



Сојуз на хемичарите и технолозите на Македонија
Society of Chemists and Technologists of Macedonia

28th Congress of The Society of Chemists and
Technologists of Macedonia

BOOK OF ABSTRACTS

23 – 26 September 2026
Metropol Lake Resort
Ohrid, R. N. Macedonia



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Society of Chemists and Technologists of Macedonia

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Dear Esteemed Colleagues and Participants,

It is our great pleasure to present the Book of Abstracts of the 28th Congress of the Society of Chemists and Technologists of Macedonia (SCTM).

As with our previous congresses held over the past two decades, this event takes place in the cradle of Slavic literacy – a region with a rich cultural heritage, a long tradition of intellectual achievement, and a history that continues to inspire generations. We hope that the remarkable heritage of Ohrid, together with the beauty of Lake Ohrid and the city itself, will make your stay both enjoyable and memorable, while providing an additional source of inspiration for your scientific work.

Over the years, the SCTM Congress has developed into an important platform for researchers from across the region and beyond, bringing together scientists and professionals from all fields of chemistry and chemical engineering. We are particularly honored to welcome 13 plenary and invited speakers, 28 oral presentations, and 122 e-poster presentations, representing the work of more than 700 authors and co-authors. This year's participants come not only from Macedonia, but also from Bosnia and Herzegovina, Bulgaria, Croatia, Estonia, Finland, France, Georgia, Germany, Hungary, Italy, Kosovo, Latvia, Lithuania, Poland, Romania, Serbia, Slovenia, Spain, Sweden, Turkey, the United Kingdom and the United States. It is especially gratifying to see so many colleagues returning to the Congress year after year, becoming an integral part of the SCTM community.

We hope that this Book of Abstracts will serve not only as a record of the outstanding scientific contributions presented at the 28th SCTM Congress, but also as a source of inspiration for future research and collaboration. Let us use this occasion to celebrate not only our scientific achievements, but also our resilience, determination, and steadfast commitment to advancing knowledge. Through our collective efforts, we can overcome challenges, foster innovation, and contribute to scientific developments that have a meaningful and positive impact on society.

We would like to express our heartfelt gratitude to Prof. Marina Stefova, President of the Scientific Committee, and especially to Prof. Jasmina Petreska Stanoeva, President of the Organizing Committee, whose dedication, commitment, and tireless efforts ensured that every aspect of the Congress was carefully coordinated and carried out successfully. We are equally grateful to all members of the Scientific and Organizing Committees who worked diligently, often behind the scenes, to make this Congress possible.



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We extend our special appreciation to Marinela Cvetanovska for her excellent work on the Congress website, Ivona Sofronievska for her meticulous management of the finances, and Pece Šerovski for compiling and preparing this Book of Abstracts.

Our sincere thanks also go to all reviewers and participants whose valuable contributions have been essential to the success of the Congress. Your commitment to scientific excellence demonstrates the importance of collaboration, particularly in times of uncertainty and rapid change. It is through the exchange of ideas, the sharing of knowledge and the creation of lasting professional connections that we strengthen our scientific community and advance our respective fields.

Finally, we express our sincere gratitude to all of our sponsors, whose support is acknowledged at the end of this volume. We are especially grateful to our General Sponsors, Alkaloid and Pharmachem, for their generous and continued support of the Society of Chemists and Technologists of Macedonia.

We wish all participants a successful and inspiring Congress, fruitful discussions, new collaborations, and a pleasant and memorable stay in Ohrid.

Prof. Zoran Zdravkovski, President
Society of Chemists and Technologists of Macedonia



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Plenary Lectures



PL-1

CHEMISTRY MATTERS: FROM A PUTATIVE PEPTIDE TO EFFECTIVE MEDICINES FOR DIABETES AND OBESITY

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In the 1960s and 1970s, considerable interest was directed toward understanding the role of peptides in glucose metabolism. Particular attention was given to incretins, intestinally secreted peptides that stimulate insulin release from pancreatic β -cells following food intake, thereby regulating glucose homeostasis. In parallel, research efforts focused on glucagon, a peptide secreted by pancreatic α -cells that increases blood glucose levels.

The presentation describes the research leading to the discovery of the biologically active sequence of glucagon-like peptide-1 (GLP-1), identified as the 31-amino-acid peptide GLP-1(7–37), and demonstrates that this peptide functions as an incretin with therapeutic potential for the treatment of type 2 diabetes. These findings are considered in the context of the broader body of work by other investigators that contributed to the understanding of GLP-1 biology.

Keywords: GLP-1; incretins; glucose metabolism; type 2 diabetes; obesity



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Invited Lectures



IL-1, AEC

DECODING COMPLEX MIXTURES: HOW LC-HRMS IS TRANSFORMING THE DETECTION OF EMERGING CONTAMINANTS

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The increasing complexity of environmental contamination, characterized by mixtures of hundreds to thousands of known and unknown compounds, poses significant challenges for effective monitoring and risk assessment. In this context, advances in liquid chromatography coupled to high-resolution mass spectrometry (LC-HRMS) have transformed the field of environmental analysis by enabling comprehensive and highly sensitive detection of a wide range of contaminants and molecular signatures in complex environmental matrices.

This talk will highlight the opportunities offered by HRMS for the identification of emerging contaminants, with a particular focus on suspect screening approaches. These strategies enable the systematic investigation of large numbers of compounds beyond conventional target analysis, substantially expanding the chemical space that can be explored in environmental samples. In addition, non-target HRMS approaches for the comprehensive molecular characterization of dissolved organic matter (DOM) will be presented, illustrating how these methods can reveal previously uncharacterized fractions of natural and anthropogenic organic mixtures in aquatic systems.

At the same time, the presentation will critically discuss the current challenges and limitations of LC-HRMS-based workflows. These include issues related to data complexity and dimensionality, compound annotation uncertainty, limited availability and quality of spectral libraries, false positives and negatives in suspect screening, and the lack of harmonized and reproducible data processing pipelines. Particular attention will also be given to the specific challenges associated with DOM analysis, including its intrinsic heterogeneity and the difficulty of assigning structural information to thousands of unresolved features. The importance of quality assurance, transparent reporting, and methodological standardization will also be addressed.

Analytical workflows for suspect and non-target screening will be presented, illustrating case studies involving different environmental matrices, including domestic wastewater, lake water, and urban runoff, to demonstrate the applicability of these approaches to real-world complex mixtures.

Overall, this presentation will showcase how LC-HRMS-based methodologies are advancing environmental monitoring towards more holistic and informative assessments of chemical contamination and organic matter complexity, while also highlighting the critical methodological challenges that must be addressed to fully realize their potential.

Keywords: LC-HRMS, suspect screening, non-target screening, emerging contaminants, dissolved organic matter.



IL-2, OBPC (PSSE)

LIFE ELECTRIC: FROM EXTRACELLULAR ELECTRON TRANSFER TO WASTE-TO-VALUE TECHNOLOGIES

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Life is fundamentally based on electrochemistry: in respiration, electrons from the oxidation of substrates are transferred to terminal electron acceptors, generating electrochemical gradients that drive ATP synthesis. Electrogenic microorganisms extend this principle beyond the cell membrane by transferring metabolic electrons to extracellular minerals or solid electrodes. This extracellular electron transfer forms the basis of microbial electrochemistry and enables the direct coupling of microbial metabolism to electrochemical systems.

In this talk, I will introduce the basic principles of microbial electrochemical technologies, with a focus on microbial fuel cells. Starting from microbial respiration and electron transfer in organisms such as *Geobacter sulfurreducens*, I will show how electroactive biofilms can be cultivated on electrodes and studied using electrochemical and in operando techniques.

Building on these fundamentals, the talk will discuss how microbial electrochemical technologies can contribute to sustainable water, energy, and material cycles¹. Wastewater is not merely a stream to be treated, but a large resource containing chemical energy, nutrients, and reusable water. Microbial fuel cells can convert part of this energy into electricity, while related systems may produce hydrogen or methane and support nutrient recovery, sensing, and decentralized sanitation.

Finally, I will critically address the challenges that still limit practical implementation, including scale-up, internal resistance, electrode materials, complex wastewater composition, long-term stability, and economic viability. Rather than replacing established treatment processes, microbial electrochemical technologies may find their future in targeted integration into circular, resource-oriented wastewater treatment schemes.

Keywords: microbial electrochemistry, microbial electrochemical technologies, microbial fuel cells, wastewater

References:

[1] Schröder, U. et al Waste to value: microbial electrochemical technologies for sustainable water, material and energy cycles; *Frontiers in Science*, 2026, 4:1688727. doi: 10.3389/fsci.2026.1688727



IL-3, OBPC

ONE FRAMEWORK, MANY INSIGHTS: A UNIFIED VISION OF VOLTAMMETRY

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Electrochemistry is far more than corrosion and batteries, it is embedded in entire life on Earth and in our environment.¹ Breathing involves electrochemical oxygen reduction, while cellular energy production via Adenosine Triphosphate arises from electron-transfer reactions in the Mitochondrial Electron Transport Chain. While the Membrane Potential governs cellular communication, redox enzymes drive biochemical transformations, and ion transport sustains homeostasis. Drug action is also rooted in electrochemical interactions, highlighting electrochemistry as a universal language of charge transfer and energy conversion.

Voltammetry is recognized as the most prominent electrochemical technique and it is often seen as indispensable tool in modern laboratories, enabling direct probing of electron-transfer processes through current–potential measurements.² It has provided fundamental mechanistic insights into various chemical and biochemical systems, allowing kinetic, thermodynamic, and quantitative analysis, with its importance reflected in several Nobel Prize in Chemistry recognitions.

Since the charge transfer is involved in vast majority of chemical and biological processes,³ voltammetry serves as a unifying platform across chemistry, pharmacy, biomedicine, physics, and environmental sciences. While voltammetry is easily achievable experimental technique, interpretation of voltammetric results often requires rigorous theoretical models.

This talk presents voltammetry as a unified framework addressing phenomena related to charge and mass transfer, and many other aspects such as adsorption, coupled chemical reactions, drug–drug interactions, nano-electrochemistry, and energy systems such as biofuel cells. By integrating experiments with theory, voltammetry emerges as one of the most versatile techniques, offering a unique perspective on electrochemical phenomena.

Keywords: bioelectrochemistry, ion-transfer across biomembranes, batteries, biosensors, nano-electrochemistry.

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IL-4, ICTM

INDUSTRIAL SYMBIOSIS THROUGH SECONDARY GYPSUM RESOURCES FOR CIRCULAR CONSTRUCTION

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Gypsum-containing waste is a valuable secondary resource that supports circular construction and reduces landfill disposal. Three circular gypsum streams were assessed: synthetic gypsum (SG), phosphogypsum (PG), and recycled plasterboard gypsum (RPG).

SG exhibits a considerably finer particle-size distribution than commercial gypsum (58–78% vs. ~4% below 63 μm). While this enables binder production at relatively low calcination temperatures (105–120 $^{\circ}\text{C}$), excessive fineness may increase water demand and limit direct utilization in conventional gypsum products.¹ PG consists predominantly of calcium sulfate dihydrate ($D_{50} \approx 74 \mu\text{m}$; commercial gypsum $\approx 140 \mu\text{m}$) and contains residual phosphorus compounds ($\text{P}_2\text{O}_5 \approx 0.6 \text{ wt.}\%$), which may affect hydration kinetics and prolong setting times.² RPG exhibits the highest compositional variability due to differences in plasterboard composition and additives. Following calcination at 160–180 $^{\circ}\text{C}$, RPG can be converted into a secondary gypsum binder, while high-temperature treatment ($\sim 700\text{--}800 \text{ }^{\circ}\text{C}$) may provide a route to more uniform anhydrite binders.¹

The suitability of SG, PG, and RPG as substitutes for natural gypsum was evaluated in commercial gypsum products with replacement levels ranging from 0 to 30 wt.%. Secondary gypsum resources were also incorporated into gypsum–cement–pozzolan (GCP) systems, achieving compressive strengths of up to 50 MPa after 28 days.² These materials demonstrated potential for additive manufacturing applications, partly due to their favourable pore structure, as revealed by micro-computed tomography.²

The findings highlight the potential of secondary gypsum resources to contribute to circular construction by reducing reliance on virgin raw materials and promoting the valorization of industrial and construction waste streams.^{3,4}

Keywords: secondary gypsum, synthetic gypsum, phosphogypsum, recycled plasterboard gypsum, industrial symbiosis, circular economy, sustainable construction.

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IL-5, OBPC

WATCHING NANOMATERIALS TRANSFORM ON ATOMIC SCALE: IN-SITU ENVIRONMENTAL TEM OF REDOX AND PHASE DYNAMICS

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In-situ environmental scanning transmission electron microscopy (e-STEM) provides a powerful platform for atomic-scale characterisation of materials under realistic and dynamic conditions. Such approaches are increasingly critical for advancing functional materials in energy applications, including nuclear and fusion systems, photovoltaics, batteries, and heterogeneous catalysis.

At York, we have developed open-cell environmental TEM/STEM methodologies, recently implemented on a double aberration-corrected JEOL NeoARM cold field-emission gun instrument (ARTEMIS). This system builds on our earlier environmental TEM developments and enables a broad range of in-situ experiments, combining variable accelerating voltage, controlled gas and vapour environments, 4D-STEM diffraction, and atomic-resolution EDX and EELS spectroscopy.

In this work, we highlight the capabilities of the ARTEMIS platform through three representative case studies. First, we examine redox processes in Ni/NiO and Fe nanoparticles under H₂, H₂O vapour, and O₂ environments, achieving single-atom sensitivity using HAADF-STEM under controlled temperature and gas conditions. Second, we investigate structural phase transformations in TiO₂ nanoparticles, including the formation of Magnéli phases, driven by electron-beam irradiation and influenced by environmental and thermal parameters. Third, we demonstrate in-situ, electron-beam-directed three-dimensional atomic restructuring of NiO nanoflowers via precursor-mediated β -hydroxide and nitrate-hydroxide intermediates.

These studies illustrate the unique capability of in-situ e-STEM to directly resolve dynamic processes at the atomic scale, providing insights into reaction pathways and structural evolution that are essential for the rational design of next-generation functional nanomaterials.

Keywords: Transmission Electron Microscopy, redox reactions, in-situ, phase transformations



IL-6, PPM

**FROM NATURAL POLYMERS TO FUNCTIONAL ADSORBENTS
FOR WATER AND WASTEWATER TREATMENT**

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Increasing degradation of the global aquatic environment has intensified the search for new, low-cost adsorbents with reduced toxicity, particularly those derived from natural and renewable sources. In response to these challenges, growing attention has been directed toward sustainable and biodegradable materials such as lignin, cellulose, and starch. These biopolymers, due to their abundance, low environmental impact, and favorable physicochemical properties, represent promising alternatives to conventional synthetic polymers, especially those derived from petrochemical sources. Their use aligns with the principles of green chemistry and circular economy, which aim to minimize waste generation and promote the use of renewable resources.

Numerous studies have demonstrated that polymers of natural origin can effectively replace synthetic counterparts while maintaining high adsorption efficiency. Moreover, the incorporation of such biopolymers into advanced material systems allows for the design of functional adsorbents with tunable properties, improved selectivity, and enhanced environmental compatibility.

This study presents a comprehensive approach to the development of eco-friendly adsorbents based on natural and renewable biopolymers, including lignin, cellulose, and starch, incorporated into functional polymer matrices. These materials were synthesized using monomers such as ethylene glycol dimethacrylate (EGDMA), triethylene glycol dimethacrylate (TEGDMA), vinyl acetate (VA), and triethoxyvinyl silane (TEVSi), enabling the formation of crosslinked, porous microspheres with tailored surface properties. The obtained materials were thoroughly characterized and demonstrated effective removal of toxic dyes, such as C.I. Basic Yellow 2, C.I. Basic Blue 3, C.I. Basic Red 46, and C.I. Acid Violet 1. The adsorption behavior was found to be influenced by factors including lignin content, the presence of surfactants and electrolyte, confirming the strong potential of these materials as sustainable and cost-effective adsorbents for wastewater treatment applications.

Keywords: dyes removal, adsorbents, wastewater treatment, biopolymers.



IL-7, PSSE

**INFLUENCE OF MOISTURE ON THE MOLECULAR STRUCTURES OF
PYRAZOLE-BASED CADMIUM HALIDE COMPLEXES**

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Due to the aromatic nature of the pyrazole ring, pyrazole derivatives are potentially applicable as luminescent materials, sensors, and functional materials. The flexible coordination behavior of Cd(II), combined with the tunable electronic properties of pyrazole-based ligands, enables the formation of different structures with attractive photophysical characteristics. In this work, a series of cadmium halide complexes (CdX_2 , $\text{X} = \text{Cl}, \text{Br}, \text{I}$) with ethyl 5-amino-1-methyl-1H-pyrazole-4-carboxylate was synthesized under different reaction conditions and characterized by structural, spectroscopic, and thermal methods. Structural investigations revealed that the presence of water significantly affects the coordination environment of the Cd(II) centers and the resulting crystal structures, leading to the formation of different compounds from the same precursors. These moisture-induced differences demonstrate the sensitivity of the complexes to environmental conditions and highlight the role of water in the formation of the coordination compounds. Except for CdI_2 , synthesis with other halides yielded the coordination polymers, promising for light-harvesting applications. These findings contribute to a better understanding of the relationship between synthesis conditions, solid-state structure, and material properties, which is essential for the rational design of coordination compounds with tailored functionalities and potential applications in optical and advanced functional materials.

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Keywords: pyrazole derivative, cadmium complex, moisture, structure.

IL-8, ICTM**CONTROLLING REACTIVITY IN MECHANOCHEMISTRY: FROM ADVANCED MOFS TO SCALABLE MATERIALS**Bahar Karadenize-mail: bahar.karadeniz@irb.hr

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Mechanochemistry has emerged as a sustainable and versatile platform for the synthesis of functional materials, offering solvent-free and energy-efficient alternatives to conventional synthetic approaches.¹ Beyond its green metrics, mechanochemistry provides unique opportunities to control chemical reactivity by tuning parameters such as temperature, mechanical input, and reaction environment.

Here we highlight recent advances in controlling mechanochemical reactivity for the synthesis of advanced materials, including metal–organic frameworks (MOFs),² MOF-based composites,³ and scalable inorganic–organic systems.⁴ Recent studies demonstrate how controlled mechanochemical methods can modulate reaction pathways, rates, and selectivity, often enabling access to products unattainable by conventional solution-based synthesis.^{2,3} Mechanochemical approaches have enabled precise control of composition and phase purity in porous materials, facilitating the incorporation of guest species and the formation of functional composites with tailored properties. Finally, the scalability of these processes will be discussed by examining the translation of laboratory-scale milling to continuous production methods, demonstrating improved energy efficiency, throughput, and prospects for industrial implementation.

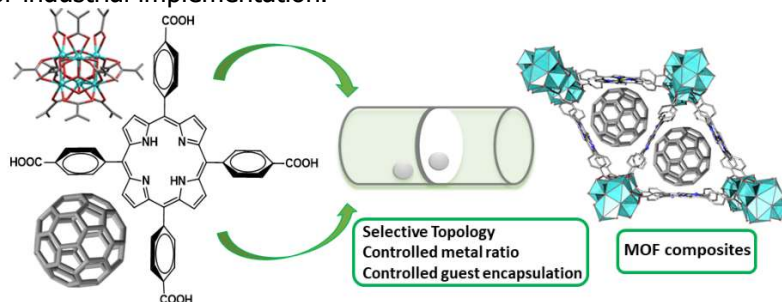


Figure 1. Scheme for a mechanochemical synthetic route for the formation of a MOF composite⁵

Keywords: mechanochemistry, solid-state, metal-organic frameworks, scale-up

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IL-9, AEC

TRACKING PFAS IN WATER: FROM MONITORING TO RISK PRIORITISATION

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Per- and polyfluoroalkyl substances (PFAS) are among the most challenging contaminants of emerging concern due to their persistence, structural diversity, and complex toxicological profiles. Their widespread use has led to global occurrence in aquatic environments, while differences in physicochemical properties across the PFAS class complicate both monitoring and environmental interpretation. This lecture presents a stepwise framework for tracking PFAS in surface waters, beginning with high-resolution mass spectrometry (HRMS)-based suspect screening analysis to expand PFAS coverage beyond conventional target lists and capture known, emerging, and previously overlooked PFAS. Screening results are then linked to hazard- and exposure-based prioritisation, integrating QSAR-derived indicators of persistence, bioaccumulation, and toxicity with occurrence-related metrics such as detection frequency and concentration magnitude. This prioritisation step supports the identification of the most relevant PFAS for follow-up analysis. A subset of prioritised compounds was then selected for targeted (semi)quantification based on both prioritisation outcomes and the availability of analytical standards, enabling experimental confirmation and refinement of the assessment. The approach is illustrated through recent investigations¹ of urban-impacted river systems in Serbia, representing one of the first comprehensive PFAS assessments in this part of the Danube River Basin. Initial HRMS screening revealed additional PFAS beyond the conventional target list, including ultra-short-chain compounds i.e. trifluoroacetic acid (TFA), which has recently gained particular regulatory relevance in the EU and was often detected at higher levels than legacy PFAS. Overall, the lecture demonstrates how a workflow progressing from broad screening to prioritisation and targeted confirmation can strengthen PFAS monitoring and provide a more robust basis for environmental risk assessment and regulatory decision-making.

Keywords: per- and polyfluoroalkyl substances, suspect screening, risk-based prioritization.

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Acknowledgement: This study is conducted under the project TwiNSol-CECs that has received funding from Horizon Europe programme under grant agreement no.101059867.



IL-10, OBPC

CLOSING THE WATER LOOP IN MINERAL PROCESSING: IMPACTS OF RECYCLED-PROCESS-WATER ON (CU-MO) SULFIDE MINERAL FLOTATION

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Flotation remains the primary technique for extracting valuable sulphide minerals, but its reliance on water presents a massive challenge amid rising global water scarcity and environmental restrictions. While recycling process water offers a sustainable path forward, accumulated species like metal ions, sulphates¹, and natural organic materials² fundamentally alter water properties and threaten flotation performance³⁻⁵.

This presentation delivers a comprehensive evaluation of how recycled and low-quality water influences the floatability of sulphide minerals (copper and molybdenum). From the lab-scale to full-scale operation, the underlying mechanisms using a dual approach were investigated: laboratory single-mineral flotation of chalcopyrite and molybdenite, and complex ore testing using process water sourced from real beneficiation plant in Peru. Utilizing surface-sensitive analytical techniques such as zeta potential and X-ray photoelectron spectroscopy (XPS), the physicochemical characterization was mapped driving the mineral-water-bubble interactions. The findings establish a predictive workflow for identifying how specific water-borne species impact positively or negatively metallurgical performance.

Keywords: process water, mineral flotation, recycled water, sulphides

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IL-11, PSSE

PEROVSKITES: FROM SYNTHESIS TO FUNCTIONAL PROPERTIES

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Over the last few decades, perovskite-type compounds (ABX_3) have attracted considerable scientific interest owing to their remarkable structural versatility and wide range of functional properties. Despite the apparent simplicity of the ideal perovskite crystal structure, this class of materials exhibits enormous compositional and structural flexibility, giving rise to a variety of intriguing physical and chemical properties. Consequently, they find applications in many fields, including catalysis, electrocatalysis, electronics, energy conversion and storage, sensing, and information technologies. Depending on their composition and structure, they may exhibit ferroelectricity, piezoelectricity, high-temperature superconductivity, colossal magnetoresistance, and many other technologically relevant properties. More recently, hybrid organic–inorganic perovskites have emerged as a new generation of semiconducting materials with outstanding performance in photovoltaic and optoelectronic applications.

The first part of this lecture will provide a general overview of the perovskite structure, major classes of perovskite materials, commonly used synthesis methods, and selected functional properties. The second part will focus on our research on complex inorganic perovskites synthesized by the solution combustion method using different fuels. Their crystal structures were refined by the Rietveld method using powder X-ray diffraction (PXRD) data, while various crystallographic parameters related to structural stability and distortion were calculated and analyzed. Structural, compositional, morphological, electrical, and electrocatalytic properties were systematically investigated using complementary characterization techniques. Particular attention was devoted to understanding how structural and microstructural factors influence the electrical conductivity and electrocatalytic performance of the synthesized materials, especially in reactions relevant to sustainable energy technologies, such as the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER).

The final part of the lecture will present selected results from our studies on bulk materials and thin films of hybrid organic–inorganic lead halide perovskites containing different organic cations. Their composition, crystal structure, morphology, optical properties, and electrochemical stability were investigated. Optical band-gap energies were determined from UV–Vis absorption spectra of the thin films using Tauc analysis, and the potential of these materials for photovoltaic applications was evaluated.

Keywords: perovskites, solution combustion synthesis, crystal structure, electrocatalysis, hybrid organic–inorganic perovskites, photovoltaic applications



IL-12, ICTM

INDUSTRIAL WASTE AS A SECONDARY RAW MATERIAL AND ITS APPLICATION IN ACCORDANCE WITH THE CIRCULAR ECONOMY

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The transition toward a circular economy requires the transformation of industrial waste streams into valuable secondary raw materials, reducing dependence on primary resources while minimizing environmental impacts associated with waste disposal. Among industrial by-products, coal fly ash represents one of the most significant residues generated from thermal power production and has considerable potential for resource recovery and sustainable material production.

This study aims to evaluate the potential of Macedonian coal fly ash as a secondary raw material through quantitative assessment and comprehensive chemical characterization, with particular emphasis on its suitability for the recovery of valuable elements and its further application within circular economy strategies. The estimated volume of fly ash generated from the investigated thermal power plant reaches 106.8 ± 5.1 million m³, indicating a significant secondary resource base. Chemical characterization revealed that the investigated fly ash samples are predominantly silicate-based materials, containing approximately 50 wt.% SiO₂, 19–20 wt.% Al₂O₃, and 15–16 wt.% Fe₂O₃, together with other alkali and alkaline earth metal oxides.

The assessment of potentially valuable and critical elements demonstrated the presence of significant concentrations of selected metals, including manganese (1100–5038 mg kg⁻¹), arsenic (31–191 mg kg⁻¹), gallium (30–35 mg kg⁻¹), as well as rare earth elements such as cerium (147–153 mg kg⁻¹) and lanthanum (60–78.1 mg kg⁻¹). These findings indicate that coal fly ash may represent a promising alternative source of valuable elements and contribute to the diversification of critical raw material supply chains. Furthermore, after the selective extraction of rare earth elements and other valuable metals, the remaining aluminosilicate-rich fraction retains significant potential for the synthesis of geopolymer materials, enabling a sequential valorization pathway and maximizing resource utilization.

These findings provide relevant information for researchers, industrial stakeholders, and potential investors interested in developing sustainable recovery and utilization technologies.

Keywords: coal fly ash, critical raw material, waste valorisation



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Inorganic chemistry and technology,
inorganic materials and metallurgy (ICTM)



ICTM-O1

SYNTHESIS OF SILVER NANOSPIRALS

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The unusual geometry of spiral nanocrystals gives rise to unique optical, electronic, and mechanical properties. Spiral growth of noble metals was demonstrated for gold decades ago but no information about silver nanospirals was reported. Here present novel approach for preparation of silver nanospirals with yields of over 90%, based on application of 3-mercaptopropionic acid (MPA) ligand. Addition of H₂O₂ results in formation of different morphologies of silver such as dendrites, nanoribbons, nanospirals or nanoflowers, depending on MPA concentration. Formation of such variety of structures is result of MPA coverage-dependent conformational change and decrease of total nanoparticle surface area during H₂O₂ addition, causing sudden change from repulsion to attraction of silver nanoparticles. Consequently, rapid 2D oriented assembly launches diffusion-limited auto-accelerated process. When random dendrite arms overlap due to mismatch caused by a rapid growth, this represents the point of spiral formation. Silver morphology can be fine-tuned via MPA/silver nanoparticles ratio, providing therefore a bottom-up route for twisted nanocrystal synthesis within minutes.

Keywords: silver nanospirals, 3-mercaptopropionic acid, synthesis

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ICTM-O2

**SUSTAINABLE CONSTRUCTION MATERIALS THROUGH ALKALI
ACTIVATION OF FLY ASH AND METAKAOLIN**

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Alkali-activated composites based on fly ash (FA) and metakaolin (MK) were designed as sustainable low-carbon construction materials. The fly ash was mechanically activated in a planetary mill for 20 min to enhance its reactivity, while metakaolin was produced by the thermal treatment of kaolin at 700 °C for 2 h. Sodium hydroxide and sodium silicate solutions were used as alkaline activators. The curing regime consisted of 24 h at 50 °C, followed by curing at room temperature up to 28 days. Different alkali-activated composites were designed using as-received fly ash, mechanically activated fly ash, and mechanically activated fly ash with the addition of metakaolin at 10, 25, and 50 wt.%. The raw materials and the synthesized alkali-activated composites were characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), and scanning electron microscopy (SEM). In addition, bulk density, capillary water absorption, and compressive strength were determined for all alkali-activated composites. The physical and mechanical properties of the alkali-activated composites were evaluated after 28 days of curing. The bulk density of the hardened products ranged from 1.05 to 1.50 g/cm³, depending on the precursor composition and metakaolin content. The compressive strength varied between 8 and 32 MPa. Among the investigated formulations, the composite containing 25 wt.% metakaolin exhibited the highest compressive strength (32 MPa) and the most compact microstructure, indicating a synergy between mechanically activated fly ash and metakaolin. The results demonstrate that the combined use of mechanically activated fly ash and metakaolin is an effective approach for producing alkali-activated materials with enhanced performance. The study supports the green transition and the principles of the circular economy by valorizing fly ash, an industrial by-product, as a secondary raw material for design of sustainable low-carbon construction materials.

Keywords: fly ash, metakaolin, alkali-activation, circular economy, compressive strength



ICTM-O3

**SUSTAINABLE GEOPOLYMER COMPOSITES INCORPORATING
MUNICIPAL CONTAINER**

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Ordinary Portland cement (OPC) production significantly contributes to global greenhouse gas emissions. Geopolymers synthesized from metakaolin offer an eco-friendly alternative, though unreinforced matrices can exhibit microstructural brittleness under load. Incorporating fiber reinforcement enhances mechanical performance and structural behavior. This study analyzed the effect of fibers derived from recycled municipal solid waste containers on the compressive strength of a geopolymer matrix composed of metakaolin and sand.

Geopolymer composites were synthesized using metakaolin and sand (1:1 mass ratio) activated with a 10 M NaOH and aqueous sodium silicate solution. Shredded white or green container waste fibers were incorporated at 5% and 7% volume fractions, and mechanical testing was performed after 28 days of curing. Two series of geopolymer samples were tested: fibers of a white waste container and fibers of a green waste container. In the white container series, adding 5 vol.% fibers increased compressive strength from 35.0 MPa (reference) to 37.5 MPa, while a 7 vol.% content produced a 14% enhancement – 39.9 MPa. For the green container series, a 7 vol.% fiber content successfully raised compressive strength by 4% compared to the reference sample (27.9 MPa).

The test results indicate that addition of shredded waste from waste containers effectively improves the compressive strength of metakaolin-based geopolymers, confirming the potential for recycling municipal plastics from containers to provide functional reinforcement for sustainable building materials.

Keywords: geopolymers, fiber reinforcement, waste fibers, sustainable materials

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ICTM-O4

CIRCULAR UTILIZATION OF RECYCLED CONCRETE FINES FOR SUSTAINABLE AND LOW-CARBON MORTARS

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The construction sector is under increasing pressure to reduce greenhouse gas emissions, decrease its reliance on virgin raw materials, and implement circular economy principles. The valorization of recycled concrete fines (RCF) as a supplementary cementitious material offers a promising route for reducing clinker consumption and natural raw materials, lowering the carbon footprint of cement-based products, and improving resource efficiency in the construction industry

This study investigates the mechanical activation of RCF and its utilization as a partial replacement of Portland cement (PC) in cement mortars. RCF derived from waste concrete was mechanically activated using different milling protocols employing both a conventional ball mill and a high-energy planetary mill. Various material-to-ball ratios, milling speeds, and activation times were evaluated to identify the most effective activation pathway. The optimal activation conditions were achieved using a ball mill with a material-to-ball ratio of 10.4, milling speed of 70 rpm, and activation time of 20 min. Structural and geometrical activity were evaluated through chemical and mineralogical characterization, particle size distribution, and surface area analysis, while the reactivity of the activated material was assessed using the activity index. The mechanically activated RCF was incorporated into cement mortars as a replacement for PC at levels from 5 to 15 wt.%. The fresh and hardened properties of the mortars were evaluated, and the microstructure of the hardened mortars was also examined. All mortars containing activated RCF exhibited longer setting times and lower mechanical properties in comparison to the reference mortars; however, all mixtures satisfied the performance requirements for mortar applications.

Keywords: Recycling concrete fines (RCF), mechanical activation, mortars, circularity, decarbonization



ICTM-P1

SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF Pr_{1-x}A_xCoO₃ TYPE OF PEROVSKITES, A = K AND Ca

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Cobalt-based perovskites incorporating rare-earth elements at the A-site, partially substituted with alkali and alkaline-earth cations, have attracted considerable attention for their potential applications in solid oxide fuel cells and catalytic processes [1]. Among them, praseodymium-cobalt perovskites stand out as a particularly interesting class of materials, combining structural complexity with promising functional properties. This study focuses on their synthesis and characterization, and the influence of the rare-earth substitution on their structural stability and properties.

For the synthesis of Pr_{1-x}A_xCoO₃, where A = K and Ca, the EDTA-citric acid complexing method was used. In this approach, EDTA acts as a chelating agent [2], ensuring controlled distribution of metal ions and promoting the formation of homogeneous particles with nanoscale dimensions, while citric acid is used as fuel.

The obtained perovskites were investigated by X-ray powder diffraction (XRD) and Infrared (IR) spectroscopy. The diffraction patterns confirm their purity and the degree of crystallinity, while the comparison with the unsubstituted Pr-perovskites with the corresponding metals indicates that the obtained compounds adopt an orthorhombic structure.

Further investigation and characterization was carried out using vibrational spectroscopy techniques such as IR spectroscopy in the mid-infrared (MIR) and far-infrared (FIR) region in order to probe the lattice dynamics and structural features of the obtained perovskites.

Keywords: complex perovskites, edta-citric complexing method, PXRD, IR spectroscopy

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ICTM-P2

**THE EFFECT OF DOPING WITH Sm AND Nd IONS ON THE
CHEMICAL, PHYSICAL, STRUCTURAL AND OPTICAL PROPERTIES
OF GEOPOLYMERS**

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The geopolymer obtained by the standard procedure of alkaline activation of metakaolin is doped with samarium (Sm) and neodymium (Nd) ions. The mass concentration of the dopant in both cases is 5%. After doping, the obtained materials were thermally treated at 600°C in a tube furnace in a stream of argon for 1 hour [1]. After cooling, the obtained materials were characterized using: Scanning Electron Microscopy (SEM), High Resolution Transmission Electron Microscopy (HR-TEM), Fourier Transform Infrared Spectroscopy (FTIR) and Spectroscopic Ellipsometry (SE). SEM analysis revealed that thermal exposure induces dehydroxylation, crystallization, and sintering processes, which are reflected in both morphological (SEM) and chemical (EDS) changes. The SEM micrographs also present a low degree of geopolymerization, as evidenced by the presence of numerous unreacted particles, indicating limited dissolution of the precursor material. HR-TEM clearly shows the differences between the crystal planes in the geopolymer, the presence of Al and Si phases as well as the polycrystalline structure of the doped geopolymer even after thermal treatment [2]. FTIR spectroscopy was performed to examine the structural evolution, and confirmed existence of hydroxyl groups bonded within the gel in the range of about 3450 cm⁻¹ was. Spectroscopic ellipsometry (SE) showed absorption of Nd and Sm dopants in the UV region in the range from 290 nm to 373 nm. It is indicative that both dopants representing rare earths show activity in the UV region.

Keywords: Geopolymer, rare earth, HR-TEM, optical properties

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ICTM-P3

**INFLUENCE OF SAMARIUM(III) OXIDE CONTENT ON THE
PHYSICOCHEMICAL AND THERMAL PROPERTIES OF
METAKAOLIN-BASED GEOPOLYMERS**

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Aluminosilicate materials are widely recognized for their high mechanical strength, corrosion resistance, and thermal stability.¹ In this study, metakaolin-based geopolymers were synthesized by alkali activation and doped with samarium(III) oxide (Sm_2O_3) in order to investigate its influence on their physicochemical and thermal properties. Two samples containing 1 wt% and 5 wt% Sm_2O_3 were prepared and denoted as S_1 and S_2 , respectively. The synthesized materials were characterized using energy-dispersive X-ray fluorescence spectrometry (EDXRF), diffuse reflectance infrared Fourier transform spectroscopy (DRIFT), X-ray diffraction analysis (XRD)², and photothermal beam deflection (PBD). The obtained results indicate that Sm_2O_3 was successfully incorporated into the aluminosilicate matrix, without causing significant changes in the density or porosity of the geopolymers. However, the addition of Sm_2O_3 altered the material's thermal response, thereby enhancing thermal conductivity. These findings suggest that Sm_2O_3 -doped metakaolin-based geopolymers may be considered promising candidates for applications requiring improved thermal stability and thermal management, including potential use as functional insulating materials.

Keywords: Aluminosilicate materials, EDXRF, XRD, PBD, DRIFT

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ICTM-P4

EFFECT OF WOOD ASH ADDITION ON THE HIGH-TEMPERATURE PERFORMANCE OF ALKALI-ACTIVATED FLY ASH MATERIALS

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Alkali-activated fly ash-based materials have attracted considerable attention as sustainable alternative binders due to their ability to partially replace ordinary Portland cement while exhibiting favorable mechanical properties, durability, and resistance to aggressive environmental conditions. Furthermore, the investigation of alkali-activated materials at temperatures exceeding 1000 °C is essential for assessing their thermal stability, phase evolution, and microstructural transformations, thereby providing valuable insights into their potential application as high-performance binders and refractory materials under extreme thermal conditions. In this study, two systems were prepared: pure fly ash (FA) and a blend of wood ash (WA) and fly ash (10 wt.% WA and 90 wt.% FA), which were subsequently subjected to alkali activation to enhance precursor reactivity through their calcium- and alkali-rich composition. The high-temperature behavior of fly ash and fly ash–wood ash alkali activated materials was evaluated following thermal treatment at 1000, 1100, and 1200 °C. X-ray diffraction analysis revealed the formation of thermally stable crystalline phases, including nepheline, quartz, and gehlenite in both systems, while albite was additionally identified in the FA–WA samples. Both alkali activated systems maintained structural stability up to 1100 °C; however, significant degradation and collapse of the formed structural network were observed at 1200 °C. Scanning electron microscopy demonstrated progressive densification, reduced porosity, and the transformation of the initially amorphous geopolymeric matrix into a ceramic-like structure with increasing temperature. These findings highlight the influence of wood ash incorporation on phase development and microstructural evolution, as well as the high-temperature performance of alkali-activated fly ash-based materials.

Keywords: Fly ash; Wood ash; Alkali-activated materials; High-temperature treatment; Thermal stability; Microstructural evolution

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ICTM-P5

**STRUCTURAL AND MORPHOLOGICAL EVALUATION OF
GEOPOLYMER–PA12 HYBRID COMPOSITES**

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This research addresses the synthesis and characterization of geopolymer–PA12 composites developed to enhance material performance. Two systems were developed: geopolymer–PA 2200 (GP_2200) and geopolymer–PA 3200 GF reinforced with glass beads (GP_3200 GF). Structural and morphological characterization was performed using XRD, FTIR, and SEM techniques. XRD confirmed the amorphous nature of the geopolymer and the semi-crystalline structure of PA12, while composite patterns exhibited features of both phases. FTIR spectra indicated the presence of characteristic functional groups of each component with no significant chemical changes.

The results indicate that the geopolymer and PA12 phases remain chemically distinct, interacting only at their interfaces through physical and morphological effects. In the glass bead–modified composite (GP_3200 GF), the silicon content increased, but no major structural changes were observed in either the matrix or the composite. A key challenge, however, is the poor compatibility between the inorganic geopolymer matrix and the organic PA12 phase. To improve interfacial bonding and achieve better phase integration, adjustments to processing conditions and the use of compatibilizers or surface treatments may be necessary.

Keywords: Geopolymer composites; Polyamide 12; Hybrid materials; Glass bead reinforcement; Interfacial bonding; Morphological analysis

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ICTM-P6

EFFECT OF MgO ON THE LUMINESCENT PROPERTIES OF SiO₂-B₂O₃-Eu₂O₃ SOL-GEL GLASSES

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The sol-gel method has a number of advantages over traditional high-temperature synthesis methods. The resulting materials exhibit high purity, homogeneity of nanosized particles, thermal stability, and chemical resistance. The advantages of the method are mainly expressed in the easy control over the structure and properties of the obtained glasses, as well as the low synthesis temperature.

The rare earth elements are of particular interest due to their excellent optical properties when incorporated into the glass matrix. Alkaline earth elements, when added to the glass matrix, improve the thermal stability and optical activity of rare-earth-doped sol-gel glasses.

In this work, the sol-gel process was used to synthesize a series of Eu-doped silica-boron glasses, and their luminescent properties were investigated both prior to and following MgO incorporation.

Several techniques were used to analyze the structural and optical properties of the as-obtained samples. DTA was employed to gain information about their thermal stability. IR spectroscopy was used to identify the vibrations of the structural units, while UV-Vis spectroscopy and photoluminescence spectrometer were carried out to investigate the optical properties of the synthesized materials. XRD and SEM-EDS were used to characterize the structure and surface morphology of the glass samples.

Because of their excellent optical properties, the investigated materials find wide application in optical and photonic devices, such as lasers, fiber optics and LED devices.

Keywords: sol-gel, glasses, luminescent properties

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ICTM-P7

CHARACTERIZATION OF HYDROGEN BLISTERING IN A LOW-CARBON STEEL STORAGE TANK

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Hydrogen damage in the shape of blistering was noticed on the first shell course of a low-carbon steel atmospheric storage tank for petroleum products. The blisters were identified both on the internal and external surfaces of the plates, whereas no blistering was observed on the remaining shell courses. To investigate the influence of the blistering on the structural integrity of the tank shell, samples were taken out from areas of the plates affected with blisters and without any visible blistering. Tensile and bend tests were performed on the samples, as well as metallography and chemical composition analysis.

The investigation showed reduced mechanical properties, with both the ultimate tensile strength (R_m) and elongation (A) being lower than the standard defined values for low-carbon steel grade VSt3ps6. The bend test yielded visible cracks on the specimen during a bending angle $<90^\circ$. The chemical composition analysis showed slight differences in the blistered and non-blistered samples, most notably higher content of S and P on the blistered surface. Comparing the obtained values with the chemical composition of the steel grade VSt3ps6 revealed that while the analyzed samples were mostly within the standard specifications, the S and Si content in the blistered area was slightly above the defined limits, while the Mn content was on the upper limit. These findings are in line with the conditions required for hydrogen damage, as both MnS inclusions and segregation of P along the grain boundaries present hydrogen trapping sites. The metallography revealed crack initiation sites on the edges of the blister, consistent with hydrogen-induced blistering, as well as visible presence of non-metallic inclusions.

The results revealed significant degradation caused by hydrogen, manifested by deterioration of the mechanical properties and alterations in the chemical composition of the steel. The research demonstrated that the combined application of mechanical testing, chemical composition analysis, and metallographic examination constitutes an effective approach for the detection and characterization of hydrogen damage in low-carbon steel atmospheric storage tanks. Furthermore, the findings provide valuable insight into the mechanisms governing hydrogen blister formation and establish a basis for future investigations aimed at determining the root causes of hydrogen-induced blistering.

Keywords: hydrogen blistering, low-carbon steel, mechanical properties



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Organic chemistry, biochemistry and
pharmaceutical chemistry (OBPC)



OBPC-P1

**VALORISATION POTENTIAL OF PROKUPAC GRAPE POMACE:
MINERAL PROFILE AND LC–MS-BASED CHARACTERISATION OF
BIOACTIVE COMPOUNDS IN AQUEOUS EXTRACT**

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Grape pomace represents an important winery by-product with significant potential for valorization as a source of minerals and bioactive compounds. In this study, an aqueous extract of grape pomace obtained from the autochthonous Serbian cultivar Prokupac was analyzed in order to evaluate its mineral profile determinate by ICP-OES method and phytochemical composition determined by LC–MS analysis. The plant material was prepared by drying the grape pomace and seeds in a drying oven at 40°C, followed by grinding in a mill. Subsequently, an aqueous extract of the plant material (1:20, w/v) was obtained at 50°C for 30 minutes using a magnetic stirrer. The extract was then centrifuged and filtered through 0.45 µm filters. The mineral profile, expressed in ppm, showed that phosphorus, calcium and magnesium were the dominant elements, with concentrations of 96.9, 84.2 and 32.66 ppm, respectively. Lower concentrations of silicon, sodium, iron, zinc, copper and manganese were also detected, indicating the presence of nutritionally relevant macro- and microelements. Cadmium, arsenic and lead were not detected, which is favorable from the perspective of potential application in food, nutraceutical or cosmetic products. LC–MS analysis revealed the presence of several bioactive compounds, including tartaric acid, taxifolin, gallic acid hexoside, aromadendrin isomer, dihydrophaseic acid hexoside, *p*-coumaric acid hexoside, quercetin hexoside, syringetin hexoside, isorhamnetin hexoside, trihydroxy-octadecenoic acid and dihydroxy-octadecadienoic acid. The detected compounds belong mainly to organic acids, phenolic acid derivatives, flavonoids and oxidized fatty acid derivatives, which may contribute to the antioxidant and functional potential of the extract.

The obtained results indicate that aqueous extraction can be an effective and environmentally acceptable approach for recovering mineral constituents and polar bioactive compounds from Prokupac grape pomace. This supports the potential use of this by-product as a sustainable raw material for the development of value-added food, nutraceutical or cosmetic formulations within the concept of circular bioeconomy.

Keywords: Prokupac; grape pomace; aqueous extract; minerals; ICP-OES, LC–MS.



OBPC-P2

**INFLUENCE OF DNA EXTRACTION METHODS ON DNA QUALITY,
POLYPHENOL CONTENT AND PCR-HRM PERFORMANCE IN
STACHYS SPECIES**

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Species of the genus *Stachys* (Lamiaceae) are widely distributed medicinal and aromatic plants characterized by considerable morphological diversity and rich phytochemical composition. Molecular identification of *Stachys* species requires high-quality DNA. However, the presence of secondary metabolites, particularly polyphenols, may interfere with DNA isolation and downstream molecular analyses. This study compared three DNA extraction approaches: a cetyltrimethylammonium bromide (CTAB)-based protocol, the Edwards method based on sodium dodecyl sulfate (SDS), and a commercial QIAGEN DNA extraction kit.

Genomic DNA was isolated from dry *Stachys* samples and evaluated in terms of DNA yield, purity, polyphenol content, and suitability for quantitative PCR (qPCR) and PCR-high resolution melting (PCR-HRM) analysis. Species-specific primers targeting the ITS1 region were used for amplification and HRM analysis.

The Edwards protocol yielded the highest DNA concentration (248.3 ± 27 ng/ μ L), followed by the CTAB method (108.5 ± 16 ng/ μ L), while the commercial QIAGEN kit produced substantially lower DNA concentrations (52.5 ± 7 ng/ μ L). DNA purity (A₂₆₀/A₂₈₀) was relatively low for both the Edwards and CTAB methods (1.1) and slightly higher for the commercial kit (1.3). The concentration of co-extracted polyphenols was highest in Edwards extracts (22.6 ± 2.3 mg GAE/L), followed by CTAB extracts (7.1 ± 0.6 mg GAE/L), and lowest in DNA isolated using the commercial QIAGEN kit (4.8 ± 0.2 mg GAE/L).

Despite providing the highest DNA yield, the Edwards extracts exhibited pronounced qPCR inhibition, whereas DNA isolated using the CTAB protocol and the commercial kit showed efficient amplification. Additional purification of Edwards extracts with chloroform/isoamyl alcohol reduced polyphenol content (9.4 ± 0.7 mg GAE/L) and markedly improved qPCR performance, suggesting that co-extracted inhibitors, potentially including residual SDS, affected polymerase activity. PCR-HRM analysis produced comparable melting profiles among successfully amplified samples.

These findings demonstrate that DNA yield alone is not a reliable indicator of DNA suitability for molecular applications. Although the Edwards method enables rapid and efficient DNA recovery, additional purification may be required prior to PCR-based analyses of *Stachys* species.

Keywords: DNA extraction; CTAB; Edwards method; PCR-HRM analysis, *Stachys* species



OBPC-P3

**DETERMINATION OF TOTAL PHENOLIC CONTENT IN
PELARGONIUM GRAVEOLENS L. LEAF EXTRACTS OBTAINED
UNDER DIFFERENT EXTRACTION CONDITIONS USING THE
FOLIN–CIOALTEU ASSAY**

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Pelargonium graveolens L. is a medicinal and aromatic plant known to possess phenolic compounds with significant antioxidant potential. The extraction efficiency of these bioactive compounds depends on several experimental parameters such as the type of extraction, the solvent used for extraction, the characteristics of the plant material and the solvent-solid ratio. The aim of this study was a preliminary assessment of the influence of different extraction conditions on the total phenolic content (TPC) of extracts from *Pelargonium graveolens* L. leaves.

Fresh and dried leaves were extracted using two polar solvents, absolute methanol and ethanol. Three extraction techniques were investigated: maceration, ultrasound-assisted extraction and Soxhlet extraction. The influence of different solid-solvent ratios was analyzed to determine their effect on the extraction efficiency of phenolic compounds. TPC was determined spectrophotometrically using the Folin-Ciocalteu method and expressed as gallic acid equivalents (GAE) based on a calibration curve prepared with gallic acid as a reference standard.

From the previous studies, it is evident that Soxhlet extraction method (using ethanol as a solvent) represents an efficient system to recover a high content of phenolic compounds.³ The largest amount of TPC (4.40 ± 0.06 mgGAE/g dw) was obtained with the Soxhlet extraction using the ethanol as a polar solvent. These results may be attributed to prolonged exposure of the *Pelargonium graveolens* L. leaves to heated solvent and repeated solvent cycling, which can enhance the release of phenolic compounds.

The information obtained will help in optimizing the extraction of phenolic constituents from *Pelargonium graveolens* L. and will help in selecting extraction conditions to obtain extracts with increased phenolic content and antioxidant potential.

Keywords: *Pelargonium graveolens* L., total phenolic content, Folin-Ciocalteu method, maceration, ultrasonic extraction, Soxhlet extraction



OBPC-P4

SELECTIVE MANGANESE ACCUMULATION BY SACCHAROMYCES CEREVISIAE UNDER OLEANDRIN-INDUCED STRESS

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Saccharomyces cerevisiae is a valuable eukaryotic model for elucidating mechanisms of metal transport, accumulation, and homeostasis. In this study, we investigated the cellular response of yeast cells to oleandrin exposure, with particular emphasis on their capacity to accumulate heavy metals. Multi-elemental analysis revealed a selective and significant increase in intracellular Mn^{2+} levels upon oleandrin treatment, while the concentration of other metals (Co^{2+} , Cu^{2+} , Fe^{3+} , Zn^{2+}) remained largely unaffected.

The enhanced accumulation of Mn^{2+} was shown to be dependent on the plasma membrane transporter Smf1, a member of the NRAMP family with high affinity for divalent metal ions². The experiments demonstrated that Mn^{2+} uptake by yeast cells is rapid and dosedependent, occurring within minutes after oleandrin exposure. Importantly, *smf1Δ* mutants failed to accumulate Mn^{2+} , confirming the essential role of this transporter in metal uptake.

Moreover, other mutants with defective manganese homeostasis (e. g., *pmr1Δ*, *ahp1Δ*) exhibited increased Mn^{2+} accumulation and also increased sensitivity to oleandrin, indicating that intracellular metal overload directly contributes to oleandrin cytotoxicity. Conversely, depletion of extracellular Mn^{2+} alleviated the toxic effects of oleandrin, further supporting the link between metal accumulation and oleandrin stress.

These findings demonstrate the yeast capacity to selectively accumulate metal ions under chemical stress and emphasise the key role of membrane transport systems in metal homeostasis, also highlighting the role of yeast as a model for studying biologically-mediated metal uptake, with applications in bioremediation, bioaccumulation, and toxicity assessment.

Keywords: manganese, oleandrin, *Saccharomyces cerevisiae*.

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OBPC-P5

POLYPHENOLIC ANTIOXIDANTS MODULATE CELLULAR METAL ACCUMULATION BY SACCHAROMYCES CEREVISIAE

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The interplay between polyphenolic antioxidants and metal homeostasis is a complex and increasingly relevant topic with significant implications for biotechnology and environmental applications. While polyphenols are widely recognised for their antioxidant and metal-chelating properties, their role in modulating intracellular metal accumulation remains insufficiently explored.

In this study, we used *Saccharomyces cerevisiae* mutants defective in metal transport to investigate how polyphenolic antioxidants influence the cellular accumulation of essential metals. We show that flavonoids such as morin and quercetin¹ modulate Mn²⁺ and Zn²⁺ homeostasis, augmenting cell tolerance and, in certain cases, intracellular metal retention. These findings indicate that polyphenols not only reduce metal toxicity via chelation but also act as buffering agents that regulate bioavailable metal ions, enabling more controlled and physiologically-compatible accumulation without immediate toxicity. Moreover, metal supplementation (especially Zn²⁺) demonstrated that polyphenols can shift the accumulation dynamics from beneficial to toxic, highlighting their potential to modulate metal uptake through antioxidant–metal combinations.

Overall, our results support the idea that polyphenols can facilitate controlled cellular bioaccumulation of metals, with promising applications in bioremediation, metal recovery, and microbial cell factories, while requiring careful optimisation to avoid toxicity.

Keywords: antioxidants, *Saccharomyces cerevisiae*, heavy metals.

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OBPC-P6

**ANTIPLASMODIAL *IN VITRO* ACTIVITY AND MAMMALIAN CELL
CYTOTOXICITY OF PHYTOCANNABINOIDS: ROLE OF REDOX
POTENTIAL OF PHENOXY RADICAL/PHENOL COUPLE**

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Not presented.



OBPC-P7

PCR-HRM DISCRIMINATION OF GLUTEN-CONTAINING AND GLUTEN-FREE CEREALS

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The production and consumption of gluten-free food products have significantly increased due to the global rise in celiac disease and non-celiac gluten sensitivity. Ensuring the safety of these products remains a critical challenge, as accidental cross-contamination can occur during manufacturing, storage, or transport.

While conventional detection relies heavily on immunochemical methods like ELISA, these techniques face limitations when analyzing highly processed food matrices. Molecular DNA-based methods, particularly PCR combined with High-Resolution Melting (PCR-HRM), offer an alternative approach for the detection and discrimination of target cereal species. The aim of this study was to develop and evaluate specific PCR-HRM primers targeting the internal transcribed spacer (ITS) region for the discrimination of gluten-containing cereals from gluten-free cereals. Three primer sets (P1, P2, P3) were designed and experimentally evaluated for their specificity toward gluten-containing cereals, including wheat, barley, and rye, and their ability to discriminate them from gluten-free cereals, including oat, rice, and maize.

The first primer pair (P1) demonstrated insufficient specificity, as amplification was also observed in non-target cereal samples, limiting its ability to reliably discriminate gluten-containing from gluten-free cereals. The second primer pair (P2) improved performance but still exhibited non-specific amplification in oat samples. In contrast, the third primer set (P3) demonstrated high specificity, with clear discrimination between gluten-containing and gluten-free cereal samples. Primer performance was further evaluated by comparing amplification cycle threshold (C_t) values and the shape and characteristics of the amplification and melting curves. The selected primer set produced distinct PCR-HRM profiles: T_m in the range of 87.8 – 89.1 for wheat, barley and rye, T_m in the range of 77.9 – 81.6 for oat, rice and maize.

These results demonstrate that careful primer design and selection within the ITS region can provide a specific PCR-HRM system for the differentiation of gluten-containing and gluten-free cereals. Further optimization and validation using a broader range of reference materials and processed food matrices will be performed to determine the analytical sensitivity, detection limit, and applicability of the developed method.

Keywords: Gluten-containing cereals, PCR-HRM, ITS region, Primer specificity, Food safety



OBPC-P8

SYNTHESIS AND CHOLINESTERASE INHIBITORY EVALUATION OF NOVEL ARYL DERIVATIVES OF 2-(1H-IMIDAZOL-1-YL)ACETIC ACID

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Nitrogen-containing heterocyclic compounds based on the imidazole scaffold are frequently utilized in crop protection and medicinal chemistry due to their exceptional capacity to interact with diverse biological targets.¹ In the field of agrochemicals, compounds disrupting the cholinergic nervous system through the inhibition of acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE) serve as vital tools for pest management and toxicological assessment. Therefore, exploring both enzymes is crucial for determining the efficacy, selectivity, and environmental safety of potential new screening candidates.² In this study, a new series of arylamide derivatives of 2-(1H-imidazol-1-yl)acetic acid was synthesized using a modified Steglich amidation procedure under mild reaction conditions. The synthetic approach involved the use of 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride (EDC × HCl) as the coupling reagent and 4-dimethylaminopyridine (DMAP) as the catalyst. Structural variation was achieved through the incorporation of differently substituted aromatic amines bearing electron-donating and electron-withdrawing groups, with the aim of exploring preliminary structure–activity relationships. The obtained compounds were characterized by melting point determination, ¹H and ¹³C NMR spectroscopy, and mass spectrometry. In addition, the synthesized derivatives were evaluated for their inhibitory activity against AChE and BuChE to assess their potential as cholinesterase inhibitors.

Keywords: 2-(1H-imidazol-1-yl)acetic acid, Steglich amidation, acetylcholinesterase, butyrylcholinesterase, cholinesterase inhibition

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OBPC-P9

**NOVEL ALKYL IMIDAZOLE-4-CARBOXYLIC ACID DERIVATIVES:
SYNTHESIS AND EVALUATION OF CHOLINESTERASE INHIBITON**

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Imidazole derivatives are important heterocyclic pharmacophores in medicinal chemistry, well known for their broad spectrum of biological activities and therapeutic potential.¹ In agricultural applications they target cholinesterases (acetylcholinesterase, AChE and butyrylcholinesterase, BuChE), which are important for the normal function of the nervous system in humans, other vertebrates and insects. Consequently, dual evaluation AChE and BuChE inhibition characterizes the potency, selectivity, and toxicological safety of newly synthesized imidazoles as agrochemicals.²

In this work, a series of novel alkylamide derivatives of 1H-imidazole-4-carboxylic acid were synthesized using a modified Steglich EDC × HCl/DMAP amidation method under mild reaction conditions. Structural modifications included the incorporation of selected aliphatic amines in order to investigate structure–activity relationships. All compounds were characterized by melting point determination, ¹H and ¹³C NMR spectroscopy, and mass spectrometry. To achieve a comprehensive understanding of their cholinesterase inhibition profiles, the synthesized derivatives were screened for dual inhibitory activity against AChE and BuChE.

Keywords: acetylcholinesterase, butyrylcholinesterase, imidazole, 1H-imidazole-4-carboxylic acid

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OBPC-P10

DESIGN OF NOVEL ARYL IMIDAZOLE-4-CARBOXYLIC ACID DERIVATIVES AS POTENTIAL CHOLINESTERASE INHIBITORS

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Imidazole derivatives are well known for their broad spectrum of biological activities and significant applications in medicinal and agrochemical research, including anticancer, antifungal, antibacterial, anti-inflammatory, and neuroprotective effects.¹ In addition to their medicinal importance, acetylcholinesterase (AChE) inhibitors are widely used as active ingredients in insecticidal plant protection products, while butyrylcholinesterase (BuChE) is also known to be inhibited by organophosphate and carbamate pesticides and is frequently used as a biomarker of pesticide exposure. Consequently, the evaluation of both AChE and BuChE inhibition provides valuable insight into the potency, selectivity, and potential safety of newly synthesized compounds in agrochemical research.² In this work, a series of novel arylamide derivatives of 1H-imidazole-4-carboxylic acid was synthesized using a modified Steglich amidation method with EDC × HCl and DMAP under mild reaction conditions. Structural modifications included the incorporation of aniline and *meta*- or *para*-substituted aniline moieties containing electron-donating or electron-withdrawing groups in order to investigate structure–activity relationships. All compounds were characterized by melting point determination, ¹H and ¹³C NMR spectroscopy, and mass spectrometry. The synthesized derivatives evaluated for their inhibitory activity against both AChE and BuChE, in order to obtain a more comprehensive insight into their cholinesterase inhibition profile.

Keywords: acetylcholinesterase, butyrylcholinesterase, imidazole, 1H-imidazole-4-carboxylic acid

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OBPC-P11

**SPECTROPHOTOMETRIC KINETIC STUDY OF *N*-ACETYL CYSTEINE
ADDITION TO 2-FLUOROBENZYLIDENE CURCUMINE ANALOGS IN
DIFFERENT MEDIA**

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Not presented.



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OBPC-P12

**ASSESSMENT OF THIA-MICHAEL REACTION OF MONOCARBONYL
ANALOGS OF CURCUMIN AND *N*-ACETYLCYSTEINE**

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Not presented.



OBPC-P13

**SYNTHESIS, COMPARISON OF SPECTROSCOPIC PROPERTIES AND
IN SILICO ANALYSIS OF SOME ACYCLIC DERIVATIVES OF C5-
CURCUMINOIDS**

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Although curcumin (CUR) has significant beneficial effects and biological activity, its clinical applications are limited due to its poor bioavailability, low absorption, rapid metabolism and low chemical stability. One approach to enhance the bioavailability of CUR is through the structural modification of its molecule. C5-curcuminoids (C5-CUR) that lack a β -diketone moiety in their structure possess greater metabolic stability and bioactivity than CUR, increased stability *in vitro*, and improved pharmacokinetic profile *in vivo*. These compounds have been extensively studied and exhibit various beneficial biological properties.

In this study, six C5-CUR were synthesized and their biological activity was predicted *in silico* using the online platforms SwissADME and Protox-3.0. The synthesis was carried out via Claisen-Schmidt condensation reaction between various aromatic aldehydes and acetone, catalyzed by sodium hydroxide. The synthesized compounds were characterized using melting points and spectroscopic techniques. The indicative spectroscopic characteristics of these cross-conjugated derivatives is the C=O stretching band that is below 1700 cm⁻¹. They all show UV-Vis absorption peak above 300 nm.

The drug-likeness analysis confirmed that most of the synthesized compound fulfilled the criteria of Lipinski's Rule of Five, indicating favorable pharmacokinetic properties and potential oral bioavailability. Furthermore, the *in silico* toxicity assessment revealed a low predicted toxicological risk, suggesting that the synthesized C5-curcuminoid derivatives represent promising candidates for further biological evaluation.

Keywords: C5-curcuminoids, spectroscopic properties, *in silico* analysis.



OBPC-P14

***IN SILICO* PHARMACOKINETIC STUDIES OF SYMMETRICAL
ACYCLIC AND CYCLIC OF C5-CURCUMINOIDS CONTAINING 3-
BROMOBENZYLIDENE AND 3-(TRIFLUOROMETHYL)BENZYLIDENE
MOIETY**

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The process of developing of new drugs is greatly hampered by their inadequate physicochemical, pharmacokinetic, and intrinsic characteristics. In this regard, the selected to were subjected to SwissADME. For the investigated compounds, the BOILED-Egg pharmacokinetic model predicted favorable gastrointestinal absorption, with selected compounds showing potential for blood–brain barrier (BBB) penetration and p-glycoprotein interaction. The physicochemical analysis indicated generally favorable drug-like properties and oral absorption potential. Although the compounds showed interactions with several major CYP450 isoforms, the predicted profiles suggest potential CYP450 inhibition and substantial plasma protein binding, which may contribute to their distribution and overall pharmacokinetic behavior. Overall, these findings support the compounds as promising candidates for further pharmacokinetic and drug-likeness evaluation.

Keywords: C5-curcuminoids, *In silico analysis*, SwisaADME.



OBPC-P15

**COMPUTER-AIDED DESIGN, ADMET PREDICTION,
AND TOXICITY ASSESSMENT OF NOVEL SYNTHETIC FLAVANONES**

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This study presents a two-step *in silico* strategy for the rational design of flavanone derivatives with improved antioxidant activity and favorable pharmacokinetic properties.¹ Experimental vitamin C equivalent antioxidant capacity (VCEAC) data for flavanones were used to develop QSAR models based on ChemSketch descriptors. The models showed excellent statistical performance, with R^2 values exceeding 0.99 and low prediction errors, confirming their suitability for antioxidant activity prediction.² The results indicate that antioxidant activity is influenced by electronic, structural, and physicochemical properties, including polarity, molecular size, and hydroxyl substitution.³

A ChemSketch-based QSAR model was further evaluated of *in silico* design of six new flavanone derivatives. The designed compounds were assessed based on predicted antioxidant activity, Lipinski drug-likeness parameters, and GUSAR toxicity profiles. Increasing hydroxyl substitution significantly enhanced predicted antioxidant capacity, showing a strong linear relationship with VCEAC ($R^2 = 0.9995$).

The most promising derivative was identified based on the combined evaluation of antioxidant potency, predicted safety, and drug-like properties. Overall, the findings show the potential of integrated QSAR-guided *in silico* design for developing new flavanone-based antioxidant candidates.

Keywords: flavanones, QSAR, VCEAC, *in silico* design, descriptors, toxicity.

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OBPC-P16

**ENANTIOSELECTIVE OXIDATION AND CHIRAL
CHROMATOGRAPHIC PROFILING OF SULFOXIDES FOR CHIRAL
BIOANALYSIS**

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Not presented.



OBPC-P17

**COMPARATIVE EVALUATION OF DRYING METHODS IN THE
MANUFACTURING OF GRANULES FOR ORAL SUSPENSION**

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The critical quality attributes of the drug product and the efficiency of the manufacturing process for production of granules for oral suspension, can be affected by the drying process. The impact of three different drying technologies single-pot vacuum, fluid bed, and tray drying on granules produced by wet granulation was evaluated. An immediate-release formulation containing a BCS class IV active pharmaceutical ingredient was prepared, and granules were characterized in terms of particle size distribution, loss of drying, porosity, and flowability, while the finished product was evaluated for assay and related and degradation products.

Single-pot and fluid bed drying improved process efficiency compared to tray drying, while vacuum drying enabled lower product temperature. Loss of drying met the specified acceptance criterion ($\leq 2.0\%$) for all systems, with improved moisture homogeneity under dynamic conditions. Drying technology affected particle size distribution, whereas porosity and flowability remained comparable.¹

Despite differences in granule characteristics, final product quality attributes were consistent across all drying technologies. XRPD and FT-IR analyses indicated that the crystalline form of the active substance remained unchanged, suggesting the absence of polymorphic transformation. Overall, drying technology influences granule properties and process efficiency without significantly affecting critical quality attributes.^{1,2}

Keywords: drying technology; granules for oral suspension; particle size distribution; loss of drying; process efficiency

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OBPC-P18

**CONFIGURATION AND VALIDATION OF METHOD FOR
DETERMINATION OF SULPHATED ASH IN LabX SOFTWARE**

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The determination of sulphated ash is a compendial analytical method, as prescribed in the European Pharmacopoeia, for the quantification of inorganic impurities in pharmaceutical and chemical substances.¹ This study describes the configuration and validation of a sulphated ash calculation method using the LabX laboratory software system.²

The method enables automated data capture and calculation based on predefined variables and formulas, supporting data integrity throughout the data life cycle while ensuring that system-generated results comply with the ALCOA+ principle. Validation was performed independently using Microsoft Excel with experimental datasets from two samples subjected to repeated ignition. The results showed excellent agreement between LabX and Excel calculations, confirming the correctness and reliability of the configured method.

The study highlights the importance of proper configuration, traceability, and independent validation in ensuring compliance with regulatory requirements and improving analytical accuracy.^{3,4,5}

Keywords: Sulphated ash, LabX, software, configuration, validation.

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OBPC-P19

RISK ASSESSMENT FOR REDUCING THE NUMBER OF ONGOING STABILITY STUDIES IN ORDER TO IMPROVE PROCESS EFFICIENCY AND REDUCE CHEMICAL AND PHARMACEUTICAL WASTE

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In the pharmaceutical industry, ongoing stability monitoring of commercial batches is a mandatory requirement that often generates a large volume of samples and analytical tests, many of which provide redundant data for well-established products. This paper explores a quality risk management (QRM) approach, aligned with ICH Q1A (R2) and Q9 guidelines, aimed at streamlining ongoing stability protocols.

The study defines risk-based criteria to support the reduction of the number of batches included in the ongoing stability program, as well as the implementation of reduced testing frequency for products with well-established historical stability data. This strategic optimization improves operational efficiency within the Quality Control (QC) laboratory by reducing sample throughput and shortening analytical lead times. Furthermore, it significantly contributes to sustainability efforts by minimizing the consumption of organic solvents (e.g. HPLC waste) and reducing overall pharmaceutical and chemical waste. The proposed model provides a robust framework that maintains strict GMP compliance while enhancing cost-effectiveness and reducing environmental impact.

Keywords: stability studies, risk assessment, process efficiency, quality control

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OBPC-20

**COMPARATIVE STUDY OF TWO MEDICAL-GRADE HDPE RESINS
(BORMED HE7541PH AND PURELL ACP6541A) FOR
PHARMACEUTICAL PACKAGING APPLICATIONS BORMED™
HE7541PH VS PURELL ACP6541A**

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The comparative evaluation between Bormed HE7541 PH and Purell ACP6541A as medical grade resins is important because both materials are widely used in Pharmaceutical packaging applications where mechanical performance, processability and regulatory compliance are critical. **Bormed™ HE7541-PH** is a bimodal high density polyethylene intended for evaluation for use in Healthcare applications and is typically used in articles produced via injection moulding. Typical applications are (caps, closures, shoulders for tubes, containers for tablets, powder or granules). Exceptional organoleptic properties and outstanding balance of stiffness, toughness and environmental stresscracking resistance make **Purell ACP6541A** appropriate for the production of closures for still mineral and sparkling water, CSD (soft carbonated drinks) and many other types of food and non-food caps and closures (incl. hinge caps) as well as tube shoulders and compression moulding applications. Purell ACP6541A is additionally used in injection moulding applications.

Property	BORMED HE7541PH	PURELL ACP6541A
Polymer type	HDPE	HDPE
Density (g/cm ³)	0,954	0,954
Melt Flow Rate (190°C/2,16kg (g/10min)	4	1,45
Tensile Modulus (1mm/min) (MPa)	1150	1100
Tensile Stress at Yield (50mm/min) (MPa)	26	22
Tensile Strain at Yield (50mm/min) (%)	9	10
Flexural Modulus (MPa)	1250	/
Melting Temperature (DSC) (°C)	129	/
Heat Deflection Temperature 0,45MPa (°C)	71	/
Environmental Stress Crack Resistance (Igepal 10%, F50, h)	40	/
Hardness Shore D	61	55

The objective of this abstract is to evaluate key mechanical and processing properties of two medical-grade HDPE resins BORMED™ HE7541PH and PURELL ACP6541A. The significantly higher MFR (Melt Flow Rate) of Bormed™ HE7541PH indicates lower melt viscosity and easier processability. PURELL ACP6541A with lower MFR, suggests higher molecular weight providing improved mechanical robustness. Similar tensile modulus values indicate comparable stiffness. Differences in hardness and tensile strength reflect variations in material rigidity and flexibility. Both HDPE resins demonstrate suitability for pharmaceutical packaging applications, but significant differences in melt flow rate and mechanical properties indicate that material substitution should be carefully validated based on processing conditions, performance requirements and regulatory compliance.

Keywords: HDPE, Injection moulding applications, Melt Flow Rate, Tensile properties of plastic.



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Analytical and environmental chemistry (AEC)



AEC-O1

**LC-ESI-MS/MS DETERMINATION OF POLYPHENOLS IN
KRATOŠIJA WINE**

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Polyphenols are important compounds in red wine that determine the color, stability, sensory characteristics, astringency and bitterness as well as stabilizing wine during the aging period. This study is focused on the determination of polyphenols, including flavonoids (anthocyanins, pyranoanthocyanins, flavonols and flavan-3-ols) and non-flavonoids (phenolic acids and stilbenes), in red Kratošija wines, applying HPLC-ESI-MS/MS method. The wines were produced using two commercial yeasts for fermentation in order to study the effect of the yeast on the phenolic compounds profile and content. The chromatographic separation of compounds was performed by using a mobile phase consisting of acetonitrile as solvent A and formic acid (pH 2.8) as solvent B, in a gradient mode, as follows: 0-3 min 10% A, 3-10 min 20% A, 10-15 min 25% A, 15-31 min 90% A and 31-50 min 100% A. Wine samples were injected directly into the HPLC system, after filtration through 0.20 µm polyester membrane, using Kinetex C18 column (100 x 2.1 mm, 2.6 µm) for separation. The accuracy and precision of the method were evaluated and the LOD, LOQ and correlation coefficient were determined. The method showed satisfactory characteristics for the analysis of phenolic compounds in red wine. In the wine samples, analytes were identified based on the knowledge of their fragmentation pathway and by comparing the retention times with their reference standards. Quantification was performed by constructing calibration curves for the available standards and for the other compounds, relative amount was calculated based on the peak area calculation from the appropriate ion peak chromatogram. It was found that the content of polyphenolic compounds was significantly influenced by the yeast strain suggesting that the phenolic profile of wine can be modulated through the appropriate selection of yeast for fermentation.

Keywords: Polyphenols, red wine, HPLC-ESI-MS/MS.



AEC-O2

**NATURAL DEEP EUTECTIC SOLVENTS AS SUSTAINABLE
EXTRACTION MEDIA FOR BIOACTIVE COMPOUNDS FROM
MEDICINAL AND ENDEMIC PLANTS OF KOSOVO**

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This study focuses on the extraction and evaluation of bioactive compounds from medicinal and endemic plant species of Kosovo, including *Thymus praecox*, *Urtica dioica*, *Juniperus communis*, *Hypericum perforatum*, *Campanula albanica*, and *Xeranthemum annuum*, using Natural Deep Eutectic Solvents (NADES) as environmentally friendly extraction media. The research aims to investigate the potential of NADES as sustainable alternatives to conventional organic solvents for the recovery of antioxidant-rich extracts. The experimental work includes optimization of extraction conditions, phytochemical characterization of the obtained extracts, and evaluation of their antioxidant potential using standard in vitro assays based on free radical scavenging activity and reducing power. Particular attention is given to the extraction efficiency of phenolic compounds, flavonoids, and other secondary metabolites known for their biological activity.

In addition, the performance of NADES-based extracts is being compared with extracts obtained using conventional solvents in order to assess differences in extraction yield, phytochemical composition, and antioxidant capacity. The study also examines the suitability of NADES for the stabilization and preservation of bioactive compounds during the extraction process.

The expected outcomes will contribute to a better understanding of the applicability of NADES in green extraction technologies and their potential for the development of high-value natural products. The findings may support future applications of medicinal and endemic plant extracts in pharmaceutical, cosmetic, and functional food formulations while promoting sustainable and environmentally responsible extraction approaches.

Keywords: Natural Deep Eutectic Solvents (NADES); green extraction; medicinal and endemic plants; bioactive compounds; phytochemical characterization; antioxidant activity; green chemistry.



AEC-03

EVALUATION OF TOTAL POLYPHENOLIC CONTENT AND ANTIOXIDANT CAPACITY (DPPH, ABTS, AND FRAP) OF EXTRACTS FROM DIFFERENT BEAN VARIETIES

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Beans are an important source of nutrients and bioactive compounds, particularly phenolic compounds, which contribute to their antioxidant properties and potential health benefits. The content of these compounds and their antioxidant potential may vary among different bean varieties, making their comparative evaluation important for nutritional and functional food research. The aim of this study was to comparatively evaluate the total polyphenol content (TPC) and antioxidant activity of bean extracts obtained from different bean varieties. Bean samples were extracted with 70% ethanol using ultrasound-assisted extraction for 30 minutes. The TPC of the extracts was determined using the Folin-Ciocalteu method and expressed as milligrams of gallic acid equivalents per gram of dry weight (mg GAE/g DW). Antioxidant activity was evaluated using three spectrophotometric assays: DPPH radical scavenging activity, ABTS radical cation decolorization assay, and ferric reducing antioxidant power (FRAP)¹. In addition, correlation analysis was performed to investigate the relationship between total polyphenol content and antioxidant activity. The results revealed differences in TPC and antioxidant activity among the investigated bean extracts. A strong positive correlation was observed between TPC and the antioxidant assays, indicating that phenolic compounds contribute substantially to the overall antioxidant potential of the extracts. The findings of this study contribute to a better understanding of the antioxidant characteristics of bean extracts and support their potential application as natural sources of bioactive compounds in functional foods².

Keywords: beans, total polyphenol content, antioxidant activity, DPPH, ABTS, FRAP, Folin-Ciocalteu assay.

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AEC-O4

**TRANSFORMATION PATHWAYS OF PERFLUOROOCTANOIC ACID
UNDER PHOTOCATALYTIC AND BIOELECTROCHEMICAL
CONDITIONS: INSIGHTS FROM TARGET AND NON-TARGET
ANALYSIS**

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Perfluorooctanoic acid (PFOA) is one of the most persistent per- and polyfluoroalkyl substances (PFAS), requiring advanced treatment technologies and reliable analytical approaches to elucidate transformation mechanisms. In this study, photocatalytic degradation using immobilized rGO-doped TiO₂ coatings and long-term bioelectrochemical treatment in sediment microbial fuel cells (MFCs) were comparatively investigated.

Targeted LC-MS/MS analysis revealed progressive chain shortening of PFOA and formation of shorter-chain perfluoroalkyl carboxylic acids in both systems. Photocatalytic treatment produced perfluoroheptanoic acid (PFHpA), perfluorohexanoic acid (PFHxA), perfluoropentanoic acid (PFPeA), accompanied by fluoride release, while high-resolution mass spectrometry confirmed additional intermediates.¹ Ten months of MFC operation resulted in a 94.9 % decrease in extractable PFOA, with PFHpA and PFHxA detected as major products.²

The results demonstrate that both abiotic and bioelectrochemical systems promote stepwise shortening of the fluorinated carbon chain, whereas complete mineralization could not be confirmed. The study highlights the importance of combining targeted and non-target analytical approaches to distinguish apparent removal from actual degradation and improve understanding of PFAS transformation pathways.

Keywords: PFAS, PFOA, LC-MS/MS, high-resolution mass spectrometry, photocatalysis, microbial fuel cells, transformation products

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AEC-05

**BIOMARKERS OF EXPOSURE TO POLYCYCLIC AROMATIC
HYDROCARBONS IN WASTEWATER-BASED EPIDEMIOLOGY**

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Not presented.



AEC-06

**EVALUATION OF DIFFERENT SOLVENTS FOR LIQUID–LIQUID
EXTRACTION OF SELECTED PESTICIDE RESIDUES FROM WATER
SAMPLES**

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The determination of pesticide residues in water requires efficient sample preparation procedures¹ to ensure reliable analytical results. Therefore, the aim of this study was to evaluate the extraction efficiency of different organic solvents for the liquid–liquid extraction (LLE) of selected pesticides from water samples.

Fortified distilled water samples containing 2,4-dichlorophenoxyacetic acid (2,4-D), atrazine, malathion, fenitrothion and parathion were used as model samples. Three concentration levels were investigated for each pesticide, and for each concentration level, four samples ($n = 4$) were prepared. Liquid–liquid extraction was performed using dichloromethane, diethyl ether, petroleum benzine and a mixture of *n*-hexane and acetone (4:1, *V/V*). The extracts were analyzed by reversed-phase high-performance liquid chromatography (RP-HPLC) method and the extraction efficiency was evaluated through recovery values.

Among the investigated solvents, dichloromethane exhibited the highest overall extraction efficiency, providing recoveries between 96.09 % and 106.52 % for all analytes except malathion, for which a lower but still satisfactory recovery of 78.89 % was obtained. Diethyl ether also showed good performance, with recoveries ranging from 90.73 % to 106.99 %, except for malathion (71.95 %). Petroleum benzine proved unsuitable for the extraction of 2,4-D (only 5.24 % recovery), while recoveries for the remaining pesticides ranged from 57.27 % to 83.18 %. The *n*-hexane/acetone mixture (4:1, *V/V*) demonstrated high extraction efficiency for malathion, fenitrothion and parathion (96.59 % – 105.78 %), moderate efficiency for 2,4-D (84.17 %), and lower efficiency for atrazine (74.06 %).

The overall extraction efficiency decreased in the following order: dichloromethane > diethyl ether > *n*-hexane/acetone (4:1, *V/V*) > petroleum benzine. The obtained results indicate that dichloromethane is the most suitable extraction solvent for the investigated pesticides and provide a basis for future application of the proposed procedure to environmental, drinking and irrigation water analysis.

Keywords: extraction efficiency, LLE, pesticide residues, water samples.

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AEC-07

COMPARATIVE EVALUATION OF THREE VALIDATED RP-HPLC METHODS FOR ASSESSING LIQUID–LIQUID EXTRACTION EFFICIENCY OF SELECTED PESTICIDES

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Reliable evaluation of extraction efficiency is essential for the development of analytical procedures for pesticide residue determination in water. This study compares the applicability of three previously validated RP-HPLC methods for assessing the efficiency of liquid–liquid extraction (LLE) of 2,4-dichlorophenoxyacetic acid (2,4-D), atrazine, malathion, fenitrothion and parathion from water samples.

Fortified distilled water samples containing selected pesticides at three concentration levels were subjected to LLE using dichloromethane, diethyl ether, petroleum benzine and a mixture of *n*-hexane and acetone (4:1, V/V). The extracts were analyzed using three validated RP-HPLC methods^{1,2} employing RP-8 columns of different dimensions under optimized isocratic chromatographic conditions.

All three methods provided satisfactory separation of the investigated pesticides, with resolution values for the closest eluting peaks exceeding 1.5. Although the shortest column reduced the analysis time from approximately 10 to 4 min, it maintained chromatographic performance and analytical sensitivity comparable to those of the longer columns. Furthermore, all three methods provided similar recovery values and identical ranking of extraction solvent efficiency, identifying dichloromethane as the most efficient solvent, followed by diethyl ether, *n*-hexane/acetone (4:1, V/V) and petroleum benzine.

The results demonstrate that all three validated RP-HPLC methods are suitable for evaluating LLE efficiency. Their consistent analytical performance confirms the reliability of the proposed approach, while the shortest RP-8 column offers a practical advantage for routine analysis owing to its substantially shorter analysis time.

Keywords: RP-HPLC, LLE, pesticide residues, water analysis.

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AEC-08

COMPARISON OF ICP-AES AND XRF TECHNIQUES FOR THE ANALYSIS OF CHEMICAL ELEMENTS IN MOSS SAMPLES FROM KOSOVO

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The aim of this research was to analyze the concentrations of some chemical elements (Al, Ca, Cu, Fe, K, Mn, P and Zn) in moss samples, using two different analytical techniques (ICP-AES and XRF), to compare their compatibility, correlation and suitability^{1,2}. The mean and median values for some chemical elements (Ca, K and Mn) were higher in the ICP-AES method, compared to XRF, while for the chemical elements (Fe, P and Cu) these values are very close from both analytical techniques. The comparison between ICP-AES and XRF measurements demonstrates generally strong agreement for most elements. Very strong positive correlations were observed for Al ($r=0.885$), Fe ($r=0.899$), Mn ($r=0.837$), P ($r=0.842$) and Zn ($r=0.977$), indicating that both analytical techniques capture similar spatial and concentration trends among moss samples³. The moderate correlations between analytical techniques were for Ca ($r=0.701$) and K ($r=0.680$). The appearance of copper with very weak correlation ($r=0.012$), suggests that the concentrations were close to the limits of analytical detection and are therefore more affected by analytical uncertainty. In general, both analytical methods show good correlation with each other for most chemical elements, as XRF offers comparable trends with the advantage of rapid and non-destructive analysis of samples, while ICP-AES remains preferable when maximum analytical accuracy is required.

Keywords: ICP-AES, XRF, moss, Kosovo, Pearson correlation.

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AEC-O9

VALIDATED ANALYTICAL APPROACH FOR SOIL CARBON MONITORING: MULTI-CROP EVIDENCE FROM CARBON FARMING SYSTEMS

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Reliable and affordable determination of soil organic carbon (SOC) is essential for evaluating carbon-farming practices and developing scalable soil-carbon monitoring systems. This study aimed to validate an effective analytical approach for routine SOC determination and demonstrate its applicability through multi-crop field monitoring under carbon-farming conditions in North Macedonia.

The classical Walkley-Black method and its spectrophotometric modification were evaluated through linearity, precision, accuracy, repeatability, reproducibility, and analysis of reference soil material. The titrimetric method demonstrated excellent linearity over 0.3-3.0% OC ($R^2 = 0.999$), while spectrophotometric determination of Cr^{3+} at 600 nm showed similarly strong linearity ($R^2 = 0.9996$). Validation using reference soil produced OC values of 1.75% by titrimetric WB and 1.78% by spectrophotometric determination, both within the accepted reference interval (1.72-2.14%), demonstrating good analytical agreement and supporting the applicability of the rapid spectrophotometric approach for routine monitoring.

The analytical approach was further applied to track soil-carbon dynamics under carbon-farming (CF) and conventional management systems (CMS) across corn, sunflower, barley, and chickpea. Under CF, soil C increased from 1.20 to 1.89% in corn, 1.19 to 1.42% in sunflower, 1.25 to 1.68% in barley, and 1.18 to 1.57% in chickpea. In contrast, CMS showed consistent depletion, reaching final values of 0.93, 0.76, 0.89, and 0.91%, respectively. Final carbon concentrations under CF were approximately 73.1-103% higher than under corresponding conventional systems.

The combination of analytical validation and field application demonstrates that validated, cost-effective carbon determination can provide sufficient analytical performance for repeated soil monitoring. Such approaches could substantially increase monitoring frequency and spatial coverage while supporting future measurement, reporting and verification (MRV) frameworks for carbon farming.

Keywords: soil organic carbon, method validation, Walkley-Black, spectrophotometry, carbon farming.



AEC-O10

**THE ASSESSMENT OF METAL CONTENT TO CUERCUS PETRAEA
WOOD ASH, PROPERTIES AND THE IMPACT IN AIR QUALITY**

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In most parts of Kosova during winter time, in many living spaces, by choice, woods are used for heating. Apart from warming atmosphere, wood burning affect air quality, inner and outer atmosphere. This is the main reason to this study.

Cuercus Petraea, sessile oak or cornish oak wood ash is chosen as sample of research. Atomic absorption spectrometry is used as method. 20 wood ash samples were collected from home fire places, day after burning.

Measurements detected metals Fe, Zn, Cu, Pb, Cd, Ni, Cr in different concentrations. Cu, Cd, Cr in smaller concentrations. Ranges from 2 – 2, 62 mg/kg for Cu, Cr and Cd were in much lower concentrations, Cr in range from 0.01 – 0.03 mg/kg, while Cd concentrations in range from 0.08 – 0.26 mg/kg. Fe, Zn and Ni concentrations were much higher; from 180.55 – 520 mg/kg for Fe; 35.24- 65.9 mg/kg for Zn and 38.4 – 68.5 mg/kg for Ni, all in dry weight.

Other parameters: LOI (0.1 - 9.5%), pH (10.2 – 10.79), EC (3.18 – 9.61), and total alkalinity (240 – 436.8 mg/L), % DM (81 – 98), % Ash (83 – 98.9) and % OM (0.01 – 0.33) are also different regardless the same type tree wood ash.

Keywords: concentrations, AAS, metals, pollution, toxicity, wood ash



AEC-O11

**UNRAVELLING THE ENERGY–AIR POLLUTION–CLIMATE–HEALTH
NEXUS IN KOSOVO: IMPLICATIONS FOR SUSTAINABLE ENERGY
TRANSITION AND PUBLIC HEALTH**

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Kosovo represents a unique case for investigating the interconnections between energy systems, air pollution, climate-related factors, and public health outcomes due to its high dependence on lignite-based electricity generation, widespread use of solid fuels for household heating, and persistent air quality challenges.

This study aims to examine the complex interactions between energy production and consumption patterns, air pollutant emissions, climate-related conditions, and population health through an integrated nexus approach. Specifically, the research investigates the contribution of electricity generation, household heating, biomass use, and transport to ambient air pollution; assesses the influence of meteorological and climate-related factors on pollution patterns; and evaluates the associations between air pollution exposure and respiratory and cardiovascular health outcomes. The conceptual framework links energy-related emissions of particulate matter (PM_{2.5}), sulfur dioxide (SO₂), nitrogen oxides (NO_x), and carbon dioxide (CO₂) with climate-related factors, including temperature inversions, heat waves, droughts, seasonal variability, and stagnant air conditions, which together influence air quality and human exposure.

Preliminary results indicate substantial seasonal and spatial variations in PM_{2.5} concentrations across Kosovo. In 2022, annual average PM_{2.5} concentrations reached 18.1 µg/m³ in Prishtina, 16.4 µg/m³ in Drenas, 20.4 µg/m³ in Mitrovica, and 20.1 µg/m³ in Obiliq, exceeding the World Health Organization annual guideline value of 5 µg/m³. Winter pollution episodes were particularly pronounced, with monthly average PM_{2.5} concentrations exceeding 30 µg/m³ in several locations and maximum hourly concentrations reaching 167.2 µg/m³ in Obiliq.

The findings are expected to provide evidence on the interconnected nature of energy use, climate variability, air pollution, and health impacts in Kosovo, highlighting the public health co- benefits of sustainable energy transition pathways. The study emphasizes the need for integrated energy–climate–health policies to support decarbonization, improve air quality, strengthen climate resilience, and protect population health.

Keywords: energy transition; air pollution; PM_{2.5}; climate change; public health; lignite; sustainable development; energy–climate–health nexus.

AEC-P1

**NMR PROFILING OF EUROPEAN OAK HONEYDEW HONEYS:
SACCHARIDE DIVERSITY AND GEOGRAPHICAL DIFFERENTIATION**

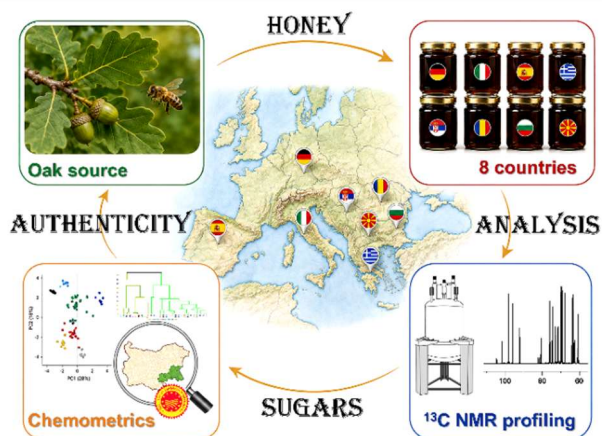
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This study investigates whether the chemical composition of European oak honeydew honeys reflects the geographical origin. Sixty samples from Bulgaria, Germany, Greece, Italy, North Macedonia, Romania, Serbia, and Spain were analyzed using semiquantitative ¹³C nuclear magnetic resonance (NMR) spectroscopy. The protected designation of origin (PDO) Strandzha honey was compared to honey from other regions in Bulgaria. Statistical analysis differentiated country groups through combinations of variables rather than a single marker.



A new pattern that had not previously been observed in European honey was identified: two coordinated saccharide networks showed that minor sugars fluctuate together rather than independently. Conventional honeydew-associated indicators were re-examined and it was found that melezitose is not a necessary component of oak honey. In contrast, 1-kestose was present in all samples. While extended ¹³C NMR profiling may support geographical characterization, independent validation is required before it can be used for authentication purposes.

Keywords: European oak honey, geographical origin, NMR metabolomics

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AEC-P2

RIBOFLAVIN AND THIAMINE CONTENT IN COMMERCIAL ALMOND MILK

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Long valued for its distinct taste, almond beverage has recently emerged as one of the leading plant-based milk alternatives. Vegans and people with lactose intolerance use almond milk as a healthy substitute for dairy products. Almond milk offers fewer calories than cow milk, mainly because it has less protein and fewer carbohydrates when unsweetened. Almond milk is produced by blending water with almond paste or powder. It generally contains water, almonds, salt, added vitamins and minerals, and stabilizers and preservatives. During commercial manufacturing, almond liquid undergoes high-pressure homogenization and pasteurization to enhance product stability and shelf life. However, recent studies indicate that these thermal and mechanical treatments can alter the physical properties of the beverage¹.

Riboflavin (vitamin B2) and thiamine (vitamin B1) are essential water-soluble B-vitamins which are coenzymes in cellular energy metabolism, support normal growth, and maintain a healthy nervous system. The aim of this work was to determine the riboflavin and thiamine content in commercial almond milk.

Commercial almond milk with 1.1% fat and 2% of almonds was from the local market. HPLC analysis with fluorescence detection was conducted on the C18 column using the mobile phase consisting of 30.0% methanol and 70.0% 0.005M NH₄Ac (pH 5.0). The sample was prepared by protein precipitation using perchloric acid. After vortexing and centrifugation, a clear supernatant was obtained. Riboflavin was analyzed directly after filtration through a membrane filter. To analyze thiamine, the supernatant was derivatized with 1% potassium ferricyanide in 15% sodium hydroxide.

The concentration of riboflavin in commercial almond milk was found to be 1.884 ± 0.124 µg/ml (RSD 6.6%), while thiamine content was 1.20 ± 0.13 ng/ml (RSD 10.8%). In the almond milk sample, the concentration of riboflavin was significant, while thiamine was present in very low concentrations. The findings confirm that almond milk may be a good source of riboflavin in a vegan/plant-based diet.

Keywords: riboflavin, thiamine, almond milk

References:

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AEC-P3

**OPTIMIZATION AND APPLICATION OF A METHOD FOR
DETERMINING THE AROMATIC PROFILE OF MACEDONIAN WHITE
WINES USING GAS CHROMATOGRAPHY COUPLED WITH MASS
SPECTROMETRY**

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Wine aroma is one of the most important characteristics of wine quality and is determined by a complex mixture of volatile compounds. In this work, volatile aromatic compounds in Macedonian white wines were investigated using gas chromatography coupled with mass spectrometry (GC-MS) and two capillary columns with different stationary-phase polarities (HP5-MS with 5 % phenyl, and DB-1701 with 14 % - cyanopropyl-phenyl). Liquid-liquid extraction with dichloromethane was selected as the most suitable sample preparation procedure and was subsequently optimized to obtain optimal extraction conditions starting from 10 mL of wine and 1 mL dichloromethane and addition of 1 g of (NH₄)₂SO₄ for pH control and 1-octanol as an internal standard.

The developed method was tested with a standard mixture of alcohols, esters, acids and terpenes and showed good sensitivity and reproducibility, with LOD values between 0.04 and 0.29 µg/mL and LOQ values of 0.41–2.93 µg/mL. Most investigated compounds showed RSD values below 10 %, indicating good analytical precision. The two columns showed complementary chromatographic characteristics. HP-5MS provided better detection of less polar compounds, particularly terpenes and long-chain ethyl esters, while DB-1701 showed improved detection and peak shape for more polar compounds, especially for carboxylic acids.

Application of the method to different Macedonian white wine varieties revealed a complex profile of alcohols, esters, terpenes, and carboxylic acids. Hexan-1-ol, 2-phenylethanol, isoamyl acetate, and several ethyl esters were consistently detected and represented important components of the wine aroma. The results demonstrate that the combined use of HP-5MS and DB-1701 enables more reliable identification and comprehensive characterization of the different classes of volatile aromatic compounds in Macedonian white wines.

Keywords: GC-MS, white wine, volatile compounds, HP-5MS, DB-1701, alcohols, esters, terpenes.



AEC-P4

**COMPARISON OF DEEP EUTECTIC SOLVENTS FOR THE
EXTRACTION OF POLYPHENOLIC COMPOUNDS FROM
SALVIA OFFICINALIS L.**

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Polyphenolic compounds derived from medicinal plants have attracted considerable attention due to their antioxidant, antimicrobial, and pharmacological properties. In recent years, deep eutectic solvents (DESs) have emerged as environmentally friendly alternatives to conventional organic solvents for the extraction of bioactive compounds, supporting the principles of green chemistry.

The extraction of polyphenolic compounds from *Salvia officinalis* L. (sage) was investigated using a series of deep eutectic solvents (DESs) as sustainable alternatives to conventional organic solvents. Nineteen choline chloride-based DES systems were prepared and evaluated, while 70% methanol was used as a reference solvent. Plant samples were subjected to ultrasound-assisted extraction, and the resulting extracts were analyzed by high-performance liquid chromatography coupled with diode-array detection and mass spectrometry (HPLC-DAD-MS).

Quantitative analysis focused on the major classes of bioactive compounds present in sage extracts, including phenolic acids, flavonoids, procyanidins, and terpenoids. The results demonstrated that 70% methanol provided the highest extraction yield of phenolic acids (26.55 mg/g) and terpenoids (1.64 mg/g). However, several DES systems exhibited superior selectivity toward specific classes of compounds. In particular, choline chloride–tartaric acid [ChT(1:2)] achieved the highest flavonoid content (81.31 mg/g), substantially exceeding that obtained with methanol (16.49 mg/g). Choline chloride–urea [ChU(1:2)] and choline chloride–acetic acid [ChA(1:2)] also showed enhanced flavonoid extraction efficiency. The extraction of procyanidins remained relatively low in all investigated systems, although ChA(1:2) and ChU(1:2) provided slightly higher yields than methanol.

The findings indicate that the composition and physicochemical properties of DESs strongly influence their extraction performance and selectivity. While methanol remains highly effective for the extraction of phenolic acids and terpenoids, DES systems based on tartaric acid and urea represent promising green alternatives for the selective extraction of flavonoids. Their low toxicity, biodegradability, and tunable properties support their potential application in sustainable extraction processes for natural bioactive compounds.

Keywords: *Salvia officinalis* L.; deep eutectic solvents (DESs); green extraction; polyphenolic compounds; flavonoids; HPLC-DAD-MS; sustainable solvents



AEC-P5

VOLATILE COMPOUND DIVERSITY IN *SALVIA* SPECIES REVEALED BY HS–GC–MS ANALYSIS

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Plants belonging to the genus *Salvia* are well known for their aromatic properties, which arise from a diverse mixture of volatile compounds. These compounds, primarily monoterpenes, oxygenated monoterpenes, sesquiterpenes, and oxygenated sesquiterpenes, represent the major constituents of *Salvia* essential oils and contribute significantly to their characteristic aroma and biological activity. The present study aimed to characterize and compare the volatile profiles of 33 *Salvia* species using headspace gas chromatography–mass spectrometry (HS–GC–MS).

Volatile compounds were identified by comparison of the obtained mass spectra with the NIST spectral database. A total of 132 volatile compounds were detected, demonstrating the remarkable chemical diversity within the investigated species. Among the identified compounds, 19.7% were classified as monoterpenes, 16.7% as oxygenated monoterpenes, 36.4% as sesquiterpenes, 14.4% as oxygenated sesquiterpenes, while the remaining 12.9% belong to other compound classes, including aldehydes, ketones, alcohols and esters. Sesquiterpenes represented the dominant class in most species, although considerable interspecific variation was observed.

The highest number of volatile constituents (48 compounds) was identified in *Salvia officinalis* Purpurens. Its volatile profile was characterized by the predominance of (–)- β -pinene (11.33%), Z,Z,Z-1,5,9,9-tetramethyl-1,4,7-cycloundecatriene (10.23%), α -thujone (7.53%), camphor (7.04%), cyclofenchene (5.85%), and camphene (5.53%).

Comparison of the volatile profiles revealed substantial qualitative and semi-quantitative differences among the investigated species. The observed variability reflects both species-specific characteristics and the influence of environmental factors, highlighting the importance of volatile compound profiling for understanding the chemical diversity of the genus *Salvia* and supporting its potential applications in pharmaceutical, cosmetic, food, and aromatic plant research.

Keywords: *Salvia*, sesquiterpenes, monoterpenes, essential oils, HS-GC- MS, *Salvia officinalis* Purpurens

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AEC-P6

OPTIMIZATION OF A NOVEL EXTRACTION METHOD FOR THE ISOLATION OF ANTHOCYANINS FROM BERRY FRUIT POMACE

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The valorization of berry pomace (aronia, blueberry, blackberry, raspberry) as a secondary raw material rich in biologically active compounds has become an attractive topic in recent years.¹ Circular economy principles are driving numerous studies aimed at finding ways to transform this industrial by-product into a raw material for various applications.

In this study, the extraction of anthocyanin pigments, present in high concentrations in these samples, was approached using novel solvents prepared on the principles of green chemistry. Several different solvents with the properties of deep eutectic systems (DESs) were prepared, and the most chemically stable ones were selected for the extraction experiments. For the solvent preparation, choline chloride, choline dihydrogen citrate, and sodium acetate were used as hydrogen bond acceptors (HBAs), while glycerol and polyethylene glycol were used as hydrogen bond donors (HBDs). The efficiency of the tested solvents was compared to that of methanol used in the conventional extraction method performed on the same samples.^{2,3} In both cases, anthocyanin quantification was carried out using UV/VIS spectrometry.

Obtained results showed significant improvement of extraction efficiency, compared to the control sample: the highest extraction efficiency was achieved for blackberry samples using the choline chloride/polyethylene glycol solvent system.

The results of this study confirm that the proposed solvent systems are promising extraction tools that can significantly contribute to reducing the food industry's environmental footprint and fostering sustainable resource management.

Keywords: anthocyanins, deep eutectic solvents, UV/VIS spectroscopy, circular economy.

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AEC-P7

**SUSTAINABLE VALORIZATION OF ORANGE PEEL WASTE BY
SUPERCRITICAL CO₂ EXTRACTION: GC–MS AND RAMAN
SPECTROSCOPIC CHARACTERIZATION**

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Not presented.



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AEC-P8

**DETERMINATION OF MICROELEMENTS IN CENTAURIUM
UMBELLATUM GILIB. HERB**

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AEC-P9

**DETERMINATION OF POTENTIALLY TOXIC ESSENTIAL ELEMENTS
IN THE FLOWER OF HYPERICUM PERFORATUM L.**

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Not presented.



AEC-P10

ASSESSMENT OF HEMOLYSIS EFFECTS ON POTASSIUM AND LACTATE DEHYDROGENASE MEASUREMENTS AND VALIDATION OF A HEMOLYSIS INDEX-BASED CORRECTION MODEL

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Hemolysis is a common preanalytical source of interference that affects laboratory test results, particularly potassium (K) and lactate dehydrogenase (LDH) measurements [1,2]. This study investigated the impact of hemolysis on K and LDH results in routine laboratory practice and evaluated the performance of a hemolysis index (HI)-based correction method [3].

A retrospective analysis was performed using anonymized data generated by a Roche Cobas analyzer. Potassium, LDH, sodium (Na), and corresponding HI values were evaluated. Linear regression analysis was used to assess the relationship between hemolysis and analyte concentrations. Regression-based correction models were subsequently applied to estimate and reduce hemolysis-induced analytical bias. The correction models were derived from routine clinical samples and therefore reflect real-world laboratory conditions.

A total of 111 serum samples were included in the study. Higher HI values were significantly associated with increased potassium concentrations ($R^2 = 0.224$, $p < 0.001$) and LDH activity ($R^2 = 0.088$, $p = 0.002$), whereas sodium showed no significant correlation with HI ($R^2 = 0.002$, $p = 0.623$). Potassium concentrations differed significantly across hemolysis categories (ANOVA, $p < 0.001$), increasing from 4.03 mmol/L at HI 0–10 to 4.63 mmol/L at HI >60. LDH activity increased from 279.9 to 402.6 U/L across the same categories. Application of the correction models substantially reduced these differences, with potassium differences decreasing from 0.60 to 0.04 mmol/L and LDH differences from 122.7 to 4.0 U/L.

These findings confirm the significant impact of hemolysis on potassium and LDH measurements and indicate that locally derived HI-based correction models may improve the interpretation of hemolyzed samples in routine laboratory practice.

Keywords: hemolysis, hemolysis index, potassium, LDH, analytical interference, clinical biochemistry, regression analysis, correction model

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AEC-P11

**DEVELOPMENT AND OPTIMIZATION OF AN HPLC-UV-DAD
METHOD FOR SIMULTANEOUS QUANTIFICATION OF CEFIXIME
AND SODIUM BENZOTE IN ORAL SUSPENSION**

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Antibiotics, particularly cephalosporins, represent an important group of drugs with wide application in modern medicine. Cefixime, a semisynthetic third generation cephalosporin, is commonly used in the form of an oral suspension, where sodium benzoate is used as a chemical preservative. Existing internal quantification procedures are based on separate analytical methods employing different chromatographic conditions due to the differing nature of the active substance and the preservative.

The aim of this study is development, optimization and validation of a simple, rapid, sensitive and specific HPLC method for simultaneous determination of cefixime and sodium benzoate in oral suspensions. Several HPLC and UHPLC columns were evaluated, with detailed assessment of their performance in terms of resolution, efficiency, stability and durability. The results demonstrated that the UHPLC columns, although enabling faster analysis, do not provide sufficient robustness when analyzing a complex, sugar-rich matrix, like the oral suspension, which limits their suitability for routine quality control applications. The HPLC Waters XBridge C18 column proved to be the most appropriate, providing stable and reproducible chromatography, satisfactory resolution, appropriate peak shape and short analysis time. Furthermore, forced degradation studies under acidic, basic and oxidative conditions confirmed the specificity and selectivity of the developed method. In addition, the method was validated according to relevant ICH guidelines, including evaluation of linearity, accuracy, precision, specificity, filtration effects, stability, and robustness.^{1, 2}

The obtained results indicate that the proposed HPLC method is suitable for routine use in quality control laboratories as well as for regulatory purposes.

Keywords: cefixime, sodium benzoate, RP-HPLC, C18.

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AEC-P12

**ANALYTICAL VERIFICATION OF A PHARMACOPOEIAL HPLC
METHOD FOR RELATED SUBSTANCES IN METAMIZOLE SODIUM
MONOHYDRATE**

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Metamizole sodium monohydrate is a widely used non-opioid analgesic and antipyretic, for which effective control of related substances is essential to ensure product quality. Although pharmacopoeial HPLC methods are established for this purpose, verification is required to confirm their suitability under routine laboratory conditions.

The aim of this study was to verify a pharmacopoeial HPLC method for the determination of related substances in metamizole sodium monohydrate. Method verification was performed in accordance with Ph. Eur. General Chapter 5.26, with evaluation of precision, specificity, and limit of quantification. Method precision was assessed using six independent samples, yielding a relative standard deviation (RSD) of the main peak area not exceeding 10 %. System precision, determined by six injections of the reference solution, demonstrated $RSD \leq 5\%$. Specificity was confirmed by chromatographic separation of the active substance from relative impurities with no observed interference at the retention time of the principal peak. The limit of quantification complied with the Ph. Eur. reporting threshold, providing a signal-to-noise ratio of approximately 10:1 and acceptable precision ($RSD \leq 10\%$).

The results of the verification study confirm that the pharmacopoeial HPLC method is suitable for its intended use in the routine quality control. This study supports reliable method implementation in quality control environment and contributes to compliance with pharmacopoeial and regulatory requirements for impurity profiling.

Keywords: Metamizole sodium monohydrate, specificity, precision, limit of quantification.

References:

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AEC-P13

**OPTIMIZATION OF AN HPLC METHOD FOR RISPERIDONE
QUANTIFICATION FOR CLEANING VALIDATION PURPOSES**

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Risperidone is a widely used atypical antipsychotic acting primarily through antagonism of dopamine D₂ and serotonin 5-HT₂ receptors, indicated for the treatment of schizophrenia, bipolar disorder, and related psychiatric conditions.¹ Cleaning validation is a critical requirement in pharmaceutical manufacturing to prevent cross-contamination and ensure patient safety. This study focuses on the optimization of the swabbing procedure and HPLC conditions for risperidone cleaning validation.

A key aspect of swab method development is the selection of an appropriate extraction medium that ensures high and reproducible recovery from equipment surfaces. Due to its potency, even trace residues of risperidone may lead to cross-contamination; therefore, sensitive and reliable analytical methods are required for its quantification in cleaning validation studies.

Risperidone is a weak base with pH-dependent solubility and significantly higher solubility under acidic conditions. In this study, recovery efficiency was evaluated using methanol and phosphoric acid-acidified methanol as swabbing media. The acidified medium significantly improved desorption from the swab matrix, achieving recoveries above the 80% acceptance criterion,² whereas unacidified methanol showed lower recovery.

The analysis was performed using a validated HPLC method optimized for cleaning validation. Improved separation of risperidone from adjacent peaks was achieved by increasing the proportion of inorganic mobile phase in combination with acetonitrile, which provided better resolution compared to methanol-based systems.

In conclusion, the use of an acidified extraction medium ensures robust and reproducible recovery, while the optimized HPLC method provides accurate and reliable quantification suitable for routine cleaning validation in risperidone manufacturing.

Keywords: Risperidone, Cleaning validation, Swab-recovery, HPLC method optimization.

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AEC-P14

APPLICATION OF COUNTER-PROPAGATION ARTIFICIAL NEURAL NETWORKS IN PREDICTION OF MARBOFLOXACIN, CLOTRIMAZOLE AND DEXAMETHASONE CONCENTRATIONS IN OTOXOLAN EAR DROPS, SUSPENSION FOR DOGS

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Marbofloxacin is a potent antibiotic synthesized for veterinary use and treatment of advanced infections, which is often dosed in combination with other substances such as clotrimazole and dexamethasone. UV/Vis spectrophotometry, with its widespread and available instrumentation in research and testing laboratories, along with simple sample preparation, offers rapid analysis, which enables its application in quality control of pharmaceutical and veterinary preparations¹.

But simultaneous determination of these three compounds without prior separation can be challenging due to extensive overlapping spectra. In order to minimize the influence of the overlapping spectra on the results, principal components (PCs) extracted from the original UV spectra were used for the training of counter-propagation artificial neural networks (CPANN)². The performances of the CPANN models were examined by (1) changing the number of principal components used for training as well as (2) the relative importance of the selected PCs. Cross-validation was used for control of the generalization performances of the CPANN models.

The developed models have excellent predictive performance for all three compounds with simultaneous quantification of marbofloxacin and clotrimazole with correlation coefficients of 0.99 for calibration and dexamethasone with a correlation coefficient of 0.95.

The results presented in this work demonstrate that analyzing complex mixtures is achievable using inexpensive instrumentation. The proposed UV spectrophotometric method assisted by CPANN represents a cost-effective tool for multicomponent pharmaceutical analysis, which has potential application in routine analysis in quality control laboratories while implementing artificial intelligence in analytical chemistry.

Keywords: Marbofloxacin, clotrimazole, dexamethasone, counter-propagation artificial neural networks, chemometrics, multicomponent analysis.

References:

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AEC-P15

**PERFORMANCE EVALUATION OF DIFFERENT HPLC COLUMNS IN
ANALYSIS OF NICOTINE FROM E-LIQUIDS**

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Not presented.

AEC-P16

INTERNAL STANDARDS USE IN ANALYSES OF CANNABINOIDS

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The dominant analytical techniques are of HPLC group of methods, predominantly with UV-PDA detecting for routine QC analyses in labs. Almost all of them are based on External Method of calculation of results. In this way, all standards and prepared samples are injected in replicates, which eliminate or minimize the errors of equipment malfunction or complexity and skills of analyst for sample preparation. Using of adequate Internal Standards substance may reduce these expenses by improvement of cost-efficiency of analysis by reducing number of injections, without jeopardizing the accuracy of results. We tested many substances and found 2 interesting of them, one more polar eluting as first significant peak on chromatogram, 4-methoxystilbene, and second is pentachlorobenzene, which in RP-C18 elution with acidified acetonitrile elutes near after the CBD molecule. The Response Factors Area/Conc were calculated for both Internal Standards and 5 main cannabinoids, CBDA, CBD, CBN, THC and THCA, for plotting calculation linearity curve. If second IS2-pentachlorobenzene is used, monitoring is at UV=220nm, while if we use IS1-4-methoxystilbene, Response Factor RF at 309-310nm gives slightly different results, which can be neglected if we use high peaks of Internal Standards. These supplantation of Internal Standards might simplified and create cheaper and Green-er methods

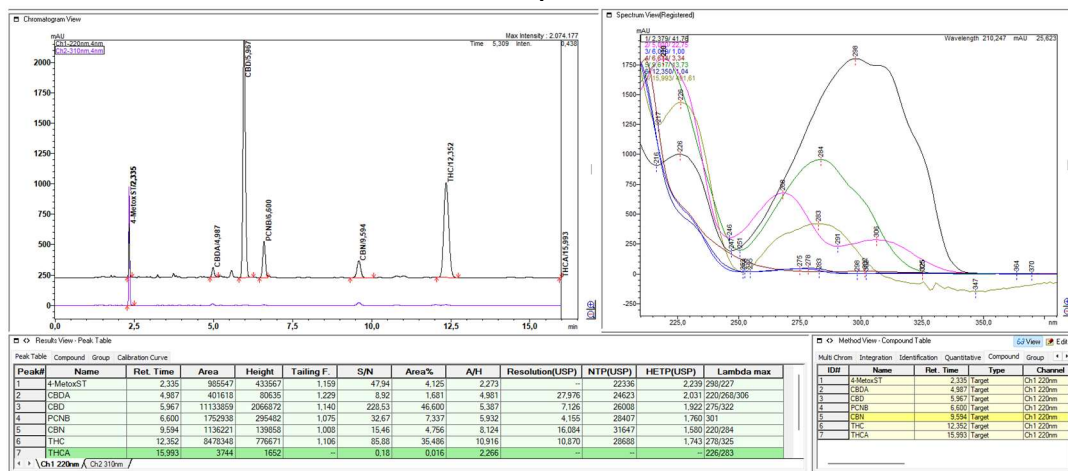


Figure 1. Characteristic Chromatogram of 5 CBDS and two Internal Standards.

Keywords: Cannabinoids, Quantification, HPLC, UV, PDA, Method, Internal Standard

References: ¹ PhEur 2026, ² USP 2026, ³HPLC for Practicing Scientist(II);M.Dong.



AEC-P17

**COMPARATIVE EVALUATION OF LABORATORY-DEVELOPED AND
PHARMACOPOEIAL HPLC METHODS FOR CANNABINOID
QUANTIFICATION**

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Cannabis is a complex phytochemical matrix rich in active cannabinoids such as Δ^9 -tetrahydrocannabinol (Δ^9 -THC) and Cannabidiol (CBD). Their accurate quantification is critical for quality control, patient safety, and regulatory compliance in medical cannabis.

A laboratory developed High Performance Liquid Chromatography – Diode Array Detector (HPLC-DAD) method was compared with the pharmacopoeial reference HPLC method described in Ph. Eur. 11.5. The laboratory method featured an Agilent 1260 Infinity II HPLC system calibrated with a Cayman Chemicals 11-cannabinoid certified reference mixture; by comparison, the pharmacopoeial method incorporated Herbal Reference Standard (HRS) and Cannabidiol Chemical Reference Standard (CRS).

Both methods demonstrated comparable limit of detection (LOD) and limit of quantification (LOQ), confirming equivalent sensitivity. The laboratory developed method achieved a shorter analysis time of 13 minutes with satisfactory precision, whereas the pharmacopoeial method required 35 minutes but ensured superior reproducibility and regulatory reliability.

In summary, the laboratory developed method provides a rapid and efficient solution for routine analysis, while the pharmacopoeial reference method remains indispensable for compliance. Their complementary strengths support robust quality assurance in cannabinoid quantification.

Keywords: Cannabinoid quantification, cannabis flos, HPLC-DAD, pharmacopoeial reference method, quality control, regulatory compliance



AEC-P18

OPTIMIZATION OF AN ANALYTICAL METHOD FOR THE DETERMINATION OF CALCIUM AND MAGNESIUM CONTENT USING INDUCTIVELY COUPLED PLASMA (ICP) TECHNIQUE

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Lifecycle monitoring of analytical procedures described in ICH Q14¹ encompasses all activities from method development and validation to routine application and continual improvement. This study describes the optimization of an ICP analytical method for the determination of calcium and magnesium content during its lifecycle, based on continuous monitoring of result trends, which indicated the need for improved accuracy and robustness.

The optimization focused on critical sample preparation parameters, including filtration, calibration range, and the type of standards used. The results demonstrated that the type of filter (blue dot paper or regenerated cellulose (RC) 0.45 µm) does not significantly affect the accuracy or precision of the results, enabling the use of RC filters for routine analysis.

Extension of the calibration range improved linearity and correlation coefficients. However, discrepancies in assay values were observed when using externally sourced solution standards. This was successfully resolved by introducing in-house solid-state standards prepared from API materials, which ensured accurate recoveries (~100%) and improved agreement with expected results.

The optimized method was verified across multiple batches, placebo-spiked samples, and API combinations, demonstrating acceptable specificity, precision, accuracy, and reproducibility, including inter-analyst consistency.

Overall, this study illustrates how a lifecycle-based approach to method optimization can significantly enhance method performance and reliability. The use of in-house solid secondary standards combined with optimized sample preparation conditions ensures a robust and fit-for-purpose analytical method suitable for routine quality control.

Keywords: ICP, lifecycle management, method optimization, secondary standards, sample preparation, accuracy.

References:

[1] International Council for Harmonisation of Technical Requirements for Pharmaceuticals for Human Use (ICH). *ICH Harmonised Guideline Q14: Analytical Procedure Development*. 2023. Available from: https://database.ich.org/sites/default/files/ICH_Q14_Guideline_2023_1116.pdf



AEC-P19

VOLTAMMETRIC STUDY OF CAFFEINE: MECHANISM AND ANALYTICAL APPLICATION

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Caffeine is a naturally occurring purine alkaloid commonly found in coffee, tea, and cocoa, and is widely recognized for its stimulating effects on the central nervous system. Due to its widespread consumption and biological activity, accurate determination of caffeine content is essential in the food, pharmaceutical, and analytical chemistry industries for quality control, product labeling, and monitoring of commercial formulations [1,2]. Therefore, the development of reliable, sensitive, and cost-effective analytical methods for caffeine determination remains an important area of research.

In this study, a voltammetric method for the quantitative determination of caffeine was developed and validated using a boron-doped diamond (BDD) electrode as the working electrode and 0.1 M acetate buffer solution as the supporting electrolyte. Experimental conditions were optimized in order to enhance the sensitivity and selectivity of the analytical response. The electrochemical behavior of caffeine was investigated using the advantageous properties of BDD electrodes, including a wide potential window, low background current, excellent chemical stability, and high resistance to surface fouling. The developed method demonstrated excellent analytical performance, including good linearity, high sensitivity, satisfactory precision, and reproducibility. Furthermore, the method was successfully applied to the determination of caffeine in real samples, yielding accurate and reproducible results.

Obtained findings confirm that voltammetric techniques combined with boron-doped diamond electrode technology provide an efficient, rapid, and economical alternative to conventional analytical methods for routine caffeine analysis in commercial and pharmaceutical products.

Keywords: caffeine, square-wave voltammetry, electrode, validation, real samples

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AEC-P20

**HUMAN BIOMONITORING OF ORGANOCHLORINE PESTICIDES
AND POLYCHLORINATED BIPHENYLS IN BREAST MILK:
OPTIMIZATION OF ANALYTICAL PROCEDURES AND TRACE-LEVEL
DETERMINATION**

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Human biomonitoring is an important approach for assessing human exposure to environmental contaminants and evaluating potential health risks associated with persistent organic pollutants (POPs). Among the most relevant POPs are organochlorine pesticides (OCPs) and polychlorinated biphenyls (PCBs), which are characterized by their persistence, bioaccumulation potential, and ability to transfer from mother to infant through breastfeeding.

This study aimed to develop and optimize an analytical procedure for the determination of selected OCPs and PCBs in human breast milk and to apply the optimized method to samples collected from breastfeeding mothers in North Macedonia. Due to the complexity and high lipid content of the matrix, different extraction, clean-up, and concentration procedures were systematically evaluated. The optimized method was subsequently validated by assessing key analytical performance parameters, including linearity, precision, recovery, limits of detection and quantification, reproducibility, and matrix effects.

Breast milk samples were collected from 30 breastfeeding mothers residing in different cities across North Macedonia. Prior to participation, informed consent was obtained from all mothers. In addition, participants completed a structured questionnaire designed to collect demographic information, lifestyle characteristics, dietary habits, and potential sources of environmental and pesticide exposure. Samples were stored at $-20\text{ }^{\circ}\text{C}$ until analysis.

The determination of OCPs and PCBs was performed using gas chromatography coupled with an electron capture detector (GC-ECD). Data processing and statistical evaluation are currently ongoing and will provide valuable information on the occurrence of these contaminants in breast milk, potential exposure patterns, and factors influencing their presence in the studied population. The findings are expected to contribute to the limited data available on human exposure to POPs in North Macedonia and support future biomonitoring initiatives.

Keywords: Biomonitoring, POPs, breast milk, optimization, validation.



AEC-P21

ANTIBIOTIC RESIDUES IN AGRICULTURAL SOILS

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Antibiotics are indispensable in the treatment of infectious diseases in humans and are extensively applied in veterinary practice, animal husbandry, and aquaculture worldwide. Their growing discharge into aquatic and terrestrial ecosystems, however, raises concerns about adverse effects on native microbial communities. Within this context, agricultural soils remain an insufficiently explored pathway of environmental contamination, as residues originating from partially unmetabolised pharmaceuticals can be introduced into cropland through manure, digestate, treated sewage sludge, and reclaimed irrigation water.

In the Hungary-Serbia border region, where organic fertilizers and irrigation are important inputs to crop production, the contribution of these practices to antibiotic loads in soils, their potential uptake by plants and the associated risk of antimicrobial resistance (AMR) development has not been systematically assessed. This work, developed in the framework of cross-border cooperation established through the Interreg IPA Hungary-Serbia (HU-SRB) Programme and aligned with the proposed PLANTSAFER project, aims to generate a shared evidence-base on antibiotic occurrence in agricultural soils and to support risk-informed management of the soil-plant continuum within a One Health approach. An advanced LC-HRMS-based workflow designed for multi-residue determination, combining optimized extraction and clean-up of soil samples with targeted and suspect screening analysis, is used for determination of selected antibiotics in soil samples from the Vojvodina Province (Serbia). The results are compared with relevant literature data. This preliminary work provides a basis for the next project phase, which will integrate chemical, microbiological and molecular biological tools to assess antibiotic transfer, AMR risk, pollution reduction options, and biodiversity protection measures in the HU-SRB border area.

Keywords: antibiotic residues, agricultural soil, LC-HRMS, IPA HU-SRB, antimicrobial resistance, One Health.

Acknowledgement: This work is connected to the Interreg VI-A IPA Hungary-Serbia Interreg Programme project proposal PLANTSAFER (HUSRB/25S/12/013). The presented research builds on the knowledge and analytical capacities reinforced at the Faculty of Technology Novi Sad through the Horizon Europe twinning project TwiNSol-CECs (101059867, 2022-2025).



AEC-P22

**MONITORING THE ORGANIC MATTER CONTENT IN
BOTTOM SEDIMENT SEGMENTS ALONG THE STRUGA SHORELINE
OF LAKE OHRID**

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This study examines the organic matter content of bottom sediments collected from five selected locations along the Struga shoreline of Lake Ohrid, with the objective of identifying its potential sources. Organic matter in lake sediments is an important indicator of ecosystem productivity, sedimentary processes, and anthropogenic influence^{1,2}. Each sampling location comprised five sampling points situated at distances of 5, 10, 15, 20, and 25 m from the shoreline. Total organic matter content was determined using the loss-on-ignition (LOI) method through gravimetric analysis, with sediment samples combusted at 600°C for 1 hour. In parallel, sediment moisture content was measured to assess the primary medium associated with organic matter accumulation. The results revealed substantial spatial variability in organic matter content, ranging from 5.54% to 16.17% across all samples. Comparison of moisture and organic matter data suggests that organic matter is predominantly associated with the water-rich fraction of the sediment, while a smaller proportion is adsorbed onto mineral particles. Elevated organic matter concentrations were observed at sites exposed to pronounced anthropogenic influence or to a combination of natural and anthropogenic factors.

The highest values were recorded near the mouth of the Sateska River, indicating that the river is a significant source of organic matter entering Lake Ohrid. This pattern is most likely related to the transport of organic pollutants and other anthropogenic inputs originating from the Sateska River catchment.

Keywords: Organic matter, lake sediment, Lake Ohrid, anthropogenic impact

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AEC-P23

EVALUATING HEAT TRANSFER DISTRIBUTION IN SOIL PROFILES

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The present study investigates heat transfer and heat distribution within soil profiles under controlled non-adiabatic experimental conditions, with particular emphasis on the effects of soil moisture content, porosity, mineral composition, and compaction on soil thermal behavior. The water content in soil plays a dominant role in heat transfer because of its high specific heat capacity and the phase changes that occur during heating. This effect becomes more pronounced with increasing moisture content, particularly at 15%. Experimental measurements were performed on particularly different soil samples collected from two locations, with a constant porosity of 50% and varying moisture contents of 0.2% (dry soil), 10%, and 15%.

To eliminate the influence of heat loss associated with non-adiabatic conditions, a reference water system was employed under identical experimental conditions. Analysis of heat distribution showed that thermal energy was partitioned among the mineral, water, and air phases of the soil. The specific heat capacities of the dominant mineral constituents—quartz, calcite, albite, muscovite, clinocllore, and gypsum—were determined and evaluated in relation to the overall thermal response of the soil. The results demonstrate that heat transfer in soils is controlled by complex interactions among moisture content, water phase transitions, mineralogical composition, soil structure, porosity, and bulk density. A comprehensive understanding of these mechanisms is essential for improving soil temperature modelling, evaluating its thermal potential, and supporting agricultural and environmental applications involving heat transport through the soil systems.

Keywords: soil heat transfer, thermal conductivity, moisture, porosity, mineral composition, phase transitions.



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AEC-P24

**DETERMINATION OF PHYSICO-CHEMICAL PARAMETERS AND
SOME HEAVY METALS IN SURFACE WATERS IN THE MIRUSHA
RIVER**

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Not presented.



AEC-P25

**SILVER NANOPARTICLE THIN FILMS AS POTENTIAL ADSORBENTS
FOR PASSIVE SAMPLING OF HYDROPHOBIC ORGANIC
POLLUTANTS IN WATER**

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The contamination of water resources by organic pollutants represents a significant environmental challenge worldwide. Monitoring these pollutants is essential for assessing water quality and reducing environmental risks. In this work, silver nanoparticle (Ag NP) thin films were investigated as functional substrates for the extraction of organic pollutants from aqueous samples prior to chromatographic analysis.

The Ag NP thin films were deposited on polyester substrates and glass using a cost-effective bottom-up synthesis method¹, yielding nanostructured surfaces with low porosity and a high density of active sites capable of interacting with organic molecules. The structural and morphological properties of the films were characterized by X-ray diffraction (XRD) and atomic force microscopy (AFM), confirming the formation of nanostructured silver domains with a high surface area.

The Ag NP thin films deposited on polyester sheets were tested as potential passive samplers for organochlorine pesticides (OCPs) and polychlorinated biphenyls (PCBs) by spiking them with 22 OCPs and 7 PCBs and then desorbing them by extraction with 5% diethyl ether in hexane. Recoveries from 38 to 115% were obtained for OCPs and between 88 and 120% for PCBs. Further, when exposed to spiked aqueous solutions, they showed a higher affinity for retaining aromatic organochlorine compounds than alicyclic ones. The Ag NP thin films were then exposed to surface water for one month and Ag NP on polyester sheets were found as more stable for further tests compared to ones on glass. During this exposure period, the films captured 10 target OCPs and PCB congeners. In addition, 51 other organic contaminants were detected: 14 PAHs, 13 fragrance-related compounds, 9 industrial and plasticizer-related compounds, 5 pyrethroids, 4 antioxidant additives, and two additional compounds (a UV filter and an OCP). 86% contained an aromatic ring, consistent with the higher retention of aromatic compounds observed in the laboratory affinity tests. The reusability of the Ag NP-coated polyester sheets was also evaluated over three exposure–desorption cycles, with no statistically significant differences among the cycles.

Results suggest that Ag NP thin films on polyester sheets show potential for application as passive samplers for monitoring aromatic organic compounds in water media.

Keywords: Ag NP thin films, functional substrates, AFM, XRD, water pollutants, passive samplers, organochlorine pesticides, polychlorinated biphenyls.



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AEC-P26

**WOOD WASTEWATER PURIFICATION WITH ACTIVATED CARBON
AND PURITY ANALYSIS VIA GC-MS AND CAPILLARY
ELECTROPHORESIS WITH DIRECT UV DETECTION**

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Not presented.



AEC-P27

PROFILING OF THE LIQUID PHASE FROM HYDROTHERMAL CARBONIZATION OF WASTE WOOD: ANTIOXIDANT PROPERTIES AND PAH CONTENT

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Hydrothermal carbonization (HTC) is increasingly recognized as a promising thermochemical process for the valorization of biowaste, enabling the conversion of lignocellulosic residues into a carbon-rich solid hydrochar and an aqueous liquid phase containing various organic compounds. In this study, HTC of waste wood was investigated, with particular emphasis on the chemical composition, antioxidant properties, and safety-related aspects of the resulting liquid phase. The process was performed at temperatures of 200 and 250 °C, liquid-to-solid ratios of 5:1 and 15:1, and residence times ranging from 30 to 165 min, under pressures between 192 and 584 psi.

Four selected liquid-phase samples obtained under different HTC conditions were characterized. The samples were strongly acidic, with pH values ranging from 2.7 to 3.1, and contained total organic carbon (TOC) concentrations between 211 and 550 mg C/L. Phenol concentrations varied from 16.9 to 75.8 mM, while total polyphenol content ranged from 0.352 to 0.588 g GAE/g. Pronounced antioxidant activity was observed in all samples, with DPPH radical scavenging values between 70.8 and 87.0%, indicating the presence of redox-active organic compounds formed during HTC.

To evaluate potential safety concerns, the liquid phase was analyzed for the 16 US EPA priority polycyclic aromatic hydrocarbons (PAHs) using gas chromatography–mass spectrometry (GC–MS) after liquid–liquid extraction.

The presence of PAHs was confirmed, suggesting that aromatic and potentially hazardous compounds may be generated or transferred into the aqueous phase during the HTC process.

Overall, the results indicate that the liquid phase obtained from HTC of waste wood is a chemically active by-product with both valorization potential and environmental relevance. Although its antioxidant activity suggests the presence of potentially valuable organic compounds, its acidic character, organic load, and confirmed PAH content emphasize the need for careful assessment and appropriate treatment before reuse or discharge.

Keywords: PAHs, hydrothermal carbonization, antioxidants properties, waste wood

Acknowledgement: This work is accomplished within the Program of the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (number: 451-03-34/2026-03/ 200134 , and 451-03-33/2026-03/ 200134), and it is also supported by the capacities reinforced through TwiNSol-CECs project (101059867).



AEC-P28

ROLE OF SURFACE MODIFICATION COAL IN ENHANCING THE PROPERTIES OF REVERSE OSMOSIS MEMBRANES

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High-performance reverse osmosis membranes are expected to simultaneously exhibit high solute rejection, elevated water permeability, excellent chemical stability, and strong resistance to compaction, particularly in aqueous separation applications.¹ For several decades, aryl diazonium salts have been employed as reagents to modify a wide range of substrates, including carbons, metals, metal oxides (e.g., ZnO, Al₂O₃), nanomaterials, semiconductors, and polymer surfaces, with aryl moieties.² The resulting grafted layers have diverse applications, including surface modification of membranes.³ The methods used for the modification of material surfaces involve both physical and chemical processes. Membrane surface properties - including charge density, hydrophobicity/hydrophilicity, and fouling resistance - can be tuned by grafting organic molecules. Such modifications enhance separation performance while maintaining mechanical and chemical robustness.

This paper examines the role of aryldiazonium salt concentration in an aqueous acid medium in the chemical grafting of aryl moieties onto the coal surface, which is subsequently used for reverse osmosis (RO) membrane preparation. Coal particles' surfaces were modified by chemical reduction of 4-nitrobenzene diazonium salt of different concentrations at aqueous acid solution (hypophosphoric and sulfuric). The ATR-FTIR spectra show that the nitrophenyl groups were strongly bonded on the surface of coal particles. The introduction of aryl groups onto the coal surface and thus in RO membranes alters their characteristics, as shown by reverse osmosis parameters as well as SEM images. The resulting membranes showed the best results with coal particles modified with a middle concentration of aryldiazonium salt in aqueous medium with hypophosphoric acid. At an acceptable reverse osmosis salt rejection level (94.55 %) of NaCl-H₂O of concentration of 0.4 g/dm³ as a referent system at 1.76 MPa, the flux was 42.6 L/hm².

Keywords: Reverse osmosis, membranes, modification process, aryldiazonium salt.

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AEC-P29

CHROMATOGRAPHIC PERFORMANCE EVALUATION OF A BIO-RENEWABLE SOLVENT USING DESIGN OF EXPERIMENTS

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Green chemistry principles are increasingly applied in chromatographic analysis to reduce the environmental impact associated with high solvent consumption and hazardous waste generation. In this context, the use of bio-renewable solvents (BRS) in chromatographic methods offers a sustainable alternative to conventional organic eluents (ex. acetonitrile, methanol), enabling efficient separations while improving safety and reducing ecological footprint.¹

This study explored the chromatographic behavior of a selected BRS, belonging to the group of lignocellulose derivatives, whose performance remains poorly characterized, using a Central Composite Face (CCF) 2² experimental design. The effects of two critical factors (the percentage (v/v) of BRS in the mobile phase and the column temperature) on mobile phase viscosity, retention factor (k'), and column backpressure were evaluated through a set of 12 experiments generated by the design of experiments (DoE) software MODDE®, employing a 1% (v/v) toluene solution as a retention marker on a LiChrospher® 100 RP-18 column (125 × 4 mm, 5 µm).

The multiple linear regression model demonstrated excellent fit ($R^2 \approx 0.99 - 1.00$) and predictive reliability ($Q^2 \approx 0.997$) for all responses. Within the studied domain, viscosity ranged from 1.37 to 2.17 mPa·s, column pressure from 84.9 to 160.5 bar, and retention factor from 1.5 to 30.4. Optimal chromatographic performance was achieved at an intermediate percentage of BRS (≈ 45 -55%) in the mobile phase and moderate temperature (≈ 38 -42 °C), where viscosity (≈ 1.5 mPa·s), retention factor (≈ 4.7), and pressure (≈ 122 bar) were simultaneously balanced.

These findings provide a rational basis for selecting sustainable chromatographic conditions, supporting safer and more environmentally responsible analytical practices.

Keywords: bio-renewable solvent, green chemistry, liquid chromatography, CCF experimental design

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<https://doi.org/10.1007/s00216-016-9726-2>



AEC-P30

**FROM MONITORING TO PRIORITISATION: THE EnviLife
FRAMEWORK FOR EMERGING CONTAMINANTS**

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The growing presence of contaminants of emerging concern (CECs) in aquatic environments poses a significant challenge for environmental protection and sustainable agriculture. This issue is particularly critical in intensively agricultural regions where surface water is widely used for irrigation, such as the Danube-Tisa-Danube (DTD) hydro-system in Vojvodina, northern Serbia. Despite increasing awareness and regulatory efforts at the European level, significant knowledge gaps remain regarding the occurrence, distribution, and prioritisation of CECs in complex agro-environmental systems.

Within the EnviLife project, a multidisciplinary framework has been developed to detect and prioritise CECs in surface water and arable soil. A central component of this framework is the application of wide-scope high-resolution mass spectrometry (HRMS), integrating suspect screening with target analysis to achieve comprehensive chemical characterisation and reliable quantification of prioritised contaminants in environmental samples.

This analytical approach is further supported by an advanced data processing workflow, a prioritisation strategy, and the development of predictive models based on machine learning and environmental datasets. The resulting data enable the formulation of a region-specific watch list of CECs, supporting the monitoring of prioritised compounds and improving understanding of potential contaminant transfer pathways between water and soil.

The proposed framework supports the design of future monitoring strategies and advances understanding of CEC occurrence in the DTD hydro-system. While developed for a specific hydro-system, the approach and findings are broadly applicable to other agro-environmental systems facing similar contamination pressures.

Keywords: surface water, arable soil, CECs, DTD canal, screening and target analysis.

Acknowledgement - This research is supported by the Science Fund of the Republic of Serbia, #GRANT No. 7335, Sustainable environmental monitoring and prediction of pollutants spread – EnviLife. The analytical capacities used in this work were established and strengthened through the TwiNSol-CECs project, whose long-term impact continues to support HRMS data processing and environmental analysis.



AEC-P31

OPTIMIZATION OF DEEP EUTECTIC SOLVENT-BASED EXTRACTION OF PERSISTENT ORGANIC POLLUTANTS FROM HUMAN HAIR

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Human hair is increasingly used as a non-invasive biomonitoring matrix for persistent organic pollutants (POPs), providing information on long-term exposure to environmental contaminants. Determination of organochlorine pesticides (OCPs) and polychlorinated biphenyls (PCBs) in human hair is important due to their persistence, bioaccumulation potential, and adverse effects on human health. However, efficient extraction and clean-up procedures remain challenging due to the complexity of the hair matrix and the low concentrations of target analytes.

In this study, extraction and clean-up conditions for the determination of OCPs and PCBs in human hair were optimized. Method development and optimization were performed using human hair samples previously exposed to elevated concentrations of pesticides.

Ten conventional organic solvents and mixtures, together with one deep eutectic solvent (DES) were tested. Hexane:dichloromethane (4:1, *V/V*) and DES composed of menthol and levulinic acid (1:1 molar ratio) provided the highest extraction efficiency. To align with the principles of green chemistry, DES was selected for further optimization steps.

Different extraction techniques were subsequently compared, including thermal incubation, mechanical agitation, Soxhlet extraction and reflux extraction. The combination of thermal incubation followed by mechanical agitation resulted in the highest extraction of target analytes. Extraction parameters were optimized using response surface methodology (RSM) based on a Box–Behnken design. The effects of solvent volume (3, 5 and 10 mL), incubation temperature (30, 40 and 50 °C) and incubation time (30, 60, and 90 min), were investigated, followed by an additional mixing step. The optimal extraction conditions were established as 10 mL of DES, incubation at 40 °C for 45 min, followed by 45 min of mechanical agitation. For sample clean-up, nine different solid-phase extraction sorbents were evaluated. Deactivated alumina provided the best overall clean-up performance.

The optimized method enables efficient determination of organochlorine pesticides in human hair while reducing the use of conventional organic solvents, making it a promising approach for future environmental and human biomonitoring studies.

Keywords: organochlorine pesticides, human hair, deep eutectic solvents, biomonitoring

Acknowledgement: The authors gratefully acknowledge the financial support by the Macedonian Ecological Society for the project titled "Assessment of human exposure to persistent organic pollutants in Skopje using human hair biomonitoring".



AEC-P32

COST-EFFECTIVE SILICONE FOAM SAMPLERS FOR MONITORING ORGANIC COMPOUNDS IN AIR

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Air pollution by diverse organic compounds poses environmental and human health concerns, while personal exposure monitoring remains challenging. Conventional air sampling often relies on sorbents such as polyurethane foam (PUF) and synthetic polymers, which may have limitations related to cost, stability, and chemical interferences. Silicone-based materials offer a promising alternative due to their affinity for a broad range of organic compounds.

In this study, silicone (polydimethylsiloxane, PDMS) foam was prepared and evaluated as a low-cost sorbent for active and personal passive air sampling. PDMS foam was prepared from a two-component silicone elastomer system (elastomer/curing agent, 10:1) using sieved NaCl to generate the porous structure followed by curing and salt removal, and characterized by infrared spectroscopy. Extraction with ethyl acetate was optimized using ultrasound-assisted and Soxhlet procedures, yielding recoveries of 70–123% and 69–129%, respectively.

The prepared PDMS foam was successfully applied for active air sampling (4 L/min, 24 h) enabling the detection of 20 organochlorine compounds at concentrations of 0.91–531 pg/m³ air. In addition, to test its suitability as a personal passive air sampler, seven PDMS samplers were worn by participants in Skopje for 9 days and analyzed by GC-ECD and GC-MS following ultrasound-assisted extraction. 14 organochlorine compounds were identified by GC-ECD, including chlorobenzenes (7), HCH isomers (3), other organochlorine pesticides (2), and PCBs (2). 1,3,5-Trichlorobenzene, tetrachlorobenzene isomers, pentachlorobenzene, and PCB 180 were most frequently detected with normalized concentrations from 1.4 to 41.1 ng/g sampler. In addition, 13 of 16 target polycyclic aromatic hydrocarbons (PAHs) were detected, individual amounts ranging from 0.16 to 29.72 ng/g sampler. Fluorene, phenanthrene, chrysene, and benzo[k]fluoranthene showed the highest concentrations, reflecting combustion-related and urban sources, including traffic and tobacco smoke, as well as indoor activities such as cooking. Additionally, a diverse range of 45 other organic compounds were detected, including aliphatic and aromatic hydrocarbons, esters, oxygenated compounds, terpenes, fragrances, phthalates/plasticizers, and UV filters. Overall, these findings demonstrate the potential of PDMS foam for both active and personal passive air sampling of diverse organic compounds.

Keywords: silicone foam, air pollution, air sampling, passive sampler, GC-ECD, GC-MS



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AEC-P33

MONITORING OF THE QUALITY OF AIR IN QUARRY

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Not presented.



AEC-P34

**ASSESSMENT OF AIR POLLUTION USING MOSSES AS
BIOINDICATORS IN SELECTED LOCALITIES ALONG THE
PRISHTINA–MITROVICA AXIS**

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Not presented.



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AEC-P35

**SUSTAINABLE USE OF PESTICIDES FOR THE PURPOSE OF
ENVIRONMENTAL PROTECTION AND EMPLOYEE SAFETY**

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Not presented.



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Physical, structural chemistry, spectroscopy
and electrochemistry (PSSE)



PSSE-O1

**POSSIBILITY OF CONSTRUCTING 2T2D CORRELATION MAPS
FROM IR REFLECTANCE SPECTRA AND 2D CORRELATION MAPS
FROM CONFOCAL RAMAN SPECTRA**

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IR Specular Reflectance (IR-SR) spectroscopy is an external reflectance technique widely used in the investigation of various materials. The specularly reflected light, described by the Fresnel equations, carries the optical, dielectric and vibrational properties of the material, which can be extracted by dispersion or Kramers–Kronig analysis. IR-SR is particularly useful for thin and ultrathin films: up to a thickness of 100 nm the reflectance function can be approximated as a reflectance–absorbance function, so that the absorbance of the film is evaluated from reflectance measurements. The reflectance–absorbance (IR-RA) spectrum, calculated from the ratio-reflectance (IR-RR) spectrum of soda-lime-silicate glass coated with an ultrathin siloxane film, reveals the wavenumber positions and profiles of the film bands, from which the Si–O–Si vibrations can be assigned. To verify these results by an independent method, the construction of two-trace two-dimensional correlation spectroscopy (2T2D-COS) maps from the originally recorded IR-SR spectra was proposed. The resulting maps, particularly the asynchronous maps, show peaks that correspond well to the band maxima observed in the IR-RA spectra of the film. This approach can be used not only for films close to 100 nm, but also for films only a few nanometers thick. The 2T2D-COS maps can also be constructed from IR-RA spectra, in which case they provide information on whether two films have the same structure. Raman spectroscopy of thin films can likewise distinguish bands of the glass substrate from those of the film. However, it remains unclear whether 2T2D-COS can be applied when the intensities of the substrate and film bands vary randomly between measurements and spectral normalization is not possible. To address this, two-dimensional correlation spectroscopy (2D-COS) was applied to a series of confocal Raman spectra recorded from the same silane-modified glass sample at the same laser position. The measurements were made on a thicker part of the film ($\approx 1\ \mu\text{m}$), the perturbation being the depth of the laser focus within the film. In this way, the asynchronous map made it possible to distinguish some of the overlapping bands and assign them either to the glass substrate or to the film.

Keywords: soda-lime-silicate glass; siloxane, IR Specular Reflectance; Raman spectroscopy; Two-trace two-dimensional correlation spectroscopy; Two-dimensional correlation spectroscopy



PSSE-O2

**TWO-DIMENSIONAL CORRELATION ANALYSIS OF FANO
RESONANCE LINE SHAPES: DISCOVERING NEW SPECTROSCOPIC
FINGERPRINTS**

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Fano-type resonance phenomena originate from quantum interference between excitations involving discrete and continuum states, giving rise to characteristic asymmetric spectral response profiles, which are highly sensitive to changes in resonance energy, linewidth, discrete-continuum coupling strength, and the surrounding environment. Such line shapes are ubiquitous in atomic, molecular and condensed-matter systems, particularly in plasmonic nanostructures and nanophotonic materials. Despite the considerable interest in these phenomena, disentangling subtle spectral variations and correlated changes of the Fano parameters remains rather challenging using conventional one-dimensional spectroscopic approaches.

In the present work, we employ several variants of two-dimensional correlation spectroscopy (2DCOS) to investigate the evolution of Fano resonance line shapes under different external perturbations. Dynamic spectra generated through systematic variations of the asymmetry parameter, resonance energy, linewidth and coupling strength are used to construct the generalized synchronous and asynchronous correlation maps. Characteristic cross-peak patterns are identified, enabling discrimination between frequency shifts, linewidth variations and changes in spectral asymmetry, and allowing the construction of a corresponding library of 2DCOS fingerprints. We further establish correlations between the physical mechanisms governing the Fano line-shape evolution and the topology of the corresponding two-dimensional correlation patterns. In addition to the generalized 2DCOS approach, we present a detailed analysis based on autocorrelation moving window two-dimensional correlation spectroscopy (MW-2DCOS) and perturbation-correlation MW-2DCOS (PC-MW-2DCOS) applied to the same datasets.

The simulation results are compared with experimental data for plasmonic semiconductor quantum dots, in which pronounced plasmon – exciton coupling gives rise to distinct Fano-type features in both optical absorption and photoluminescence spectra.

These results establish 2DCOS as a sensitive tool for decoding the dynamics of Fano resonances and for elucidating the mechanisms underlying their spectral evolution, as well as probing e.g. plasmon-exciton interactions in strongly coupled nanoscale systems.

Keywords: Fano resonance, Fano line shapes, plasmonic semiconductor quantum dots, two-dimensional correlation spectroscopy (2DCOS), plasmon-exciton coupling, optical absorption, photoluminescence.

PSSE-03

WHY THE PEAK IS NOT ENOUGH: UNIVARIATE CALIBRATION BEYOND THE BEER–LAMBERT APPROXIMATION

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In spectrophotometric analysis, univariate calibration is often based on the intuitive assumption that the maximum of an absorption band provides the best analytical signal. This practice is closely connected to the Beer–Lambert relation, which suggests a linear dependence of absorbance on concentration and makes the most intense spectral position appear especially attractive because of its high sensitivity. However, peak height alone is not a reliable criterion for optimal calibration.

This lecture examines why the best univariate calibration point is frequently not located at the peak maximum. The discussion is illustrated using UV-Vis spectra of methyl orange and infrared spectra of thermodynamically ideal binary mixtures, including benzene–toluene, benzene–cyclohexane, and benzene–carbon tetrachloride. By comparing calibration performance across spectral positions and relating prediction errors to sensitivity, spectral separation, and curvature of the concentration-dependent response, it becomes clear that band flanks or apparently less prominent regions can outperform the absorbance maximum.

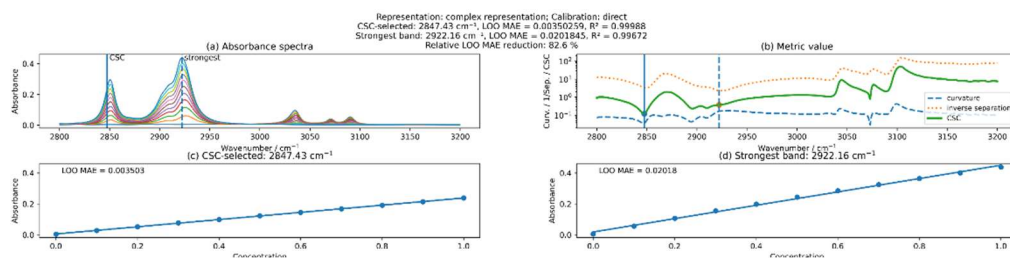


Figure 1. Calibration in the system benzene-cyclohexane.

Keywords: Spectrophotometry, Beer-Lambert Approximation

PSSE-O4

INVESTIGATION OF ELECTROACTIVE *GEOBACTER Sulfurreducens*: INSIGHTS FROM SQUARE-WAVE VOLTAMMETRY AND CYCLIC VOLTAMMETRY

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Understanding electroactive biofilms is essential to advance the development of microbial fuel cells (MFCs), biological wastewater treatment, and to comprehend the bacterial communication pathways. Although decades of research have investigated electroactive bacteria (EAB), particularly *G. sulfurreducens* and *S. oneidensis*, the exact electron transfer mechanisms between EAB and electrodes remain poorly understood.¹

This presentation highlights square-wave voltammetry (SWV) as a powerful, yet often-overlooked technique, to investigate early-stage biofilm formation and elucidate these electron transfer pathways (Fig. 1). Furthermore, these results are contextualized with traditional cyclic voltammetry.² This comparative analysis provides new insights into how biofilms exchange electrons with the electrode interface.

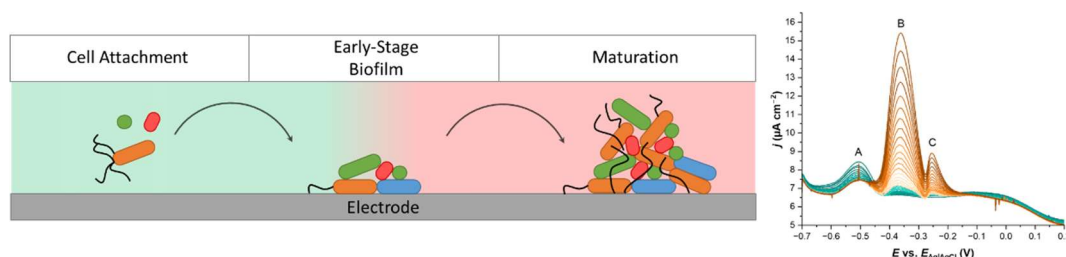


Figure 1. Different biofilm phases (left) and square-wave voltammogram of *G. sulfurreducens* (right) depicting the gradual establishing of redox systems indicated by the peaks A-C.

Keywords: Electroactive Bacteria, Square-Wave Voltammetry, Electron Transfer Mechanism

References:

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PSSE-05

SURFACE INTERACTION OF Ni BASED ELECTROCATALYST WITH HYDROGEN PEROXIDE

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In this study, non-stoichiometric Ni–O thin films were synthesized by magnetron sputtering, enabling precise control over their morphology independently of the chemical composition. X-ray diffraction indicated the presence of crystalline Ni(111) planes, while Raman confirmed amorphous nickel oxide. Samples with the various amount of crystalline Ni were grown. X-ray photoelectron spectroscopy further revealed a mixture of metallic Ni and partially oxidized Ni–O species. Electrochemical analysis demonstrated that the thin films characterized by highly abundant Ni(111) planes exhibit catalytic activity for H₂O₂ detection, with the current density of -1.64×10^{-4} A/cm². To gain deeper insight into the underlying mechanisms, density functional theory calculations were performed, showing that metallic sites on Ni(111) offer stronger interaction for OH groups than amorphous NiO, with average adsorption energies of -3.76 and -1.86 eV, respectively. The simulations also indicated that OH groups from H₂O₂ preferentially dock onto bridge sites of Ni(111). These findings highlight the significant potential of non-stoichiometric Ni–O systems for electrochemical sensing applications and provide valuable understanding of H₂O₂ interactions with oxides.

Keywords: Ni-O; DFT; Electrochemical interactions; Hydrogen peroxide; Sensors

Acknowledgement: The author gratefully acknowledges the financial support provided by the UNIC Alliance for this study and participation in the conference.



PSSE-06

**THERMODYNAMIC FOUNDATIONS OF ACTIVITY COEFFICIENTS OF
ELECTROLYTES IN ELECTROSTATIC THEORIES**

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Activity coefficients provide a measure of the non-ideality introduced by a species in a system. In electrolyte solutions, strong electrostatic interactions often cause ionic activity coefficients to deviate substantially from unity, even at low concentrations. Although the century-old Debye–Hückel theory¹ successfully predicts activity coefficients in dilute solutions, only recently has a thermodynamic decomposition of these contributions been achieved².

Within the Debye–Hückel framework, it can be demonstrated that the energetic contributions of induced repulsive electrostatic interactions and entropy are each exactly half the magnitude—but opposite in sign—to that of the direct attractive electrostatic interaction between the central ion and its ionic atmosphere. This decomposition not only deepens our understanding of how ions influence their surroundings but also establishes a direct link between activity coefficients and the microscopic behaviour of individual ions.

This work explores potential extensions of the approach to other electrostatic theories, including the non-linear Poisson–Boltzmann equation, the Hypernetted Chain (HNC) equation, and the incorporation of non-Coulombic terms. Furthermore, its applicability to polyelectrolyte solutions—of both spherical and cylindrical symmetry—is considered. Finally, the approach enables the validation of such thermodynamic dissections, ensuring consistency across theoretical frameworks.

Keywords: electrolyte solutions, entropy, attractive interactions, induced repulsive interactions.

References:

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PSSE-P1

**ELECTRODEPOSITION OF METALS FROM LUNAR REGOLITH
DISSOLVED IN RELINE**

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To enable a sustainable human presence on the Moon, it is essential to use local resources safely and economically to access strategic metals¹. This study evaluates the potential of deep eutectic solvents (DESs) for dissolving and electrochemically extracting metals from lunar regolith simulant. Lunar regolith simulant, representing Lunar Mare Soil (LMS-1), is an abundant and easily accessible material on the Moon². LMS-1 was dissolved in freshly prepared reline (ChCl:Urea) by mechanical stirring at 250 rpm for 10 h at 70 °C under an argon atmosphere. The solubility of the oxides was determined using inductively coupled plasma–optical emission spectrometry (ICP–OES). In reline, Al₂O₃ showed a solubility of 0.4 wt%, SiO₂ reached 0.98 wt%, Cr₂O₃ exhibited the highest solubility at 14.6 wt%, followed by FeO_t at 2.27 wt% and MgO at 4.1 wt%. Electrochemical measurements and electrolysis experiments were carried out in the supernatant solution using a three-electrode system: gold (Au) as the working electrode, platinum (Pt) as the counter electrode, and a platinum wire (Pt, 2 mm diameter) as the quasi-reference electrode. The equilibrium potentials of the metals were measured and correlated with the order in which the metals should be deposited on the cathode. Electrochemical investigations using cyclic voltammetry and square-wave voltammetry evaluated a highly complex system involving multiple multivalent redox processes. Selective metal recovery was subsequently achieved by potentiostatic electrolysis by adjusting the electrode potential. At more positive deposition overpotentials, the deposit was composed mainly of Si, whereas Al, Cr, and Fe, along with Si, were electrodeposited at more negative potentials, demonstrating controlled potential-dependent metal separation. These results demonstrate the possibility of controlled and selective metal deposition directly from DES electrolytes.

Keywords: Choline Chloride-Urea, Silicon, Lunar Mare Soil, Electrodeposition

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PSSE-P2

DEPOSITION OF DYSPROSIUM FROM ETHALINE DEEP EUTECTIC SOLVENT

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Rare earth elements (REEs), particularly dysprosium (Dy), are critical for development of future clean energy technologies. However, their recovery from end-of-life (EOL) NdFeB magnets faces significant challenges and has not been widely implemented at the industrial scale. Improving resource efficiency requires the development of recycling and recovery methods for REEs from EOL waste using cost-effective and environmentally friendly technologies. Deep eutectic solvents (DESSs) present a promising alternative due to their low cost, simple preparation, low toxicity, and wide electrochemical window¹, compared with conventional high-temperature molten salt electrolytes commonly used for electrolysis.

In this study, the electrochemical reduction and deposition of Dy(III) were investigated for the first time, in a choline chloride and ethylene glycol (1:2, ChCl:EG) deep eutectic solvent (Ethaline) at 70 °C using a gold working electrode. Cyclic voltammetry (CV) and square wave voltammetry (SWV) in 0.1 M DyCl₃–Ethaline electrolyte revealed a single-step, irreversible three-electron transfer process for the reduction of Dy(III) to Dy(0). Potentiostatic deposition at –0.800 V vs. Ag for 4 h produced deposits whose morphology, elemental composition, and surface chemical states were characterized by SEM, EDS, and XPS. The combined analyses confirmed the formation of metallic dysprosium. These results demonstrate the potential of Ethaline as an environmentally friendly medium for the low-temperature electrodeposition of rare earth metals. This approach offers a sustainable pathway for recovering critical materials from EOL and contributes to the development of greener recycling technologies.

Keywords: Choline Chloride-Ethylene Glycol, Dysprosium, Rare earth elements, Deposition

References:

[1] Cvetković, V.S.; Petrović, N.M.; Nikolić, N.D.; Jovićević, J.N.; Influence of Cu(II) Ion Concentration on Copper Electrodeposition from Deep Eutectic Solvent on Inert Substrate, *Metals*, 2025, **15**, 716. <https://doi.org/10.3390/met15070716>.

Acknowledgement: This research was supported by the Science Fund of the Republic of Serbia, #Grant No. 270, *Applying advanced product intellectual properties and industrialization workflows to innovative fundamental research ideas in the area of rare earth electrochemical recovery*– REMEDIS. V.S.C. and N.M.P. acknowledge the financial support received from the Ministry of Science, Technological Development and Innovation of the RS (Contract No: 451-03-33/2026-03/200026).



PSSE-P3

TERNARY THIN FILM CATALYST OBTAINED BY GALVANIC DISPLACEMENT METHOD FOR FORMIC ACID ELECTROOXIDATION

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Pollution from fossil fuels resulting from industrialization, urbanization and technological progress greatly affects the environment and human health. Thus, the main challenge confronting both the scientific community and humanity is to reduce reliance on fossil fuels by shifting energy production and consumption to renewable energy sources. The development of catalysts for the electrooxidation of small organic molecules, such as formic acid, requires an optimal balance between cost and catalytic activity and stability. Platinum (Pt) remains among the most effective choices for formic acid electrooxidation (FAO), despite its high cost, limited availability, and susceptibility to carbon monoxide poisoning. Catalysts incorporating multiple active metals can significantly enhance performance while reducing the use of Pt.

In this study, platinum-based catalysts were produced using a galvanic displacement method, in which platinum and iridium (Ir) replace nickel. The thin film PtIr@Ni catalyst was obtained via a two-step spontaneous galvanic displacement process. Following synthesis, the catalyst underwent thermal treatment to further improve activity and stability. The activity of the catalysts was tested in the formic acid electrooxidation reaction, while the influence of thermal treatment on the surface morphology was monitored using atomic force microscopy (AFM).

Catalysts obtained using this approach, in addition to being very active and stable, contain extremely small amounts of precious metal, thereby lowering the overall cost and bringing fuel cell technology closer to full commercialization.

Keywords: Galvanic displacement, formic acid, electrooxidation

Acknowledgment

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PSSE-P4

**ELECTROCHEMICAL SODIUM STORAGE IN HARD CARBONS
DERIVED FROM INDUSTRIAL LIGNIN WASTE**

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Hard carbons derived from renewable biomass are promising anode materials for sodium-ion batteries due to their low cost, sustainability, and favorable electrochemical properties. In recent years, in line with the increasingly widespread circular economy model, household biowaste has been used as raw material for the preparing of hard carbon [1].

In this work, we demonstrate industrial waste with high lignin content as precursors for the synthesis of hard carbons. Kraft lignin (from pulp and paper industry) and technical hydrolysis lignin (from filamentous yeast production) were pyrolysed on two temperature steps - at 800 and 1300 °C. The obtained materials were characterized by X-ray diffraction (XRD), differential thermal analysis (DTA-TG) and electrochemical techniques. The electrochemical performance of the lignin-derived hard carbons was evaluated in sodium half-cells using galvanostatic charge–discharge cycling in two mode: “constant current” and “constant current – constant voltage”, cyclic voltammetry, first sodiation discharge, first irreversible capacity, cycling stability. The results show reversible sodium storage, good cycling stability, and the influence of lignin precursor type on the structural and electrochemical properties of the materials. The observed differences are associated with variations in carbon disorder and pore structure. The study highlights the potential of industrial lignin waste as sustainable precursors for hard carbon anodes in next-generation sodium-ion batteries.

Keywords: kraft lignin, technical hydrolysis lignin, cycling voltammetry, sodium-ion batteries

References:

[1] S. Harizanova, I. Uzunov, L. Aleksandrov, M. Shipochka, I. Spassova and M. Kalapsazova, *Materials*, 2024, 17, 1016.

Acknowledgment: The authors thank for the financial support of the project BionN (KP-06-H-69/7 from 15.12.2022).



PSSE-P5

DECIPHERING SODIUM-ION INSERTION MECHANISM INTO HARD CARBON BY *EX-SITU* EPR SPECTROSCOPY

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Since the hard carbons (HCs) has emerged as promising negative electrode materials for sodium-ion batteries, numerous research has been done on the factors impacting their electrochemical performance. Nevertheless, one of the most debatable question remains the sodium-ion insertion mechanism. Recently, we report electron paramagnetic resonance (EPR) spectroscopy as a comprehensive method to monitor the interaction of sodium into carbons derived from spent coffee grounds and used as electrodes in sodium-ion cells [1].

Herein, we applied the ex-situ EPR spectroscopy to monitor the sodium-ion insertion into hard carbons derived from lignin precursors. As precursors industrial biowaste was selected, i.e. kraft lignin and technical hydrolysis lignin. The HCs were prepared by pyrolysis at high temperatures (800 and 1300 °C) and under a constant Ar-flow. Depending on the biomass origin and synthesis temperature, the HCs show clearly distinguishable texture. The electrochemical insertion of sodium into hard carbons were carried out in model Na-cells consisting of sodium metal as counter electrode and in presents of carbonate-based sodium electrolyte (1M NaPF₆:PC). At selected potential stages during the first electrochemical sodiation, the cells were stopped and *ex-situ* EPR spectroscopy was employed. The EPR analysis reveals the correlations between textural features - sodium intercalation - sodium cluster formation - storage performance. This insight into sodium storage mechanism can serve as a guiding point in the design of more efficient carbon electrode materials.

Keywords: hard carbon, EPR spectroscopy, sodium-ion batteries

References:

[1] R. Kukeva, M. Kalapsazova, S. Harizanova, I. Uzunov, P. Markov, I. Spassova, and R. Stoyanova, ACS Appl. Energy Mater., 2024, 7, 9543–9550.

Acknowledgment: The authors thank for the financial support of the project BionN (КП-06-H-69/7 from 15.12.2022).



PSSE-P6

**SODIUM ION MOBILITY IN CARBON DECORATED
Na₄Fe₃(PO₄)₂P₂O₇ ELECTRODE MATERIAL: COMPARATIVE STUDY**

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Sodium-ion batteries (SIBs) offer an efficient energy storage solution for large-scale applications. Na₄Fe₃(PO₄)₂P₂O₇ (NFPP) is recognized as a promising candidate for electrode material in SIBs: it is able to intercalate reversibly up to 3 moles of Na ions. The main disadvantage of NFPP is its very low electronic conductivity, which hinders the Na⁺ mobility. To increase NFPP conductivity, a conventional strategy involves its coating with various carbonaceous materials in an amount of about 10-15 wt. %. However, the presence of a large amount of electrochemically inactive carbonaceous additives in the electrode composition is a major contributor to the lower overall energy density of the battery cells, which is one of the most important characteristics for practical application.

To overcome the reduced energy density, the purpose of the present contribution is to decorate NFPP with carbon additives with a minimal amount of 1 wt. %: carbon black (CB) and reduced graphene oxide (rGO). The composites NFPP/CB and NFPP/rGO have been prepared by a dry-coating method. The galvanostatic/potentiostatic tests have been performed at 20 and 40 °C in Na half-cells. Electrochemical performance has been evaluated in terms of capacity and cycling stability, while the origin of the kinetic response is studied by electrochemical impedance spectroscopy (EIS). The contributions of the Faradaic and capacitive reactions in NFPP/CB and NFPP/rGO have been compared. The effect of the carbon additive on the Na-ion diffusion has been studied by three electrochemical methods: EIS, cyclic voltammetry (CV) and galvanostatic intermittent titration technique (GITT). The difference in the electrochemical behaviour of NFPP/CB and NFPP/rGO has been discussed based on the data for the electrolyte resistance (R_e), electrolyte/electrode interfacial resistance (R_{SEI}), and charge-transfer resistance (R_{ct}). The results show a clear distinction in the role of the two types of carbon additives.

Keywords: Sodium-ion Batteries, Electrochemical Techniques, Sodium Diffusion Kinetics

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PSSE-P7

EFFECT OF CARBON ADDITIVES FOR ELECTROCHEMICAL PERFORMANCE OF MIXED POLYANION-TYPE ELECTRODE MATERIAL $\text{NaFeVPO}_4(\text{SO}_4)_2$ FOR SODIUM-ION BATTERIES

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The rising demand for energy makes the development of new high-performance energy storage systems a major concern. Sodium-ion battery technology is one of the best alternative to the lithium analogue due to the low cost and abundance of sodium which are critical issues for large-scale application. One of the challenges facing SIBs is the exploration of new cheap electrode materials with efficient electrochemical performances suitable for practical applications. This can be achieved through design of electrode materials that allow compositional diversity in combination with both cationic and anionic substitutions. Polyanionic electrode materials with NASICON type of structure fulfill the above requirements to a great extent.

The present work is focused on the electrochemical performance of a multi-electron material sodium-iron-vanadium-phosphate-sulfate (NFVPS) that combines two abundant transition metals having multiple oxidation states with two anionic groups in a stable NASICON structure. In addition, the sulfate substitution for phosphate is known to enhance the potential of the redox reactions thus increasing the power density. In order to enhance the capacity and long-term cycling stability, NFVPS was decorated with two carbon additives, reduce graphene oxide (rGO) and carbon black (CB), using simple ball-milling treatment. The electrochemical tests of the two composites were performed in sodium half-cells in voltammetric and galvanostatic modes at 20 and 40 °C. The cycling voltammograms reveal reversible cathodic and anodic peaks ascribable to iron and vanadium redox couples. The CV-curve profile for NFVPS/rGO evidences for simultaneous occurrence of capacitive and Faradaic electrochemical reactions, while Faradaic reactions are predominant for the NFVPS/CB composite. The contribution of Faradaic and capacitive reactions in the two composites were estimated. The cycling stability (C/2 rate) and rate capability tests show that NFVPS/rGO outperforms NFVPS/CB at 20 and 40 °C. The storage performance of NFVPS/rGO is among the best performing iron-vanadium phosphates.

Keywords: Sodium-ion batteries, Electrochemical Performance, Multi-electron Reactions

Acknowledgement:

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PSSE-P8

PERI-ANNULATED DISELENIDES AS A FRAMEWORK FOR HIGH-RATE ORGANIC Li/Na ELECTRODES

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The utilisation of organic electrode materials (OEMs) as versatile redox-active hosts for lithium- and sodium-ion batteries is a recent development. The popularity of these materials is driven by their tunability, sustainability, and capacity to store both cations and anions within one framework. The structural flexibility inherent to these substances renders them far less sensitive to the ionic radius of the charge carrier in comparison to conventional inorganic intercalation hosts. This quality positions them as a particularly attractive proposition for use in sodium-ion batteries, where the larger size of Na⁺ frequently limits both diffusion and structural stability.

Here, we investigate the mechanism of bipolar redox reactions in naphthalimide (NI) derivatives when used as cathodes in lithium and sodium half-cells with ionic liquid electrolytes. To improve the low electronic conductivity, NI was composited with rGO.

Electrochemical tests were conducted in potentiostatic and galvanostatic modes within a range of potential windows spanning between 1.0-4.6 V. The results of the CV experiments demonstrate the bipolar nature of the studied NIs. The objective of the cyclic stability experiments is to ascertain the influence of the incorporated groups at the imide nitrogen and the halogen substituent in the naphthalimide core. The results demonstrate that the specific capacity of lithium cells stabilises after the 20th cycle, whereas that of sodium cells stabilises after the 5th cycle, irrespective of the halogen substituent. Furthermore, long-term cycling tests were conducted under conditions of high current loads. The investigation revealed that the specific capacity of the sodium electrolyte at a current load of 500 mA/g decreased marginally from 45 mAh/g to 35 mAh/g. This finding suggests that the cathode material exhibited consistent high-rate performance.

Keywords: Organic electrode materials; Naphthalimide derivatives; LIB; SIB; Bipolar redox reactions.

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PSSE-P9

COMPOSITE OF ZnO WITH REDUCED GRAPHENE OXIDE AS ANODE FOR SODIUM-ION BATTERIES

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Sodium-ion batteries are a promising alternative to lithium-ion batteries. They use sodium, which is less expensive than lithium. However, developing high-capacity, stable anode materials is challenging. Zinc oxide (ZnO) has a wurtzite structure and a high theoretical capacity, but it exhibits poor conductivity during charge/discharge cycles and undergoes fast degradation. However, ZnO nanoparticles functionalized with reduced graphene oxide (rGO) are promising anodes for sodium-ion batteries¹. The aim of our study is to investigate the role of rGO in improving the electrochemical parameters of ZnO and enhancing its performance as an anode in sodium-ion cells.

The electrochemical performance of ZnO/rGO composite electrodes was examined using sodium half cells with a standard electrolyte of 1 M NaPF₆ in PC. Cycling voltammetry was recorded at different speeds ranging from 1 mV/s to 0.1 mV/s to determine redox reactions. The results show that the rGO/ZnO composite outperforms the individual ZnO component in terms of cycling stability and rate capability. Thus, our study emphasizes the importance of the synergistic effect between rGO and ZnO in enhancing the structural integrity and charge-transport kinetics of anode materials for sodium-ion batteries.

Keywords: ZnO, rGO, anodes for sodium-ion battery

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PSSE-P10

RIETVELD STRUCTURAL ANALYSIS AND ELECTROCATALYTIC ACTIVITY OF $\text{GdMn}_{0.5}\text{M}_{0.5}\text{O}_3$ ($\text{M} = \text{Cr, Fe, Co, Ni, Cu}$) DOUBLE PEROVSKITES TOWARD HYDROXIDE OXIDATION AND HYDROGEN EVOLUTION REACTIONS

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$\text{GdMn}_{0.5}\text{M}_{0.5}\text{O}_3$ ($\text{M} = \text{Cr, Fe, Co}$) double perovskites were synthesized via a glycine-assisted solution combustion method. Phase purity and crystal structure were confirmed by powder X-ray diffraction, while Rietveld refinement established the formation of single-phase orthorhombic structures within the *Pnma* space group, and $Z = 4$. Structural analysis revealed significant octahedral distortions, quantified through crystallochemical parameters including the global instability index.

Far-infrared spectroscopy (FIR) supported the structural results by showing characteristic metal–oxygen vibrational modes and systematic band shifts associated with lattice distortion. Scanning electron microscopy (SEM) revealed a porous combustion-derived morphology, while successive annealing treatments enhanced grain growth and microstructural homogeneity. Energy-dispersive X-ray spectroscopy (EDX) confirmed uniform elemental distribution close to the nominal composition.

Electrocatalytic performance was evaluated by cyclic voltammetry using perovskite modified paraffin impregnated graphite (PIGE) electrodes. The investigated materials exhibited composition-dependent activity toward hydroxide oxidation and hydrogen evolution reactions, with the Co-substituted sample showing the highest catalytic efficiency and good electrochemical stability.

Keywords: Perovskites, Solution combustion synthesis; Rietveld refinement; FIR, SEM/EDX, cyclic voltammetry



PSSE-P11

**PLASMA CHARACTERIZATION AND MATRIX EFFECTS IN
HYDROPHILIC CHIA SEEDS STUDIED BY TEA CO₂ LASER-INDUCED
BREAKDOWN SPECTROSCOPY**

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Laser-induced breakdown spectroscopy (LIBS) was employed to investigate plasma characteristics and matrix-induced analytical effects in hydrophilic chia (*Salvia hispanica* L.) seeds. Owing to their gel-forming polysaccharide matrix, chia seeds represent a structurally complex material that can significantly influence plasma formation and emission stability. Pressed pellet samples were analyzed under optimized TEA CO₂ laser conditions, while elemental concentrations were validated by inductively coupled plasma–optical emission spectrometry (ICP–OES). Quantitative calibration was performed for Ca, Fe, Zn, and Mg using analyte-to-internal standard intensity ratios, yielding high linearity with correlation coefficients (R^2) of 0.989 (Ca), 0.991 (Fe), 0.997 (Zn), and 0.989 (Mg). In addition to the calibrated elements, emission lines of major constituents (P, K, Ca, Mg) and trace elements (Ba, Sr, Ti, Cu, Al, Si) were clearly detected. Plasma diagnostics revealed an electron temperature of $\sim 10,000$ K and an electron number density of $\sim 4 \times 10^{16} \text{ cm}^{-3}$, confirming stable plasma conditions despite pronounced matrix effects. The obtained results are consistent with previously developed LIBS methodologies for plant-based matrices¹ and further demonstrate that TEA CO₂ LIBS provides reliable multielemental quantification in hydrophilic food materials.

Keywords: laser-induced breakdown spectroscopy (LIBS); TEA CO₂ laser; chia; quantitative analysis; plasma diagnostics; matrix effects; ICP–OES calibration

Acknowledgments

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PSSE-P12

WHERE DO METALLIC IMPURITIES COME FROM IN INDUSTRIAL GASES DETECTED BY LASER-INDUCED PLASMA SPECTROSCOPY?

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This work builds on the previous study, which documented the initial detection of metallic impurities (vanadium and possibly Fe and Cu) in commercially available argon gas supplied in steel cylinders ¹. In the present study, the laser-induced gas plasma was spectroscopically analyzed over the spectral range 250-550 nm in argon (5.0), helium (4.6), and air at atmospheric pressure. Because vanadium exhibits a prominent spectrum in argon plasma, as identified in the NIST database ², its presence is strongly confirmed, as indicated lastly¹. Similarly, the iron line-rich spectrum overlaps with the vanadium spectrum, making reliable identification difficult but highly likely, since no other elements were identified within those ranges. For example, a number of iron lines are registered around 240 nm, and vanadium shows lines around 300 nm and 450-500 nm, where only vanadium lines are identified. Upon further examination of the updated spectra, two additional elements are detected in argon gas: copper and zinc. Those elements exhibit multiple lines across broad spectral ranges, especially copper. Zinc is identified by several lines, primarily through a persistent line at 328 and 330 nm. Compared to argon plasma, helium and air plasmas result in an almost empty line spectrum.

The main question is: what is the origin of the metal impurities detected in argon? If present, their concentrations must be extremely low yet detectable, so they can be quantified by laser-induced breakdown plasma spectroscopy.

How does metal contaminate argon gas but not helium? As we stated earlier, this could be a consequence of the purification process during gas production ¹. Now, another possible reason is the so-called dealloying process, or leaching ³.

Keywords: Laser-Induced Plasma Spectroscopy, metal detection, gases

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PSSE-P13

STRUCTURAL AND SPECTROSCOPIC DATA OF SOME AQUACHLORO COMPLEXES

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This work investigates the structural and spectroscopic characteristics of water molecules in aquachloro complexes in the solid state and analyzes the dynamics of hydrogen bonding in crystalline environments. Structural and spectroscopic data from selected aquachloro complexes were systematically extracted from crystallographic publications and comparatively analyzed. Methodologically, the study combines a review of the fundamental principles of solid-state chemistry, with particular emphasis on hydrogen bonding in confined systems, and statistical processing of structural parameters (bond lengths and coordination geometry) together with spectroscopic data in order to establish spectrum–structure correlations. The analysis highlights how confined environments in solid-state systems influence the structural flexibility of water molecules and their bonding interactions. The conclusions emphasize the role of lattice geometry in determining the efficiency of hydrogen bonding, thereby providing insights into the design of crystalline materials with controlled hydration properties.

Keywords: solid-state chemistry, structural data, aquachloro complexes, spectroscopic data, hydrogen bonding, crystal structures.



PSSE-P14

**INTERPRETING POSITIVE AND NEGATIVE IR REFLECTANCE-
ABSORBANCE INTENSITIES IN 2T2D-CORRELATION
SPECTROSCOPY OF SILOXANE FILMS ON SILICATE GLASS**

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Organosilanes can be used to engineer silicate glass surfaces, creating water-repellent coatings that enhance hydrophobicity without compromising transparency. The process involves forming a nanometric siloxane film and altering surface roughness to achieve hydrophobicity. In this work, glass substrates were modified with hydrolyzed or non-hydrolyzed 3-aminopropyltriethoxysilane (APTES). Contact angle measurements, calculated surface energy, AFM and Raman measurements demonstrated successful silanization of the surface¹. We used two-trace two-dimensional correlation spectroscopy (2T2D-COS) as a tool in distinguishing the IR bands between the substrate silicate glass and the ultrathin nano-film of siloxane formed on its surface. For that purpose, both, originally recorded IR Specular Reflectance spectra (IR-SR) and calculated IR Reflectance-Absorbance (IR-RA) spectra were used for creating the 2T2D-COS maps. While 2T2D-COS obtained from IR-SR can be used as an independent method for localizing the film band's wavenumber, compared to IR-RA spectra, the 2T2D-COS obtained from IR-RA has the advantage of comparing the structure of two siloxane films². However, since the IR-RA spectra can have positive and negative bands (contrary to the IR-SR), this has its impact on the interpretation of the positive and negative peaks in the 2T2D-COS maps. This work tries to turn attention on the consequences if this fact is not taken into account and gives solution to the problem.

Keywords: silicate glass, hydrophobicity, APTES, IR-SR, IR-RA, 2T2D-COS

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PSSE-P15

**TEMPERATURE-DEPENDENT STRUCTURAL DYNAMICS OF
MOLECULARLY ENGINEERED INSULIN DETEMIR REVEALED BY X-
RAY DIFFRACTION AND TWO-DIMENSIONAL CORRELATION
ANALYSIS OF INFRARED AND RAMAN SPECTRA**

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We report a comprehensive study of the structure, molecular organization, conformational heterogeneity, supramolecular packing and thermally-induced dynamics of insulin detemir, a long-lasting engineered insulin analogue obtained by removal of ThrB30 and covalent attachment of myristic acid chain to LysB29. Powder X-ray diffraction, temperature-dependent Fourier-transform infrared and Raman spectroscopy and generalized two-dimensional correlation analysis (GEN-2DCOS), together with moving-window (MW) and perturbation-correlation moving window (PCMW) 2DCOS approaches were employed to probe temperature-induced structural transformations.

The combined analyses reveal coupling between conformational changes of the protein backbone and rearrangements of the myristic acid chain, providing insights into the interplay between α -helical backbone adjustments, and stabilization of hexameric assemblies. The sequence of temperature-induced structural changes was established through joint analysis of synchronous and asynchronous two-dimensional correlation spectra, enabling identification of processes associated with partial unfolding, intermolecular association and fatty acid packing. Furthermore, the applied methodology provides information on the rigidity of the disulfide bonds, their rearrangements in the course of aggregation, as well as on the propagation of conformational changes through the molecule.

The results demonstrate how conformational adaptations of the insulin backbone are linked to intermolecular self-assembly and crystallization phenomena, highlighting the utility of advanced two-dimensional correlation approaches for elucidating complex relationships between structure and dynamics in engineered protein pharmaceuticals.

Keywords: insulin detemir, protein conformational dynamics, self-association, two-dimensional correlation spectroscopy (2DCOS), moving-window (MW) 2DCOS, perturbation-correlation MW 2D COS, temperature-dependent structural dynamics.



PSSE-P16

**THEORETICAL IRMPD SPECTROSCOPY OF PROTONATED GLYCINE
TAGGED WITH HYDROGEN AND HELIUM**

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Protonated glycine constitutes one of the most extensively investigated model systems in gas-phase ion chemistry due to its fundamental relevance for understanding proton localization, conformational flexibility, as well as intra- and intermolecular hydrogen-bonding interactions in biomolecular ions. Owing to its structural simplicity and rich vibrational behavior, it provides an ideal platform for developing and validating theoretical methodologies aimed at interpreting high-resolution infrared spectroscopic data. In particular, the combination of computational chemistry and infrared multiple-photon dissociation (IRMPD) spectroscopy has emerged as a powerful framework for establishing detailed relationships between structure and spectrum in isolated molecular ions.

In the present study, a comprehensive theoretical investigation of protonated glycine and its weakly bound complexes with helium and molecular hydrogen is performed with the objective of elucidating the influence of molecular tagging on structural stability, vibrational dynamics, and predicted IRMPD spectral signatures. Special attention is devoted to the limitations of the harmonic approximation and the necessity of incorporating anharmonic effects for an accurate description of highly localized X–H stretching vibrations. The vibrational dynamics is analyzed beyond the purely harmonic regime, enabling a more realistic representation of frequency shifts, mode coupling, and energy-transfer pathways that contribute to multiphoton dissociation mechanisms. To account for the coexistence of multiple low-energy conformers, Boltzmann-weighted spectral averaging is applied, allowing thermodynamic populations to be incorporated into the theoretical spectra.

Comparative evaluation of the calculated spectra reveals that helium preserves the native structural characteristics of the ion to a large extent, whereas hydrogen induces measurable perturbations that are particularly pronounced in vibrational modes associated with protonated and hydrogen-bonded sites. Beyond the specific system investigated, the study illustrates the broader role of theoretical chemistry in supporting spectroscopic characterization of isolated biomolecular ions and in guiding future studies of structurally related systems.

Keywords: protonated glycine, quantum chemistry, IRMPD spectroscopy, anharmonic vibrations, conformational analysis, molecular tagging, potential energy surface, vibrational dynamics.



PSSE-P17

BENCHTOP NMR AS A FEASIBLE AND RELIABLE TECHNIQUE FOR DETECTION OF HONEY ADULTERATION

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Honey is a natural product produced by honey bees from floral nectar or honeydew secretions, highly valued for its nutritional and functional properties.¹ Due to its high market value, honey is frequently adulterated with inexpensive sugar syrups or through indirect bee feeding practices, making the development of reliable methods for authenticity assessment and adulteration detection increasingly important.² NMR have been developed during the last three decades for the detection of honey adulterants. However, these technique require highly trained stuff and special conditions. Compared to conventional high-field NMR systems, benchtop NMR spectrometers offer several advantages, including lower cost, compact size, easier operation, minimal maintenance requirements, and no need for liquid helium or other cryogenes. Additionally, they enable rapid, non-destructive analysis on site, making them highly suitable for routine quality control and honey authenticity studies at honey collection points.³

Two different polyfloral honeys (pure – natural from beekeeper and adulterated – commercially purchased with adulteration history) were submitted to benchtop NMR analysis in order to demonstrate feasibility of benchtop NMR as a fast and easy-to-use method for adulteration determination.

The ¹H NMR spectra revealed clear differences between the pure honey sample and the sample adulterated with sucrose. Significant increase of intensity of the sucrose signal (around 5.4 ppm) was observed in the adulterated sample.

These results demonstrate the potential of benchtop NMR spectroscopy as a rapid and non-destructive tool, and first of all a cheap method for detecting honey adulteration.

Keywords: honey, adulteration, benchtop NMR analysis.

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PSSE-P18

**RAPID AUTHENTICATION OF SALEP IN COMMERCIAL PRODUCTS
USING VIS-NIR SPECTROSCOPY COUPLED BY STATISTICAL
METHODS**

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Salep powder, derived from dried tubers of wild terrestrial orchids, is a high-value ingredient used to prepare a thick, hot winter beverage valued for its many reported health benefits. However, products marketed as salep are often diluted, adulterated or falsified, unless specifically declared as pure, with low-cost ingredients such as sugars and starches. The lack of rapid and robust methods for verifying product authenticity poses a significant challenge to the protection of legal and consumer rights, emphasizing the need for the development of fast and reliable authentication techniques.

In this work, VIS–NIR spectra (350–2500 nm) recorded from commercial salep products available on the domestic market, including products spiked with pure authentic salep, were analyzed by principal component analysis (PCA) after standard normal variate (SNV) correction. Unsupervised PCA loading profiles showed the visible range (400–700 nm) as an appropriate marker region for the authentication, reflecting the contrasting color of off-white salep relative to the whiter diluents, and a near-infrared band near 1850–1900 nm, corresponding to the O–H stretch-plus-bend combination band of the hydroxyl-rich, high-bound-water glucomannan matrix. In addition to this, a Hotelling's T² analysis flagged three commercial products as containing little or no genuine salep. These results show that a single, rapid, non-destructive and low-cost VIS–NIR measurement can both quantify salep content and thus expose its near-absence in cheap commercial preparations.

Keywords: Salep, VIS-NIR spectra, authentication, statistical methods, commercial products.



PSSE-P19

REDOX CHEMISTRY OF POLYPHENOLS- GREEN SYNTHESIS OF SILVER NANOPARTICLES AND ELECTROCHEMICAL INTERACTIONS OF QUERCETIN WITH DOPAMINE

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Polyphenolic compounds exhibit diverse redox properties that determine both their ability to reduce metal ions and their interactions with biologically relevant electroactive molecules. In this study, green synthesis of silver nanoparticles using grape seeds as natural polyphenol sources and the electrochemical behavior of quercetin in the presence of dopamine were investigated. Intact grape seeds served as reducing and stabilizing agents for AgNP synthesis from aqueous AgNO₃ solutions[1]. UV–VIS spectroscopy confirmed nanoparticle formation through the characteristic localized surface plasmon resonance band at 410–430 nm, while SEM analysis revealed predominantly spherical particles with diameters of 20–50 nm.

The developed protocol represents a simple, eco-friendly approach aligned with Green Chemistry principles. The electrochemical properties of quercetin were examined in phosphate buffer (pH 7) using square-wave voltammetry. Quercetin exhibited a quasi-reversible redox process at approximately +70 mV versus Ag/AgCl, with diffusion-controlled behavior at low frequencies (1–10 Hz), whereas higher frequencies resulted in decreased responses due to kinetic limitations. Dopamine displayed a reversible redox transformation at approximately +0.20 V. Simultaneous measurements revealed weak but detectable interactions between quercetin and dopamine, while preserving sufficient peak separation for their individual identification. These findings highlight the importance of polyphenol redox chemistry in sustainable nanoparticle synthesis and biologically relevant electrochemical systems.

Keywords: dopamine; grape seeds; green synthesis; polyphenols; quercetin; redox interactions; silver nanoparticles; square-wave voltammetry.

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PSSE-P20**COMPLEXATION OF METAL CATIONS WITH THIOAMIDE CALIX[4]ARENE DERIVATIVE**

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Calixarenes are a class of supramolecular ligands that can be readily functionalized to give very efficient and even selective receptors for various ionic and neutral chemical species.^{1,2} Among them, those bearing sulfur-based functional groups form stable complexes with low-charge-density and soft metal cations.³ In the scope of this work, binding affinity of thioamide calix[4]arene derivative **L** (Figure 1) towards alkali, alkaline earth, and soft metal cations in acetonitrile was investigated by spectrophotometry, NMR spectroscopy, isothermal titration calorimetry, and X-ray crystallography. The obtained results were discussed regarding the structural characteristics of the ligand, as well the size, charge density, and polarizing power of the cations.

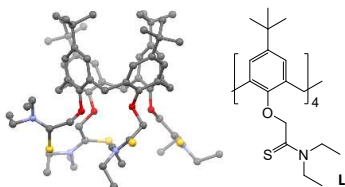


Figure 1. Molecular structure of thioamide calix[4]arene derivative **L**.

Keywords: calixarenes, metal cations, thermodynamics

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PSSE-P21

**ALMOND SHELL AS A SUSTAINABLE SENSOR MATERIAL FOR
REAL-TIME HEAVY METALS MONITORING**

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Clean water is a fundamental human need increasingly threatened by rapid population growth and industrial expansion. Among the most hazardous contaminants are heavy metal ions, which are non-biodegradable, highly toxic, and prone to bioaccumulation within food chains¹. These challenges create an urgent need for the development of sensors capable of real-time environmental monitoring². In this study, almond shells, collected near Belgrade, were enriched with Bi_{1.55}Sm_{0.45}O₃ nanoparticles and thermally converted through carbonization into a carbon-nanoparticle composite. This material was employed as a sensing platform for heavy metal detection. The materials were characterized chemically and morphologically using Scanning Electron Microscopy – Energy Dispersive X-ray Spectroscopy (SEM-EDS) and X-ray photoelectron spectroscopy (XPS). SEM images revealed a scaly carbon structure with uniformly embedded nanoparticles, while XPS confirmed the successful formation of carbon and incorporation of the surface modifier. The electrochemical performance of the sensor was evaluated in a conventional three-electrode system, with the synthesized material serving as the working electrode and unmodified carbon as the control. Cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) demonstrated enhanced electrocatalytic activity compared with unmodified carbon. The analytical performance was assessed using anodic stripping voltammetry (ASV). The novel sensor reported the limit of detection (LOD) 0.15 µg L⁻¹ (Cd) and 0.58 µg L⁻¹ in a linear range from 0.22 µg L⁻¹ to 0.11 mg L⁻¹ and from 0.41 µg L⁻¹ to 0.21 mg L⁻¹ for Cd and Pb, respectively. Supported by this data, the focus of future research will be on real sample applications.

Keywords: almond shells, sensors, carbon, heavy metals, water

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PSSE-P22

**INVESTIGATION OF THE HYDROPHOBICITY OF MODIFIED GLASS
IN GLASS–TEOS–HDTMS SANDWICH STRUCTURES**

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Soda-lime-silicate (SLS) glass is widely used in industry. To render its surface hydrophobic, it is commonly modified using different silane derivatives. Among the most widely used are alkoxysilanes, which can be anchored onto the glass surface through hydrolysis, followed by condensation between the silanol groups of the silane and those on the glass surface. Among the alkoxysilanes, tetraethoxysilane (TEOS) is unique because, after complete hydrolysis, it contains no organic groups and only OH groups attached to the Si atom. This also makes TEOS an excellent glass surface modifier, since it increases the number of active silanol groups on the glass surface, thereby making it susceptible to a higher degree of modification.

In this work, we investigated how the modification of SLS glass with hexadecyltrimethoxysilane (HDTMS), and consequently its hydrophobicity, is affected when TEOS with different degrees of hydrolysis is used as the first glass layer. In this way, a sandwich structure was built in which the first layer on the glass consisted of TEOS, onto which HDTMS was chemisorbed. The analysis was performed by recording FTIR specular reflectance spectra, from which IR reflectance–absorbance spectra and two-trace two-dimensional correlation spectra were obtained. This analysis is particularly interesting because it provides information on the IR spectra of the formed ultrathin siloxane film on top of the glass substrate, both of which possess very similar chemical structures.

The morphology of the films was analyzed using Atomic Force Microscopy, while the wetting properties were determined through measurements of the water contact angle and the calculated polar and dispersive components of the surface energy using the Owens–Wendt–Rabel–Kaelble (OWRK) method.

The obtained results show that the degree of hydrolysis of TEOS strongly depends on time, pH, and the solvent used. It will be shown that drying and curing play particularly important roles in the hydrophobicity of the modified glass, which is in connection to the content of surface silanol and siloxane groups. The hydrophobicity of the glass resulting from modification with a second HDTMS layer in each case will also be discussed.

Keywords: soda-lime-silicate glass; hydrophobicity; tetraethoxysilane; hexadecyltrimethoxysilane

Acknowledgement: This work was financially supported by the Ministry of Education and Science of the North Macedonia under National Project No. 15–6171/36.



PSSE-P23

SYNTHESIS AND CHARACTERIZATION OF THE NOVEL MIXED-HALIDE PEROVSKITE DMAPbI_{1.5}Cl_{1.5}

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Hybrid organic–inorganic perovskites are promising materials for energy-related applications owing to their tunable optoelectronic properties.¹ In this work, the novel mixed-halide perovskite [(CH₃)₂NH₂][PbI_{1.5}Cl_{1.5}] (DMAPbI_{1.5}Cl_{1.5}), within the DMAPbX₃ (X = I, Br, Cl) family, was synthesized and characterized. The compound was prepared in *N,N*-dimethylformamide from pre-synthesized DMAPbI₃ and DMAPbCl₃ precursors,² yielding a light-yellow crystalline product. Powder X-ray diffraction (PXRD) confirmed the formation of a crystalline mixed-halide phase distinct from the parent compounds. Scanning electron microscopy (SEM) revealed porous aggregated microcrystals, while energy-dispersive X-ray spectroscopy (EDX) confirmed an approximately 1:1 atomic ratio of iodine to chlorine, consistent with the targeted composition. Infrared and Raman spectroscopy confirmed the structural integrity of both the organic cation and the metal-halide framework. Cyclic voltammetry performed in dichloromethane containing tetrabutylammonium perchlorate (TBAPC) as the supporting electrolyte revealed redox activity and progressive current decay during successive scans, indicating partial electrochemical degradation of the compound.

Keywords: DMAPbI_{1.5}Cl_{1.5}, mixed-halide perovskite, PXRD, SEM-EDX, vibrational spectroscopy, cyclic voltammetry

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PSSE-P24

**STRUCTURE-PROPERTY RELATIONSHIP AND PLASMON-
ENHANCED PHOTOLUMINESCENCE IN Ag@Ag₂O CORE-SHELL
NANOPARTICLE THIN FILMS**

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Silver/silver oxide (Ag@Ag₂O) core-shell nanoparticles have attracted considerable attention due to their unique combination of plasmonic and semiconducting properties, making them promising materials for applications in sensing, photocatalysis and optoelectronics. In this work, Ag@Ag₂O NP thin films were synthesized and systematically characterized to investigate the relationship between their structural, morphological, optical and photoluminescence properties.

The crystal structure and phase composition were examined by X-ray diffraction (XRD) and selected area electron diffraction (SAED), confirming the coexistence of metallic Ag and Ag₂O phases. Raman spectroscopy revealed characteristic vibrational modes associated with Ag₂O and provided additional evidence of the composite Ag/Ag₂O structure. The enhanced Raman response observed from the nanostructured thin films indicates the presence of strong localized electromagnetic fields generated by the Ag component, highlighting the potential of the films as Surface-Enhanced Raman Scattering (SERS) active substrates. Transmission electron microscopy (TEM) revealed the formation of nanoparticles with a distinct core-shell architecture, while scanning electron microscopy (SEM) provided information on particle morphology. Atomic force microscopy (AFM) was employed to analyse the surface topography and nanoscale roughness of deposited NP thin films.

The optical properties were investigated using UV-Vis spectroscopy, revealing a pronounced localized surface plasmon resonance (LSPR) associated with the Ag core. Photoluminescence measurements demonstrated a significant enhancement of the emission intensity compared to pure Ag₂O nanostructures. The observed enhancement is attributed to the coupling between the semiconductor excitonic transitions of Ag₂O shell and the localized plasmonic field generated by the Ag core.

The results provide valuable insights into the structure-property relationships governing the optical response of Ag@Ag₂O nanostructures and highlight their potential for plasmon-enhanced photonic, sensing and SERS applications.

Keywords: Ag@Ag₂O nanoparticles, core-shell nanostructures, plasmonics, SERS substrates, photoluminescence enhancement, XRD, TEM, SEM, AFM.



PSSE-P25

SYNTHESIS, CHARACTERIZATION, AND ELECTROCATALYTIC PROPERTIES OF $\text{Pr}_{1-x}\text{Er}_x\text{FeO}_3$ ($x = 0; 0.2; 0.4$ OR 1)

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Lanthanide-based perovskites have attracted considerable attention due to their structural versatility and tunable physical and chemical properties, making them promising materials for catalytic and electrochemical applications.¹

In this work, the results of synthesis, characterization and detailed electrochemical investigations of complex perovskites with the general formula $\text{Pr}_{1-x}\text{Er}_x\text{FeO}_3$ ($x = 0; 0.2; 0.4$ or 1) are presented. These compounds are synthesized using the sol-gel combustion method, employing citric acid as fuel and chelating agent, under controlled temperature and pH conditions. The obtained samples are identified and characterized using powder X-Ray diffraction, infrared and Raman spectroscopy, while their electrochemical properties are investigated using cyclic staircase voltammetry in different electrolytes (phosphate buffer, KNO_3 , and KCl) on a glassy-carbon working electrode, modified with Nafion and corresponding perovskite.

The X-Ray diffraction patterns confirmed the formation of single-phase perovskites with high purity and crystallinity. The diffraction patterns exhibit the same sequence of diffraction maxima with slight shifts in their 2θ positions, indicating that the obtained compounds are isostructural. All of them are orthorhombic and crystallize within the space group *Pnma*.

The recorded IR and Raman spectra confirmed the partial substitution of praseodymium with erbium and the formation of Pr–O and Er–O bonds in the substituted perovskites. The incorporation of the smaller Er^{3+} in the place of the larger Pr^{3+} leads to a decrease in the lattice parameters, causing a shift of the vibrational modes.

Electrochemical investigations showed that the synthesized perovskites are electrochemically stable and exhibit significant electrocatalytic activity toward the reduction of dissolved oxygen. Among the investigated materials, PrFeO_3 displayed the highest catalytic activity. The results indicate that the electrocatalytic properties are strongly influenced by the composition of the material and the experimental conditions.

Keywords: complex perovskites, sol-gel combustion, X-ray powder diffraction, infrared spectroscopy, Raman spectroscopy, cyclic voltammetry

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PSSE-P26

**SYNTHESIS AND INVESTIGATION OF $\text{La}_{1-x}\text{Er}_x\text{Mn}_{0.5}\text{Fe}_{0.5}\text{O}_3$
($x = 0.2$ AND 0.4) COMPLEX PEROVSKITES**

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In recent decades, perovskite-type ceramic materials, with general formula ABO_3 , have attracted considerable attention due to their significant electrical, optical, magnetic and catalytic properties. Among them, mixed-cation perovskites containing two different lanthanide ions at the A-site and two transition-metal ions at the B-site have attracted particular attention because their structural and functional properties can be effectively tuned through cation substitution. In this work, the synthesis and characterization of $\text{La}_{1-x}\text{Er}_x\text{Mn}_{0.5}\text{Fe}_{0.5}\text{O}_3$ ($x = 0.2$ or 0.4) are presented.

These compounds were synthesized by the sol-gel combustion method using citric acid as fuel, while the pH value of the precursor solution was adjusted with ammonia. The obtained perovskite precursors were calcined at 900 °C for 8 hours to obtain the crystalline perovskite phase.

Powder X-ray diffraction (PXRD) confirmed the successful formation of single-phase perovskites with high phase purity and crystallinity, and revealed a systematic shift of the diffraction peaks with increasing of Er^{3+} content.

The morphology and the verification of the stoichiometry of the synthesized perovskites were performed by scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM/EDX analysis). The EDX results showed good agreement with the proposed composition. SEM micrographs revealed a typical sponge-like porous morphology characteristic for perovskites obtained by sol-gel combustion method.

In addition to structural investigations, Fourier-transform infrared (FTIR) in the mid- and far-IR regions confirmed the presence of characteristic stretching and bending vibrations of Mn/Fe-O , and Ln/Er-O . The Raman spectra of both compositions exhibit similar vibrational features in the 200–700 cm^{-1} region, indicating similar local environments around the $(\text{Mn,Fe})\text{O}_6$ octahedra. The observed broad Raman bands suggest the presence of local structural disorder and distortion of the $(\text{Mn,Fe})\text{O}_6$ octahedra, most likely arising from the Jahn–Teller activity of Mn^{3+} ions together with the random distribution of Mn and Fe cations over the B-sites of the perovskite lattice.

Keywords: Complex perovskites, PXRD, SEM/EDX, FTIR, Raman spectroscopy



PSSE-P27

STRUCTURAL DYNAMICS OF SsbA FROM *STREPTOMYCES COELICOLOR* BY HYDROGEN-DEUTERIUM EXCHANGE MASS SPECTROMETRY

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Single-stranded DNA-binding proteins (SSBs) are essential for genome maintenance across all domains of life, protecting transiently exposed single-stranded DNA during replication, recombination, and repair. While the crystal structure and biophysical properties of SsbA from *Streptomyces coelicolor* have been characterized, direct information on its solution-phase conformational dynamics has been lacking.

In this study, hydrogen-deuterium exchange mass spectrometry (HDX-MS) was used to probe the conformational dynamics of free SsbA in physiological conditions. Deuterium labeling was performed at five time points (10 s, 1 min, 20 min, 1 h, 4 h). Two proteolytic strategies were used to generate overlapping peptide maps, and data were analyzed using HDEaminer software, yielding approximately 70% sequence coverage. Regions corresponding to the N-terminal His-tag (residues 1–9) and portions of the C-terminal region (residues 152–211), which includes glycine rich region and acidic C-tip (DEPPF) were not covered, consistent with known challenges in peptide identification within low-complexity sequences

The N-terminal OB-fold domain, responsible for ssDNA binding, showed a heterogeneous exchange pattern, with the highest deuterium uptake observed in the region spanning residues 26–44, and additional regions of elevated exchange around residues 60–66 and 72–89, revealing locally flexible or solvent-exposed segments. In contrast, the glycine-rich IDL region (residues ~121–151), previously described as intrinsically disordered, exhibited consistently low deuterium uptake across all time points, suggesting reduced solvent accessibility in the free state relative to that expected for a fully disordered linker. This observation is consistent with previously reported hydrodynamic data suggesting a more globular conformation of the SsbA C-domain, and may reflect self-association or condensate-forming behavior proposed for this protein.

These findings provide the first direct evidence of the conformational dynamics of free SsbA in solution and establish a baseline for future comparative HDX-MS studies.

Keywords: SsbA, HDX-MS, *Streptomyces coelicolor*, conformational dynamics



PSSE-P28

QUANTITATIVE EVALUATION OF NUTRITIONAL AND SAFETY-RELEVANT ELEMENTS IN SESAME SEEDS USING LIBS

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Laser-induced breakdown spectroscopy (LIBS) was employed to perform rapid multielemental analysis of sesame (*Sesamum indicum* L.) seeds, focusing on both nutritional and safety-relevant elements. Pressed sesame pellets were analyzed under optimized TEA CO₂ laser conditions, while inductively coupled plasma–optical emission spectrometry (ICP–OES) measurements supported calibration and ensured reliable quantification, consistent with previously developed LIBS methodologies for plant-based matrices¹. Major nutrients (K, P) and safety-relevant elements (Sr, Al) were quantitatively determined. Additional major and trace elements were also identified, providing a comprehensive elemental profile. The oil-rich, compact matrix contributed to stable plasma formation, enhancing signal reproducibility and analytical precision. These results demonstrate that LIBS offers a fast and practical approach for multielemental profiling of sesame seeds, supporting nutritional evaluation and food safety monitoring, and highlight its potential applicability to other oil-rich plant-based materials.

Keywords: laser-induced breakdown spectroscopy (LIBS); sesame; quantitative analysis; nutritional profiling; food safety; ICP–OES calibration; oil-rich matrix

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PSSE-P29

PLASMA PROPERTIES AND MULTIELEMENTAL PROFILING OF FLAX SEEDS VIA TEA CO₂ LIBS

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Flax (*Linum usitatissimum* L.) seeds were studied to investigate their elemental composition and plasma characteristics, given their high oil and fiber content which creates a dense matrix affecting plasma formation and signal reproducibility. Laser-induced breakdown spectroscopy (LIBS) with a TEA CO₂ laser was applied to pressed flax seed pellets, while inductively coupled plasma–optical emission spectrometry (ICP–OES) provided calibration and reliable quantification. Calibration was performed for major nutrients and trace elements, including K, Ca, Mg, and Fe, using analyte-to-internal standard intensity ratios, demonstrating high linearity with correlation coefficients (R^2) above 0.98. Emission lines of additional elements such as P, Zn, and Mn were also detected, providing a comprehensive elemental profile. Plasma diagnostics indicated an electron temperature of $\sim 11,000$ K and electron number density of $\sim 5 \times 10^{16} \text{ cm}^{-3}$, confirming stable plasma conditions despite the complex flax matrix. These results highlight the applicability of TEA CO₂ LIBS for rapid, multielemental analysis of oil-rich seeds, offering valuable insight for nutritional evaluation and quality control.

Keywords: laser-induced breakdown spectroscopy (LIBS); TEA CO₂ laser; flax; quantitative analysis; plasma diagnostics; matrix effects; ICP–OES calibration

References:

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Polymers and polymer materials (PPM)

PPM-O1**ELECTROSPUN PLA/Tuff COMPOSITE MEMBRANES: FABRICATION, STRUCTURAL CHARACTERIZATION, AND POTENTIAL FOR METAL ADSORPTION**

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Electrospinning enables the fabrication of micro- and nanofibrous materials with high surface area and porosity, making them attractive for water treatment and environmental remediation applications. In this study, electrospun polylactic acid (PLA) membranes containing 0, 2, 5, and 10 wt% natural opalized tuff were successfully fabricated and evaluated as eco-friendly adsorbents for heavy metals removal. The incorporation of tuff provided active mineral sites, while the PLA matrix ensured structural stability and biodegradability. Scanning electron microscopy (SEM) revealed a uniform fibrous morphology with well-developed porosity (Figure 1, left images). X-ray diffraction and Fourier-transform infrared spectroscopy confirmed the successful incorporation of tuff without altering the chemical structure of PLA. Energy Dispersive X-Ray (EDX) spectroscopy analysis demonstrated the effective adsorption of Ni²⁺ (Figure 1, right) and Pb²⁺ ions from aqueous solutions, indicating the important role of the silicate-rich mineral phase in the metal uptake.

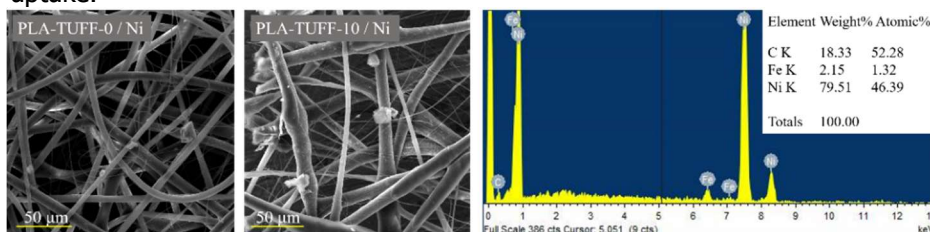


Figure 1. SEM-EDX characterization of electrospun PLA-TUFF-0 and PLA-TUFF-10 membranes after 6 h exposure to Ni²⁺ solution.

The combination of a renewable polymer and a naturally occurring mineral filler resulted in porous composite membranes with promising adsorption performance.

Keywords: Electrospinning; Polylactic acid (PLA); Opalized tuff; Heavy metals adsorption, Biodegradable composites.



PPM-O2

**GOLD-DECORATED REDUCED GRAPHENE OXIDE NANOHYBRIDS
FOR HIGH-PERFORMANCE ELECTROCATALYTIC SENSING OF
DOXORUBICIN**

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Screen-printed carbon electrodes (SPCEs) are crucial for point-of-care diagnostics but often require surface modification to meet clinical sensitivity demands. This study presents the development of high-performance electrochemical sensors utilizing reduced graphene oxide (rGO) decorated with gold nanoparticles (AuNPs) at varying concentrations (0.5, 2, and 4 wt.%). Structural and thermal analysis (XRPD, FTIR, Raman, SEM/EDS, TGA) confirmed successful nanohybrid formation, with Raman spectroscopy revealing a G-band redshift indicative of strong electronic interaction via n-type doping. The 2 wt.% AuNP/rGO hybrid demonstrated the highest graphitic ordering and thermal stability and was selected to modify SPCEs for the electrocatalytic detection of the anticancer drug doxorubicin (DOX).

Voltammetric analysis of the engineered sensor showed a highly favorable quasi-reversible redox process, resulting in a 3.3-fold increase in anodic peak current density ($18.912 \mu\text{A cm}^{-2}$) compared to bare SPCEs. Electrokinetic investigations confirmed accelerated electron transfer kinetics, yielding a reduced Tafel slope (140 mV dec^{-1}) and an elevated heterogeneous rate constant ($k^0 = 2.57 \times 10^{-5} \text{ cm s}^{-1}$). Ultimately, the sensor delivered a 1.45-fold increase in sensitivity ($0.221 \mu\text{A} / \mu\text{mol L}^{-1}$) and a 20.9% improvement in the limit of detection ($13.193 \mu\text{mol L}^{-1}$) in the low concentration range ($0.5 - 10.5 \mu\text{mol L}^{-1}$). These results highlight the potential of AuNP/rGO frameworks for next-generation, high-sensitivity screen-printed sensors.

Keywords: screen-printed electrodes, electrochemical sensor, doxorubicin, reduced graphene oxide, gold nanoparticles.



PPM-03

**DETECTION OF 2,4-DIMETHYLBENZOIC ACID USING
ZWITTERIONIC LIGNIN-BASED POLYMER COMPOSITES**

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To develop sustainable functional polymer-lignin composites, the lignin was modified with zwitterionic (L)/3-[(2-methacryloyloxy)ethyl]dimethylammonio propane sulfonate (DMAPS) oligomers grafted in situ from its surface in different mass ratios (1:1, 1:2, and 1:3) via an UV-induced thiol-ene reaction. Successful surface functionalization was confirmed by FTIR, XPS, and colloidal analysis. The L/DMAPS hybrids were subsequently employed as stabilizer in the Pickering miniemulsion polymerization of methyl methacrylate/butyl methacrylate to prepare functional polymer composites. Compared with unmodified lignin, the L/DMAPS hybrids exhibited improved dispersion within the polymer matrix, enhanced filler-matrix interactions, and promoted the formation of a more homogeneous microstructure. The composites were then functionalized with 2,4-dimethylbenzoic acid (DMBA) to be make its surface sensitive to similar compounds. The influence of L/DMAPS on adsorption behaviour and sensing performance toward DMBA was evaluated. Quartz crystal microbalance (QCM) measurements were performed to monitor the adsorption and desorption of DMBA from aqueous solutions (0.01 and 0.02 mg/mL), revealing that the 1:1 L/DMAPS/polymer composite exhibited the highest adsorption capacity while maintaining reversible binding characteristics. In comparison with the L/polymer composite, the incorporation of L/DMAPS facilitated the formation of selective recognition sites through the synergistic contribution of ionic interactions, π - π interactions, and steric complementarity. These results demonstrate that the optimized L/DMAPS hybrid composite is a promising sustainable material for the selective recognition and detection of organic pollutants.

Keywords: lignin/dmaps hybrids, pickering miniemulsion polymerization, selective adsorption



PPM-P1

**THERMAL AND FIRE PROPERTIES OF EPOXY COMPOSITES WITH
MELAMINE-BASED FLAME RETARDANTS**

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Epoxy resins are widely used polymeric materials owing to their excellent mechanical strength, chemical resistance, and adhesion properties. However, their relatively high flammability restricts their use in areas where improved fire safety is required. Therefore, modifying epoxy systems with effective flame-retardant additives is an important area of research. Among the various flame-retardant systems available, those containing phosphorus and nitrogen have attracted considerable attention. Melamine-based phosphates in particular are considered promising additives, as they promote char formation and reduce heat release during combustion¹⁻³.

This study examined the modification of epoxy composites crosslinked with amine hardeners using melamine phosphate flame-retardant additives. These modifiers were obtained through reactions between melamine and selected phosphorus derivatives. Additionally, a hybrid flame-retardant system containing melamine phosphate and hydrated zinc borate was prepared by mechanical mixing. These additives were then incorporated into epoxy resin systems to obtain polymer composites with enhanced flame-retardant properties. Thermal resistance (DSC and TGA) and flammability tests were also conducted to evaluate the thermal stability and fire behaviour of the prepared epoxy composites.

Keywords: epoxy resin, melamine, composites, thermal resistance, fire properties.

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PPM-P2

INFLUENCE OF SPIN COATING PARAMETERS ON β PHASE FORMATION IN PVDF THIN FILMS DEPOSITED ON ITO SUBSTRATES: AN ATR-FTIR STUDY

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Poly(vinylidene fluoride) (PVDF) is one of the most attractive electroactive polymers due to its piezoelectric, pyroelectric, and ferroelectric properties, which are strongly dependent on the content of the polar β crystalline phase. The development of a high β phase content is highly sensitive to processing conditions and post processing treatments.¹

The spin coating method is one of the promising routes for obtaining thin films with a high content of β phase.²

In this study, the influence of molar mass, solution concentration, and spin-coating speed on the β phase content of PVDF thin films was systematically investigated. Three PVDF samples with low, medium, and high molar mass (with different concentrations in DMF/Ac.) were used in this research. Thin films were deposited onto indium tin oxide (ITO) coated glass substrates by spin coating at rotational speeds between 1000 and 5000 rpm. The crystalline phase composition was analyzed by Fourier Transform Infrared Spectroscopy (FTIR). The experimental design enabled evaluation of the individual and combined effects of molar mass, solution concentration, and spin-coating speed on β crystal phase development. Variations in solution viscosity and chain entanglement associated with molar mass, together with differences in centrifugal stretching and solvent evaporation rates during spin coating, were found to influence the crystallization behavior of PVDF.

The results provide valuable insights into the optimization of processing conditions for enhancing β phase formation in PVDF thin films. The findings contribute to the development of high performance PVDF based piezoelectric and ferroelectric devices, fabricated through scalable solution processing techniques.

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Keywords: PVDF films , β crystal phase, spin coating, ATR-FTIR spectroscopy

PPM-P3

DEVELOPMENT OF WATERBORNE POLYMER NANOCOMPOSITES WITH MWCNT/Ag HYBRIDS FOR EMI SHIELDING APPLICATIONS

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Waterborne polymer nanocomposites have attracted considerable attention as sustainable alternatives to solvent-based materials for electromagnetic interference (EMI) shielding applications^{1,2}. In this study, nanocomposite films based on a poly(methyl methacrylate-co-butyl acrylate) matrix synthesized via miniemulsion polymerization were reinforced with multi-walled carbon nanotubes (MWCNTs) and silver-decorated MWCNT (MWCNT/Ag) hybrid fillers prepared in different mass ratios. FTIR spectroscopy confirmed the successful incorporation of the conductive fillers into the polymer matrix. The mechanical properties were assessed by tensile testing, with the MWCNT/Ag-containing nanocomposites exhibiting increased toughness compared with the neat polymer. The incorporation of conductive fillers resulted in electrical conductivities on the order of 10^{-7} S/cm, while the surface properties remained relatively stable, with water contact angles ranging from 71° to 83°. EMI shielding measurements showed improved attenuation for the MWCNT/Ag-containing nanocomposites, with the highest shielding effectiveness observed for the 0.5 wt% 1:1 MWCNT:Ag formulation. Overall, the developed waterborne nanocomposite coatings show promising potential as lightweight and environmentally friendly materials for EMI shielding applications.

Keywords: waterborne nanocomposites, miniemulsion polymerization, MWCNT/Ag hybrids, electromagnetic interference shielding.

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PPM-P4

ANTI-INFLAMMATORY EFFECTS OF GRAPE SKIN EXTRACT-LOADED HYDROGELS IN CARRAGEENAN-INDUCED PAW EDEMA IN RATS

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Inflammation is a response to tissue injury characterized by swelling, redness, and pain. Although conventional anti-inflammatory drugs are effective, polyphenol-rich natural products may offer a safer alternative. Grape skin extracts are rich in compounds that exhibit antioxidant and anti-inflammatory activities¹, however, their therapeutic potential following incorporation into topical formulations remains insufficiently investigated. This study evaluated the anti-inflammatory effects of hydrogels containing grape skin extracts obtained from *Cabernet Sauvignon* (E1) and *Shiraz* (E2) in a rat model of carrageenan-induced paw edema.

Extracts (8 mg/mL) were incorporated into alginate-gelatin hydrogels containing 3% of each polymer (1:1), followed by homogenization, sonication, freezing, cross-linking with calcium chloride, and drying. *Wistar albino* rats were assigned to four groups (n=4): control (CTRL), hydrogel base (HB), E1, and E2. Paw edema was induced by carrageenan injection, the formulations were applied immediately, and paw thickness was measured at baseline and after 1, 2, 3, and 4 hours.

CTRL animals exhibited swelling, peaking 1–2 hours after injection and declining slowly afterwards. HB produced only a minor reduction in edema. Both extract-loaded hydrogels reduced paw swelling, with E1 showing the strongest and consistent effect, lowering peak edema and accelerating recovery toward baseline by hour 4. E2 demonstrated a moderate effect that exceeded that of HB.

These findings support investigation of grape skin extracts as bioactive components of topical formulations for inflammation and wound healing.

Keywords: Grape skin extract, hydrogel, anti-inflammatory activity.

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PPM-P5

DEVELOPMENT OF HALOCHROMIC NANOFIBROUS WOUND DRESSINGS FOR REAL-TIME pH MONITORING AND WOUND HEALING APPLICATIONS

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Not presented.



PPM-P6

**LAYER-BY-LAYER ASSEMBLY OF LIGNIN-DERIVED
BIOCHAR/POLYMER COMPOSITE FILMS FOR SELECTIVE
ADSORPTION OF 2,4-DIMETHYLBENZOIC ACID**

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Activated biochar was prepared from lignin by chemical activation with NaOH followed by carbonization at 600 °C for 2 h. The resulting biochar was washed with 1 M HCl and deionized water, dried, and dispersed in water using poly(vinyl pyrrolidone) (PVP) as a surfactant. Multilayer composite films were fabricated by combining a poly(methyl methacrylate-co-butyl methacrylate), p(MMA/BMA) (30/70 wt/wt), matrix with the lignin-derived biochar using a layer-by-layer (LbL) assembly approach. Spin coating deposition enabled the sequential formation of polymer (P) and biochar (B) layers, producing films with different architectures (P, B, P-B, P-B-P, and P-B-P-B). After each deposition step, the films were rinsed to remove loosely bound material and dried at 45 °C to ensure uniform layer formation. The optical properties of the multilayer films were investigated by UV–Vis spectroscopy, revealing characteristic π – π^* and n – π^* transitions of the polymer matrix in the UV region. Increasing the number of deposited layers, particularly those containing biochar, enhanced UV absorption while reducing optical transparency, indicating successful incorporation of biochar and increased surface coverage. Surface morphology examined by optical microscopy demonstrated that spin coating produced smooth and homogeneous films, with progressive encapsulation of the biochar particles by the polymer matrix as additional layers were deposited. Among all investigated architectures, the multilayer sandwich structure (P-B-P-B) exhibited the best sensing performance, showing a selective frequency decrease of 160 Hz upon exposure to a 0.02 mg/mL solution of 2,4-dimethylbenzoic acid, whereas the simpler film configurations showed no measurable response. These findings demonstrate the potential of lignin-derived biochar/polymer multilayer films as sustainable functional materials for selective adsorption and sensing applications.

Keywords: lignin-derived biochar, multilayer coatings, adsorption.



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Biotechnology and food technology (BFT)



BFT-P1

OPTIMIZATION OF ETHANOLIC EXTRACTION CONDITIONS FROM BLUEBERRY WASTE AND IN VITRO EVALUATION OF ANTIOXIDANT POTENTIAL

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Blueberry (*Vaccinium spp.*) waste, a by-product of industrial fruit processing, represents a rich source of polyphenolic compounds, particularly anthocyanins, which may contribute to the antioxidant potential. Ultrasound-assisted ethanolic extraction is an efficient and eco-friendly approach for obtaining bioactive extracts from this raw material.¹ The aim of this study was to optimize the extraction conditions for blueberry waste and evaluate the *in vitro* antioxidant potential of three obtained extracts.

Ultrasound-assisted extraction was performed using ethanol concentrations of 40% and 60%, temperatures of 45 °C and 55 °C, and extraction times of 20–60 min. Antioxidant activity was determined by DPPH and ABTS assays (IC₅₀, µg/mL), while total phenolic content (TPC) was determined by the *Folin–Ciocalteu* method (mg GAE/g DE).

Extract E1 (60% EtOH, 55 °C, 30 min) exhibited the highest TPC (93.14 mg GAE/g DE), strongest ABTS activity (IC₅₀ = 24.19 µg/mL), and favorable DPPH activity (IC₅₀ = 304.85 µg/mL). Extracts E2 (40% EtOH, 55°C, 60 min) and E3 (60% EtOH, 45°C, 20 min) showed slightly lower but comparable antioxidant activity (DPPH IC₅₀ = 308.65 and 322.00 µg/mL; ABTS IC₅₀ = 40.47 and 33.60 µg/mL) and phenolic content (85.43 and 80.00 mg GAE/g DE).

E1 showed the most favorable overall antioxidant profile, indicating that higher ethanol concentration and temperature favored phenolic recovery and antioxidant activity within a short extraction time. E2 and E3 also demonstrated considerable antioxidant activity and phenolic content, supporting ultrasound-assisted extraction as an effective approach for blueberry waste valorization.

Keywords: Blueberry, fruit waste, ethanolic extraction, ultrasound, polyphenols.

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BFT-P2

TYROSINASE-INHIBITORY POTENTIAL OF PROKUPAC GRAPE EXTRACTS: INFLUENCE OF BERRY PART AND EXTRACTION pH

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Tyrosinase is a copper-dependent enzyme involved in melanin biosynthesis, and its increased activity is associated with hyperpigmentation. Due to the limitations of some synthetic inhibitors, natural polyphenol-rich plant extracts are increasingly investigated as safer alternatives. Prokupac grapes are of particular interest because of their specific phenolic profile and potential for the valorisation of local viticultural resources.

The aim of this study was to investigate the tyrosinase-inhibitory potential of extracts obtained from grape skin, pulp, and seeds of the Prokupac variety, with emphasis on the influence of extraction pH. The extracts were prepared using 50 mM buffer solutions with pH values ranging from 4.0 to 8.0. Tyrosinase activity was determined spectrophotometrically by monitoring dopachrome formation from L-DOPA at 475 nm, while inhibition was calculated in relation to a control sample without inhibitor. The dry residue of the extracts was also determined. Statistical analysis was performed using two-way ANOVA and Tukey's post hoc test, with $p < 0.05$ considered significant.

The results showed that tyrosinase-inhibitory activity depended significantly on both the berry part and extraction pH. Grape skin extracts exhibited the strongest activity, with inhibition ranging approximately from 70 to 95%, while seed extracts showed moderate to high activity. Pulp extracts demonstrated considerably lower inhibitory potential. The highest inhibition was recorded at pH 6, where skin, seed, and pulp extracts inhibited tyrosinase activity by 94.81%, 78.94%, and 58.20%, respectively. The highest dry residue values were also observed at pH 6, suggesting a possible relationship between the amount of extracted compounds and biological activity.

These results indicate that Prokupac grape skin and seeds are promising sources of natural tyrosinase inhibitors. Their activity may be associated with polyphenolic compounds capable of affecting enzyme activity, including through copper ion chelation. Prokupac grape extracts therefore show potential for use as natural active ingredients in dermatocosmetic formulations aimed at regulating melanogenesis and treating hyperpigmentation.

Keywords: Prokupac, grape, tyrosinase, inhibition, polyphenols, hyperpig



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BFT-P3

**ORANGE PEEL ESSENTIAL OIL AS A NATURAL SOLVENT FOR
PROPOLIS: DEVELOPMENT AND CHARACTERIZATION OF AN OIL-
BASED FORMULATION**

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Not presented.



BFT-P4

INFLUENCE OF THE ADDITION OF PORK COLLAGEN PROTEIN ON THE PARTICLE SIZE DISTRIBUTION IN COCOA CREAM PRODUCTS

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Recent dietary trends indicate a growing consumer preference for high-protein diets. Confectionery products are typically characterized by low protein content and high levels of fat and sugar, making them suitable matrices for protein enrichment. Collagen, a protein derived from animal by-products such as skin and bones, represents a highly valuable ingredient due to its recognized benefits for skin, nails, and other connective tissues.

This study investigates the incorporation of collagen derived from pork skin at different concentrations (10%, 12.5%, and 15%) for the enrichment of cocoa cream products. Particle size distribution in control (C) and collagen-enriched samples (CC10, CC12.5, and CC15) was analyzed using a Mastersizer 2000 (Malvern Instruments). Measurements were conducted with the Malvern Hydro 2000 μ P dispersion unit, with samples dispersed in sunflower oil prior to analysis.

The results demonstrated that increasing collagen concentration resulted in a progressive increase in the volume-weighted mean diameter, D[4,3], across all collagen-enriched samples, whereas the highest value (94.051 μ m) was recorded for the raw material, pork collagen powder (CP). However, in the enriched cocoa cream samples, D[4,3] values did not exceed 30 μ m. Considering that the optimal particle size range (15–30 μ m) is associated with the absence of a gritty mouthfeel, the addition of pork collagen did not negatively affect the sensory quality of the produced samples.

Keywords: protein, pork collagen, cocoa cream products, particle size distribution, functional food products

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BFT-P5

**EFFECT OF PROBIOTIC PREPARATIONS ON
ENTEROBACTERIACEAE AND MICROBIOLOGICAL SAFETY OF RAW
COW'S MILK**

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Not presented.



BFT-P6

GOOD GHG REDUCTION PRACTICES

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Reducing GHG emissions and improving waste management are key challenges for every industry. This abstract presents a practical example of GHG reduction through industrial symbiosis between ALKALOID AD Skopje¹ and Elektro Sharri – Veze Sharri Group, Tetovo².

Since 2024, ALKALOID has supplied plant-based tea production waste to Elektro Sharri's biogas cogeneration plant, where it is used as feedstock which by anaerobic digestion process is converted to renewable energy instead of being landfilled.

Over the period 2024–2025, the diversion of 13.07 tons of organic waste resulted in the avoidance of approximately 24.8 [t] of CO₂ equivalent emissions, including a significant reduction of methane that would otherwise be generated in landfill conditions^{3,4,5}. At the same time, this waste contributed to the generation of approximately 3.4 [MW] of renewable electricity, supporting low-carbon energy production^{7,8,9}.

Keywords: biological waste, anaerobic digestion process, biogas-methane cogeneration plant

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BFT-P7

TOMATO: NUTRITIONAL PROPERTIES, PROCESSING AND BY-PRODUCTS

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Not presented.



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BFT-P8

**RHEOLOGICAL, STRUCTURAL AND SENSORY PROPERTIES OF
KETCHUP AND ITS PRODUCTION FROM TOMATO BY-PRODUCTS**

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BFT-P9

**INFLUENCE OF BOTANICAL ORIGIN ON THE PHYSICOCHEMICAL
PROPERTIES OF HONEYS FROM NORTH MACEDONIA**

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Chemical engineering (CE)



CE-O1

Photocatalytic degradation of 2,5-diphenyl-1,3-oxazole and 2-(4-biphenyl)-5-phenyl-1,3,4-oxadiazole using nanoflowers

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The photocatalytic degradation of the scintillation compounds 2,5-diphenyl-1,3-oxazole (PPO) and 2-(4-biphenyl)-5-phenyl-1,3,4-oxadiazole (PBD) was studied using pure and rare-earth-modified ZnO nanoflowers (Gd³⁺, Sm³⁺, and Eu³⁺). The catalysts were characterized by SEM, EDS, XRD, and photoluminescence spectroscopy, confirming the formation of flower-like ZnO structures and successful rare-earth modification. Residual concentrations of Zn²⁺, Gd³⁺, Sm³⁺, and Eu³⁺ in the treated aqueous solutions were determined by ICP-MS to evaluate catalyst stability, while chemical oxygen demand (COD) was used to assess mineralization efficiency. The photocatalytic activity followed the order ZnO < ZnO–Gd < ZnO–Sm < ZnO–Eu, which can be attributed to the enhanced charge separation and reduced electron–hole recombination caused by rare-earth ion incorporation, with Eu³⁺ providing the most effective electron trapping. PPO showed faster degradation than PBD due to its simpler molecular structure and lower chemical stability, whereas the more rigid and conjugated structure of PBD increases its resistance to oxidative degradation. The modified catalysts also demonstrated good stability and recyclability, indicating their potential for the efficient removal of scintillation contaminants from aqueous media.

Keywords: rare earth, ZnO nanoflowers, scintillators.



CE-P1

EXPERIMENTAL STUDY OF CO₂ ADSORPTION KINETICS ON ZEOLITES USING THE BREAKTHROUGH CURVE METHOD

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The increasing concentration of carbon dioxide (CO₂) in the atmosphere is a major contributor to global climate change, creating a growing demand for efficient carbon capture technologies. Among the available separation methods, adsorption on solid porous materials has emerged as a promising alternative due to its high selectivity, low energy consumption, and operational simplicity. Synthetic zeolites, particularly 13X and 5A, are widely used for CO₂ capture because of their developed microporous structures and favorable adsorption properties.

Although zeolite-based adsorption has been extensively studied, a detailed understanding of the effects of operating conditions on adsorption kinetics is still required for process optimization. In particular, the influence of inlet CO₂ concentration, gas flow rate, and adsorbent type on breakthrough behavior remains of significant interest.

In this study, the adsorption kinetics of CO₂ on synthetic zeolites 13X and 5A were investigated using the breakthrough curve method. Experiments were performed in a fixed-bed adsorption column packed with 22.5 g of adsorbent at a bed height of 9 cm. A CO₂–air mixture was introduced under different operating conditions, with inlet CO₂ concentrations ranging from 5.2% to 15.6% and total flow rates from 14.67 to 21.83 L min⁻¹. Outlet CO₂ concentration and temperature were continuously monitored to determine breakthrough time, saturation time, adsorbed CO₂ mass, and temperature changes during adsorption.

The results showed that increasing the inlet CO₂ concentration and gas flow rate reduced breakthrough and saturation times while increasing the adsorbed CO₂ mass. The adsorption process was accompanied by a measurable temperature rise, confirming its exothermic nature. Zeolite 13X exhibited higher adsorption capacity at CO₂ concentrations around 10%, whereas zeolite 5A showed better performance at lower CO₂ concentrations (~5%). These findings provide useful insights for the optimization of adsorption-based CO₂ capture systems.

Keywords: CO₂ adsorption, zeolites, breakthrough curves, adsorption kinetics, fixed-bed column.



CE-P2

CO₂ ADSORPTION IN A DRAFT-TUBE SPOUT-FLUID BED WITH A HYDRAULIC BARRIER

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Adsorption-based CO₂ capture requires not only highly selective adsorbents, but also an efficient gas–solid contacting configuration that ensures sufficient gas residence time, effective adsorbent utilization, stable particle circulation, and enhanced heat transfer. In this work, CO₂ adsorption was investigated in a draft-tube spout-fluid bed with a hydraulic barrier. This configuration was designed to provide spatial separation between the adsorption zone and particle transport. A CO₂-containing stream was introduced into the annulus as the aeration gas, while a separate air stream was introduced at the bottom of the hydraulic barrier as the spouting gas. In the annulus, particles move downward as a moving packed bed, while the draft tube provides upward particle transport and circulation. The hydraulic barrier suppressed aeration gas bypass into the draft tube and confined adsorption to the annulus. Previous hydrodynamic investigations of this system enabled the selection of suitable geometric and operating conditions characterized by stable particle circulation, low minimum spouting gas flow rate, reduced pressure drop, and favourable gas distribution¹. In this study, the influence of inlet CO₂ concentration and gas flow rates on the breakthrough behaviour was first investigated using zeolites 13X and 5A as adsorbents. Adsorption experiments were then performed under selected optimal hydrodynamic conditions. Outlet CO₂ concentration and bed temperature were measured to determine breakthrough and saturation times, temperature response, and adsorption capacity. The results show that the investigated system can be considered a hybrid gas-solid contactor, combining the favourable contact characteristics of a moving packed bed with the process flexibility of circulating particle systems. Therefore, it represents a promising platform for CO₂ capture and future adsorption-regeneration integration.

Keywords: spout-fluid bed, CO₂ adsorption, breakthrough curves, zeolites.

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CE-P3

**EFFECT OF PYROLYSIS TEMPERATURE ON THE LEACHING
BEHAVIOR OF ENRICHED DIGESTATE BIOCHAR**

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This study aimed to valorize nutrient-rich wastewater from the corn starch industry by using it as a source of plant-relevant nutrients, primarily nitrogen and phosphorus, to enrich anaerobically digested sewage sludge (ADSS). ADSS obtained from the Public Utility Company "Vodovod i kanalizacija" Subotica, Serbia, was enriched with corn starch industry wastewater in a continuous packed-bed column containing approximately 100 g of digestate. The enrichment was carried out over 24 h in a cylindrical plexiglass column with an inner diameter of 40 mm and a height of 180 mm, while 0.7 L of wastewater was continuously mixed and circulated through the column using a peristaltic pump at a flow rate of 4 mL/min.

The enriched digestate was then subjected to pyrolysis at 400, 550, and 700 °C under an argon atmosphere to produce biochars with varying degrees of thermal transformation. The resulting materials were evaluated using a leaching test to determine how pyrolysis temperature affected nutrient release and the mobility of potentially toxic elements. Particular attention was given to balancing the retention of plant-relevant elements and the stabilization of hazardous elements within the carbonaceous and mineral matrix.

The results showed that pyrolysis temperature strongly influenced elemental leaching behavior. Biochars produced at higher pyrolysis temperatures, particularly 550 and 700 °C, generally showed reduced leaching of most potentially toxic elements, indicating improved stabilization within the solid matrix and enhanced environmental safety. This effect may be related to the incorporation of metals into stable carbonaceous and mineral phases. Meanwhile, the biochars retained key plant-relevant elements, including Ca, K, Mg, P, and, to a lesser extent, residual N.

Overall, the combination of nutrient enrichment and controlled pyrolysis produced a stabilized, mineral-enriched biochar with potential as a soil conditioner. These findings suggest that this approach may support the sustainable valorization of both anaerobically digested sewage sludge and nutrient-rich industrial wastewater from the corn starch industry.

Keywords: anaerobically digested sewage sludge, corn starch industry wastewater, pyrolysis, biochar, leaching test, soil conditioner



CE-P4

BISMUTH-MODIFIED WOOD WASTE AS A SUSTAINABLE SORBENT FOR REACTIVE BLUE 19 REMOVAL

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Water pollution is a major environmental concern due to its negative effects on aquatic ecosystems and human health. Textile dyes are particularly problematic among water contaminants because of their widespread industrial use, complex structures, and resistance to degradation, because their release into aquatic environments can reduce light penetration, disrupt aquatic organisms, and introduce potentially toxic or mutagenic substances.¹ Conventional wastewater treatment methods may be ineffective for the removal of persistent dyes, while advanced technologies often require high costs and complex operational conditions. Sorption has therefore attracted considerable interest as an efficient, cost-effective, and environmentally friendly treatment approach, particularly waste-derived materials such as wood waste represent promising sorbents.²

In this context, the present study aimed to develop a bismuth-modified wood waste sorbent and evaluate its efficiency in removing Reactive Blue 19 from aqueous solutions. The sorption performance was assessed through optimization of the sorption process by systematically investigating the influence of key operational parameters, including contact time, solution pH, pollutant concentration, initial dye concentration, and temperature, in order to determine the conditions that favor efficient dye removal. Maximal dye removal was achieved for 40 min, at pH 2, with 2 g/L sorbent dose, at 25 °C, with 300 mg/L complete dye removal indicating the high sorption efficiency and strong potential of the sorbent.

Keywords: wood waste, modification, bismuth, sorption, textile dye

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CE-P5

**FERRITE-BASED SORBENT FOR EFFICIENT REMOVAL OF
REACTIVE BLUE 19 DYE**

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Environmental contamination by organic pollutants, especially reactive textile dyes, represents a serious and persistent threat to living organisms.¹ Reactive Blue 19 (RB19) is a stable anionic dye containing electrophilic vinylsulfone groups, which may contribute to its toxic and mutagenic potential.² Sorption is widely applied for dye removal from water due to its efficiency, low cost, and simple operation. Ferrites are versatile ferrimagnetic materials whose properties depend on their composition, structure, and synthesis conditions. Among them, spinel ferrites are the most common. Their chemical and thermal stability, easy synthesis, low cost, and diverse magnetic and catalytic properties make ferrites promising materials for sorption and water purification.

The zinc–manganese ferrite carbonate was synthesized by coprecipitation. Bach experiments evaluated the influence of pH, dye concentration, contact time, and sorbent dosage on RB19 removal. Sorption mechanisms were analyzed using kinetic (pseudo-first and pseudo-second order) and isotherm (Langmuir, Freundlich and Brouers–Sotolongo) models. Optimal sorption of RB19 was achieved at pH 2 and sorbent dose of 0.25 g/L, yielding a maximal sorption capacity of 1463.1 mg/g. The process is driven by electrostatic interaction between positively charged sorbent sites and the RB19 sulfonic groups, supported by Van der Waals forces. Kinetic and equilibrium studies confirm chemisorption as the dominant mechanism, with Langmuir isotherm fitting indicating a homogeneous sorption surface.

Keywords: nanosorbent; ferrites; carbonate; sorption;

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CE-P6

INFLUENCE OF PHYSICAL AND CHEMICAL PARAMETERS ON THE RHEOLOGICAL PROPERTIES OF MODIFIED DISTARCH

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Distarch adipate is a highly utilized modified starch valued for its texturizing stability. This study aims to investigate how specific physical and chemical processing variations alter its rheological profile, providing essential data for optimizing industrial-scale starch modification. Starch modification was performed in a controlled 600 mL reactor system integrated with automated stirring, temperature, pH regulation, and precise dosing. The effects of shifting parameters—specifically acetic anhydride and adipic acid concentrations, modifier preparation time/temperature, water and sulfate levels, and various mixing intervals—were comprehensively evaluated. All rheological changes were characterized using a Brabender amylograph. The resulting Brabender amylograms demonstrated that adjustments in modifier concentration and reaction temperature directly dictate the peak viscosity and gelatinization onset. The results indicate that achieving high-performance distarch adipate requires a careful balance of all components and process conditions, as a shift in a single parameter significantly alters the overall rheological behavior. The optimized starch matrix must exhibit excellent texture, acid and shear resistance, and high water-holding capacity. Mixing time and sulfate presence primarily influenced the breakdown and setback viscosity profiles. In conclusion, this work presents a systematic overview of how chemical dosing and mechanical handling inside a reactor can be adjusted to tailor the visco-elastic performance of distarch adipate. These insights allow for precise customization of starch properties for specific food and industrial formulations requiring high stability.

Keywords: distarch adipate, rheology, Brabender amylograph, water-holding capacity, process optimization.



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Textile engineering (TE)



TE-O1

RAW WOOL SCOURING – DIFFERENT DETERGENTS AND THEIR SCOURING RESULTS

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The revival of regional wool processing requires sustainable and decentralised methods for scouring raw wool. In this context, the Department of Textile Technology of Chemnitz University of Technology is developing a compact wool scouring machine for small and medium-sized manufacturers together with environmentally friendly washing processes. The aim is to provide a resource-efficient alternative to the big, centralised wool scouring facilities.

The research focuses on a modular wool scouring system with mechanical pre-cleaning, washing and rinsing stages, and a centrifuge unit to reduce wastewater carryover. A key challenge is the machine design and the scouring parameters in combination with scouring process.

Initial laboratory trials with Saxon raw Merino wool investigated different detergents, including industrial surfactant-based detergents, traditional potash cleaning, and a plant-based solution made from horse chestnuts. Cleaning performance was evaluated using CIE whiteness and yellowness measurements.

The results showed that all washing systems improved the optical properties of the wool. The highest whiteness values were achieved with surfactant-based detergents, especially "Power Scour." The horse chestnut solution also demonstrated good cleaning performance and strong potential as a sustainable option for decentralized wool washing, while potash cleaning was less effective and partly increased fibre felting.

Overall, both surfactant-based and plant-based scouring methods are promising approaches for sustainable regional wool processing. Future work will optimise process parameters and evaluate residual grease content and wastewater sustainability.

Keywords: Wool, Scouring, Sustainable Wool Scouring, Saxon merino wool, surfactant-based detergents, bio-based detergents, CIE whiteness, yellowness index

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TE-P1

MULTIFUNCTIONAL COTTON TEXTILES MODIFIED WITH LA-DOPED TiO₂: SELF-CLEANING AND ANTIBACTERIAL PERFORMANCE

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Lanthanum-doped titanium dioxide nanopowder were successfully synthesized via sol-gel technology and deposited onto cotton textile substrates to obtain multifunctional materials. Two La-doped compositions containing 2 and 5 mol% were investigated to evaluate the influence of dopant concentration on the structural, morphological, optical, and functional properties of the coated textiles.

The prepared materials were comprehensively characterized using X-ray diffraction (XRD), Scanning electron microscopy (SEM), Transmission electron microscopy (TEM), Fourier-transform infrared spectroscopy with attenuated total reflectance (FTIR-ATR), and UV-Vis spectroscopy. The analyses confirmed the successful incorporation of La into the TiO₂ structure and the uniform deposition of the photocatalyst onto the cotton fibers while preserving the textile morphology.

The photocatalytic self-cleaning performance of the coated textiles was evaluated through the degradation of Methylene blue and Malachite green dyes. Both La-doped samples demonstrated good discoloration efficiency. Furthermore, the antibacterial properties of the functionalized textiles were assessed against *Escherichia coli*. A pronounced inhibition of bacterial growth was observed for all modified samples, with the antibacterial effectiveness increasing with the lanthanum content.

The obtained results demonstrate that La-doped TiO₂-coated cotton textiles exhibit promising self-cleaning and antibacterial properties, making them attractive candidates for advanced functional textile applications in healthcare, environmental remediation, and protective materials.

Keywords: modified textile, sol-gel, self-cleaning, antibacterial properties.

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TE-P2

USING NATURAL EXTRACTS FOR IMPARTING COLOR AND ANTIOXIDANT ACTIVITY TO COTTON, CELLULOSE ACETATE, AND POLYAMIDE FABRICS

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Potentilla erecta L., *Galium verum* L., and *Melilotus officinalis* L. extracts were prepared using ultrasound-assisted extraction under the following conditions: 70% (v/v) ethanol, 30 min, 60 °C, with a liquid-to-solid ratio of 40 mL/g. After the dilution, the UV-Vis spectra of the prepared extracts were recorded, and their antioxidant activity was determined using the ABTS test. The obtained results revealed that all extracts exhibited antioxidant activities exceeding 98%. Such characterized diluted extracts were further employed for the functionalization and/or dyeing of cotton, cellulose acetate, and polyamide fabrics. The antioxidant activities of cotton, cellulose acetate, and polyamide fabrics functionalized with *Potentilla erecta* L. extract were found to be 90.19%, 95.78%, and 99.40%, respectively. Cotton, cellulose acetate, and polyamide fabrics functionalized with *Galium verum* L. extract displayed antioxidant activities of 52.56%, 79.71%, and 99.25%, respectively. Corresponding results for antioxidant activity of fabrics functionalized with *Melilotus officinalis* L. extract were 77.60%, 88.16%, and 100%, respectively. Among examined extracts, *Potentilla erecta* L. has an affinity for dyeing fabrics, therefore, their color coordinates were determined. Colorimetric measurements pointed out that functionalized cellulose acetate manifests a lighter and greener appearance compared to cotton and polyamide fabrics, while functionalized cotton fabric demonstrated a yellower tonality in relation to the cellulose acetate and polyamide fabrics. The release of bioactive compounds from nine functionalized fabrics was monitored in a physiological saline solution at 37 °C for 24 h. Based on the results, it can be concluded that cotton fabric functionalized with *Potentilla erecta* L. extract has the highest release of bioactive compounds, making it suitable for producing high-value-added medical textiles with protective functions such as wound dressing. Additionally, all other fabrics possessing excellent antioxidant activities (>90%) can also be considered for use in disposable medical textiles.

Keywords: natural extracts; antioxidant activity; color; fabric

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TE-P3

EFFECTS OF SALT, POLYELECTROLYTE CONCENTRATION, AND pH ON THE FLAME-RETARDANT AND MECHANICAL PROPERTIES OF COATED NYLON–COTTON FABRIC

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Blended nylon–cotton (NYCO) fabric combines the comfort of cotton with the strength of nylon, but its flammability limits its use in protective clothing. In this study, a sustainable, water-based coating composed of egg white proteins (EWP), pectin (P), and guanidine phosphate (GP), a phosphorus- and nitrogen-containing salt, was applied to NYCO fabric through a two-step process. The effects of salt addition, polyelectrolyte concentration, and pH on coating deposition, flame retardancy, and mechanical properties were investigated.

The EWP/P coating without GP produced only 1.8% weight gain and did not prevent complete burning. As a salt, GP induced charge screening along the pectin macromolecules, reducing electrostatic repulsion and increasing coating deposition. It also acted as an acid source and blowing agent within the intumescent system. This behavior agrees with the effects of ionic strength, pH, and charge density on weak-polyelectrolyte deposition.¹ Increasing the EWP, P, or GP concentration improved flame retardancy. The 4% EWP/(1% P–20% GP) formulation was subsequently deposited at pH 2, 3, and 4 to evaluate the influence of pH. Although all three coatings self-extinguished, pH 3 provided the best balance between flame retardancy and mechanical performance, producing 14.8% weight gain and the lowest char length of 127 mm. At pH 2, deposition was accompanied by reduced tensile strength due to cellulose hydrolysis, whereas pH 4 preserved tensile strength but resulted in lower deposition and a longer char length. The pH 3 treatment retained a tensile strength of 1333.5 N, comparable to 1345.5 N for uncoated NYCO, while the coating slightly increased stiffness and reduced elongation and air permeability.² These findings show that controlling GP addition, polyelectrolyte concentration, and pH enables effective flame retardancy while preserving NYCO mechanical performance.

Keywords: nylon–cotton fabric, flame retardancy, polyelectrolyte complex, pH

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TE-P4

LACCASE-CATALYZED OLIGOMERIZATION OF ESCULIN FOR *IN SITU* DYEING AND FUNCTIONALIZATION OF WOOL FABRIC

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In pursuit of sustainable and environmentally friendly green dyeing processes, the use of laccases and natural polyphenolic compounds has emerged as a suitable alternative to the established synthetic dyeing protocols. Laccases are considered to be eco-friendly enzymes due to their use of molecular oxygen and production of water as the only by-product. The application of laccases in dyeing and functionalization of textile materials is based on their ability to oxidize a broad range of substrates including naturally occurring flavonoids. This reaction can yield colored flavonoid oligomers/polymers that have potential to be applied in textile industry as colorants. Additionally, these compounds can add novel functionalities to textile materials. Esculin, a coumarin glycoside with many beneficial biological activities, is among the substrates of laccase. In this work, laccase from *Trametes versicolor* was applied as a catalyst in the reaction of oligomerization of esculin to its colored oligomers enabling the *in situ* simultaneous dyeing and functionalization of wool fabric. The antioxidant activity of the dyed wool fabric was tested before and after washing cycle. Wool fabric showed moderate ABTS radical scavenging ability (53.32%) which remained in the same range after washing (50.78%). In order to improve the bioactivity, wool fabric was modified with chitosan and functionalized under the same conditions. The ABTS radical scavenging activity of dyed and functionalized chitosan-modified wool fabric was significantly improved, reaching an inhibition rate of 96.18%, while an inhibition rate of 80.12% was retained after the washing cycle. These results indicate that the applied process can broaden the applicability of laccase in textile industry for the production of colored and functional wool fabrics.

Keywords: textile dyeing; esculin, laccase; oligomerization; wool, functionalized fabrics; antioxidant activity

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Quality, Regulatory Affairs and Industrial Management (QRAIM)



QRAIM-P1

APPLICATION OF STATISTICAL TOOLS FOR TREND ANALYSIS OF NON-CONFORMITIES: EXPERIENCE FROM ALKALOID

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In the pharmaceutical industry, managing non-conformities is not only a regulatory requirement, but also essential for maintaining product quality and patient safety. As processes become more complex, there is a growing need to move from simple deviation tracking to a more structured and data-driven approach. Statistical tools play an important role in this transition by enabling better understanding of process behavior and early identification of potential risks.

At Alkaloid AD Skopje, statistical analysis is integrated into the quality management system as part of routine deviation management. The objective is not only to document deviations, but to analyze them systematically over time in order to detect recurring patterns and identify areas for improvement.

One of the main approaches is the use of trend and control charts. These tools help visualize the frequency and distribution of non-conformities and allow teams to distinguish between normal variability and signals that may indicate underlying issues. Deviations are categorized and grouped based on type, process stage, or potential cause. Correlation analysis is also used to explore possible relationships between process parameters and deviations, such as the impact of environmental conditions or raw material variability.

Experience at Alkaloid demonstrates that applying statistical tools for trend analysis helps identify meaningful patterns, minimizes repeated deviations, and contributes to continuous improvement aligned with GMP and ICH expectations.

Keywords: Non-conformities; Trend analysis; Statistical tools; Control charts; Deviation management; Process variability; Quality management system; Data analysis; Continuous improvement; GMP compliance

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QRAIM-P2

ROOT CAUSE ANALYSIS (RCA) AND CORRECTIVE ACTION/IMPROVEMENT ACTION (CAIA) AS KEY TOOLS IN MANAGEMENT OF NON-CONFORMITIES

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The pharmaceutical industry operates under strict regulatory frameworks to ensure that medicinal products meet the highest standards of quality, safety, and efficacy of the products¹. Effective management of non-conformities in the pharmaceutical industry is essential for ensuring product quality, patient safety, and regulatory compliance.

While reporting of any nonconformity is mandatory, the key objective is identifying root causes and preventing recurrence. Root Cause Analysis (RCA) and Corrective and Preventive Actions (CAPA) are therefore fundamental elements of the pharmaceutical quality system² as part of lifecycle management³.

This study focuses on the most common tool used in Alkaloid AD Skopje, Ishikawa Fishbone Diagram and 5Whys, as root cause analysis as important and powerful methods for resolving cause in the investigations and defining appropriate corrective action. RCA and CAPA represent essential tools for managing non-conformities in the pharmaceutical industry and preventing their recurrence. Based on the performed root cause identification, CAIA is implemented through clearly defined actions, tracking, and effectiveness verification. Risk-based thinking ensures proportionality of investigations and actions⁴.

The integration of RCA findings into CAPA strategies enables organizations to eliminate root causes effectively, prevent recurrence, and strengthen process robustness.

Keywords: Root cause analysis (RCA), Fishbone diagram (Ishikawa), 5 Whys, Corrective action/Improvement action (CAIA), Non - conformities

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Education (EDU)



EDU-01

**AN ANALYSIS OF SYSTEMS THINKING SKILLS IN CHEMISTRY
EDUCATION USING A BIBLIOMETRIC APPROACH**

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Chemistry education has historically developed through a reductionist approach focused on molecular structures, formulas, and reaction mechanisms. Although this approach has made significant contributions to the production of scientific knowledge and technological advancement, it is not sufficient on its own to address complex problems such as climate change, pollution, resource depletion, and sustainability. Therefore, chemistry education needs to be reconceptualized through a holistic approach that considers chemical processes in relation to social, economic, and environmental systems. In this context, systems thinking has emerged as an important approach for understanding the dynamic relationships among the components of complex structures, feedback loops, and the emergent properties of a system as a whole. Accordingly, it is important to transform chemistry curricula on the basis of systems thinking and to support students in developing systems thinking skills. The aim of this study is to examine the development, main trends, and research gaps in academic studies on systems thinking and related skills in the chemistry education literature through bibliometric analysis. Within this scope, the study was conducted in the Web of Science (WoS) database using the keywords (("systems thinking" OR "system thinking") AND ("skill" OR "skills") AND ("chemistry")), and 108 sources were retrieved. Studies outside the Education Educational Research category and book chapters were excluded from the dataset, and the analyses were conducted based on 76 articles. The study examined publication and citation trends by year, the productivity and collaboration levels of countries, and the shared citation network. The findings indicate a marked increase in the number of publications and citations after 2019, suggesting that systems thinking skills have become an emerging paradigm in chemistry education. Publication and collaboration analyses by country show that the USA, Canada, Israel, and England are the countries contributing most substantially to the field, whereas Turkey's contribution remains relatively limited. Keyword analysis reveals that "systems thinking" is located at the conceptual center of the field and that this concept reflects the current direction of the field through its strong connections with "sustainability" and "green chemistry". Co-citation analysis shows that the study by Orgill et al. (2019) is the most cited study in the field.¹ In conclusion, systems thinking skills can be considered an emerging research area in chemistry education, and further studies are needed in this field.

Keywords: System thinking skills, chemistry education, bibliometric analysis

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EDU-02

THE EFFECT OF CHEMISTRY-BASED STEM ACTIVITIES ON HIGH SCHOOL STUDENTS' ARGUMENTATION QUALITY

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The purpose of this study is to investigate the effect of chemistry-based STEM activities on students' argumentation quality. The study involved 22 tenth graders in 2023–2024. Over 10 weeks, three STEM activities were implemented, each incorporating relevant learning outcomes from the chemistry topics of "Mixtures," "Acids, Bases and Salts," and "Chemistry Everywhere." Students followed Engineering Design Process¹ and answered 16 open-ended questions across its steps. However, within the scope of this study, we focused on the responses to the five questions corresponding to the first two steps of the Engineering Design Process. The questions were written on Padlet platform and asked students to response them individually on Padlet as a homework study. The responses were analyzed using the rubric developed by Venville and Dawson (2010), which includes levels representing argumentation quality². For instance, while Level 1 includes only a claim, Level 3 includes arguments in which students use a claim, data or warrants and backing. The responses were coded independently by two researchers, and disagreements were resolved through discussion. The findings showed that in Activity 1, most individual written arguments were at Level 1, whereas fewer were at Levels 2 and 3. In Activity 2, the distribution of argumentation levels was 163, 74, and 3, respectively. In Activity 3, the corresponding frequencies were 128, 79, and 7. Although Level 1 arguments were predominant across all three activities, the frequencies of Level 2 and Level 3 arguments increased from Activity 1 to Activity 3. This finding indicates that students gradually moved beyond merely presenting claims and began to justify and support their arguments with evidence. The improvement in argumentation quality suggests that the activities may enhance students' achievement.

Keywords: STEM, Chemistry Education, Argumentation

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EDU-P1

**A STUDY OF COOPERATIVE INQUIRY-BASED INSTRUCTION
SUPPORTED BY MOLECULAR MODELS IN CARBOHYDRATE
STEREOCHEMISTRY EDUCATION**

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Understanding stereochemistry is fundamental to the study of biomolecules, as even subtle changes in their spatial orientation can lead to significant differences in their properties and biological activity. Despite its importance, stereochemistry is one of the most conceptually challenging topics in chemistry education, highlighting the need for innovative teaching approaches that enhance visualization and promote conceptual understanding.

The aim of this research was to examine how the application of the Inquiry-Based Learning (IBL) approach, implemented through cooperative work and the use of molecular models, affects the acquisition of knowledge in carbohydrate stereochemistry among high school students. The research was conducted in two parallel groups: the experimental group participated in a teaching process based on the IBL approach, while the control group followed the traditional methodological approach. Students in the experimental group worked collaboratively and engaged in a three-phase learning cycle: exploration, concept invention, and application. During the activities, they used molecular models to visualize, construct, and analyze three-dimensional carbohydrate structures, as well as to identify and interpret different structural representations of carbohydrates.

After the implemented intervention, data on students' attitudes and experiences were collected using a questionnaire, while acquisition of the teaching content was assessed through a knowledge test. The questionnaire results showed that students in the experimental group found the activity highly motivating and useful for understanding stereochemical concepts, noting increased engagement and improved conceptual understanding. They also expressed a preference for interactive and exploratory teaching approaches over traditional methods. Analysis of the knowledge test results indicated that students in the experimental group achieved a higher level of content acquisition than those in the control group. These findings highlight the importance of integrating different teaching approaches to enhance teaching quality and improve student achievement.

Keywords: carbohydrate stereochemistry, conceptual understanding, inquiry-based learning, molecular models.



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ФАРМАХЕМ Е ПРЕПОЗНАТЛИВ И ДОВЕРЛИВ ПАРТНЕР ВО ЛАБОРАТОРИСКИТЕ И ИНДУСТРИСКИТЕ РЕШЕНИЈА, СО 35 ГОДИНИ ПРОФЕСИОНАЛНО ИСКУСТВО И КОНТИНУИРАНА ПОСВЕТОСТ КОН КВАЛИТЕТОТ, ПРЕЦИЗНОСТА И ИНОВАЦИЈЕТЕ.



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