) systematically covaries with a downshift in peak positions and a pronounced increase in *FWHM* values. This quantifies a state of non-equilibrium chemical alteration, where the structural lattice strain was induced by the diffusion and substitution of larger Fe^{2+} ions in the silicate framework [3].

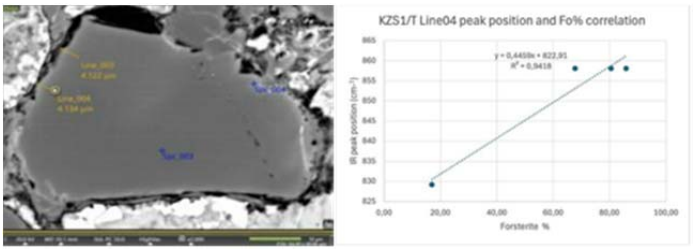

Figure 1. KZS1/T olivine grain's BSE picture and its correlation graph.

Ultimately, this work demonstrates that the coupled SEM-EDX and FTIR-ATR approach, supported by rigorous statistical analysis, serves as a powerful non-destructive tool for decoding the complex post-crystallization, secondary alteration, and structural evolution histories of primitive meteorites.

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URBAN MINING OF MOBILE PHONES: DETERMINATION OF PALLADIUM AND PLATINUM IN PRINTED CIRCUIT BOARDS BY ATOMIC ABSORPTION SPECTROMETRY

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Platinum group metals (PGMs) are strategic raw materials whose supply is associated with high risk due to limited, rapidly depleting resources, costly extraction processes, and widespread use across numerous industrial sectors [1]. Since 2011, PGMs have been included on the European Union's list of critical raw materials. Palladium (Pd) and platinum (Pt) are widely used in the automotive, chemical, and electronics industries due to their excellent electrical conductivity, corrosion resistance, thermal stability, and catalytic properties.

The rapid development of electronic technologies and the growing demand for advanced consumer devices have driven increased demand for PGMs. Mobile phones and smartphones contain significant amounts of these valuable metals, particularly in printed circuit boards (PCBs), which are considered one of the richest secondary sources of precious metals. It is estimated that the motherboard, rear camera module, speakers, display, and wireless components in a smartphone contain 60–70% of recyclable metals by weight, of which approximately 70% are precious metals. It has been reported that one ton of used mobile phones can contain up to 340 g of Au, 140 g of Pd [2], and 10 g of Pt [3]. Concentrations of these metals in electronic waste often exceed those in natural ores, highlighting e-waste as an important secondary source for precious metal recovery. The Pd and Pt content in printed circuit boards is 80 - 110 mg/kg and 25 - 70 mg/kg, respectively [3].

In this study, mobile phones, multimedia phones, and smartphones manufactured between 2005 and 2020 were collected and dismantled. Printed circuit boards (PCBs), identified as potential sources of platinum group metals, were separated and heat-treated in a muffle furnace. The resulting ash was ground and sieved into four particle size fractions (<0.12 mm, 0.12–0.20 mm, 0.20–0.30 mm, and >0.30 mm). Elemental characterisation of the samples was performed using X-ray fluorescence spectrometry (XRF). The presence of Pd and Pt was confirmed in PCB samples from mobile phones, multimedia phones, and smartphones. A high-pressure microwave-assisted system was used to leach PGMs from samples with *aqua regia*. High-resolution continuous-flame atomic absorption spectrometry (HR-CS FAAS) and electrothermal atomic absorption spectrometry (ETAAS) were used to determine Pd and Pt in e-waste. The accuracy of the method was confirmed by the analysis of the certified reference material BAM-M505a (electronic scrap) and the standard addition method.

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EFFECT OF ENVIRONMENTAL CONDITIONS ON THE STABILITY OF FORENSIC SAMPLES STUDIED BY VIBRATIONAL SPECTROSCOPY

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Forensic investigations increasingly rely on understanding the chemical evolution of evidence over time and under varying environmental conditions. Vibrational spectroscopy, with its minimal sample preparation and non-destructive nature, offers a powerful tool to monitor these dynamic changes across diverse forensic scenarios.

In this project, we investigate the influence of controlled environmental conditions (temperature, relative humidity, atmospheric composition, and light exposure) on forensically relevant samples using a custom-designed experimental chamber. Time-dependent spectral changes are monitored for model and real biological fluids (blood and saliva) deposited on various substrates. Our results indicate that both environmental factors and substrate type influence degradation processes, and selected spectral features serve as potential indicators for estimating the age of biological evidence.

Building on our characterization of the biological matrix, we subsequently apply these insights to the direct detection of exogenous compounds, specifically drugs and their metabolites, in saliva. By leveraging surface-enhanced vibrational spectroscopic approaches, we aim at sensitive identification of these targets at trace levels, while carefully accounting for the variability of biological fluids and potential spectral interferences [1].

Extending the concept of chemical stability to synthetic systems, we further examine electronic cigarette liquids (e-liquids). We assess their chemical variability across flavors and their stability under storage and thermal stress. Notably, flow-through ATR infrared spectroscopy enables real-time monitoring of generated aerosols, revealing temperature-dependent compositional shifts that mirror the dynamic changes observed in biological samples.

Collectively, these studies demonstrate that vibrational spectroscopy can effectively track chemical transformations and provide critical insights for forensic time estimation, contaminant detection, and aerosol analysis.

Acknowledgements
This work was supported by the grant of Specific university research – grant „Dynamics of Forensic Samples - Their Controlled Aging Using Vibrational Spectroscopy Optics"

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POLLUTION-DRIVEN SOIL ORGANIC MATTER RESTRUCTURING ALTERS ORGANIC MICROPOLLUTANT SORPTION IN AGRICULTURAL SOIL

László Bauer[1, 2, 3*], Zoltán Szalai[1, 2, 3], Attila Csaba Kondor[1, 3], Fruzsina Gresina[1, 2, 3], Zoltán Dévény[1, 2, 3], Gergely Jakab[1, 2, 3], Tibor Filep[1, 3], Lili Szabó[1, 3, 4]

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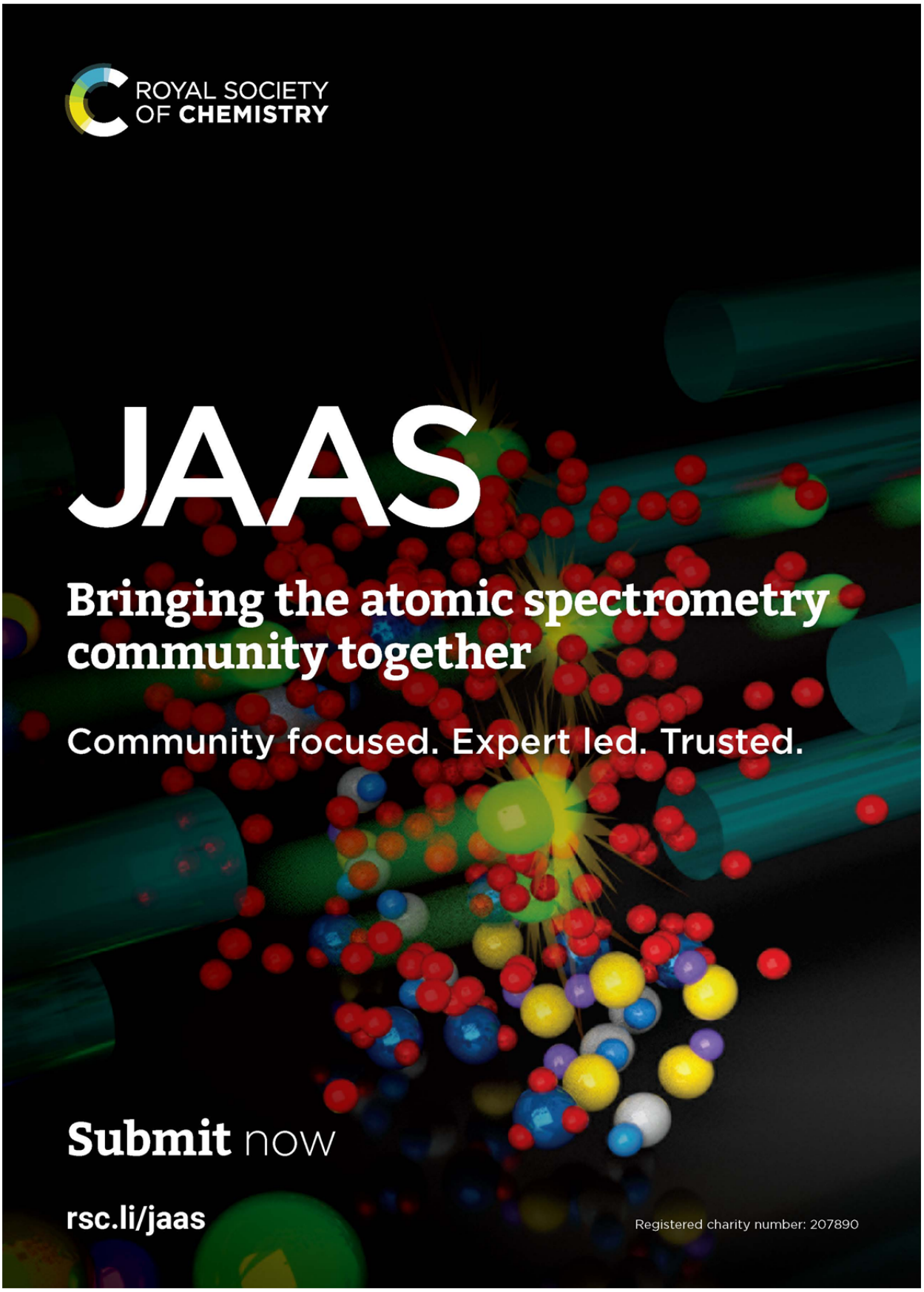
Soil organic matter (SOM) represents a heterogeneous sorbent system composed of coexisting rubbery and glassy domains, whose dynamic balance governs the environmental fate of organic micropollutants (OMPs). In this study, we employed an integrated spectroscopic–chemometric approach combining excitation-emission matrix fluorescence spectroscopy with PARAFAC decomposition (EEM-PARAFAC) and Fourier-transform infrared spectroscopy coupled with two-dimensional correlation spectroscopy (FTIR-2D-COS) to investigate OMP-induced molecular restructuring of SOM during a 92-day simulated vegetation period. Mollisol samples were exposed to an environmentally relevant mixture of pharmaceuticals, steroid hormones, fungicides, and antibiotics. EEM-PARAFAC resolved five fluorescent components, revealing contrasting dissolved organic matter (DOM) trajectories between uncontaminated and contaminated systems. Control soils exhibited progressive enrichment of humic-like fluorophores and depletion of protein-like fractions, indicating ongoing microbial humification. In contrast, contaminated soils maintained nearly constant component distributions, suggesting suppression of natural DOM turnover and stabilization of a quasi-equilibrium state. FTIR-2D-COS provided molecular-scale insight into transformations within the solid SOM fraction. In uncontaminated soils, asynchronous maps revealed a transformation sequence characterized by depletion of aliphatic and polysaccharide-rich domains followed by enrichment of aromatic, lignin-derived, and ester-linked structures. Contamination fundamentally altered this sequence, delaying polysaccharide turnover and reorganizing functional-group evolution pathways. The observed shifts indicate reduced microbial accessibility and enhanced formation of non-extractable residues (NERs), which promote structural condensation of SOM. The combined spectroscopic evidence supports a pollution-driven transition toward a more diffusion-limited, glassy SOM configuration.

Our results demonstrate that the integration of EEM-PARAFAC, FTIR-2D-COS, and multivariate chemometrics enables simultaneous characterization of liquid- and solid-phase SOM dynamics, providing insight into pollutant-driven molecular transformation pathways. The approach highlights spectroscopy-driven chemometrics as a powerful methodology for resolving environmental organic matter evolution, dual-mode sorption behaviour, and the emergence of glassy sorption domains in contaminated soils.

AUTHOR INDEX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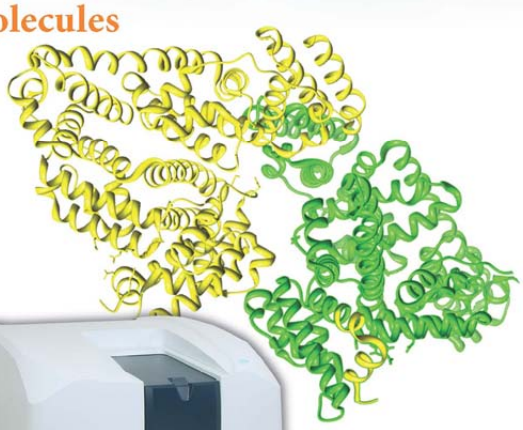

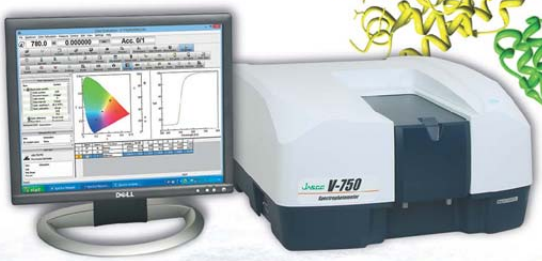

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