BOOK OF ABSTRACTS

6th International Congress
of Chemists and Chemical Engineers
of Bosnia and Herzegovina

26

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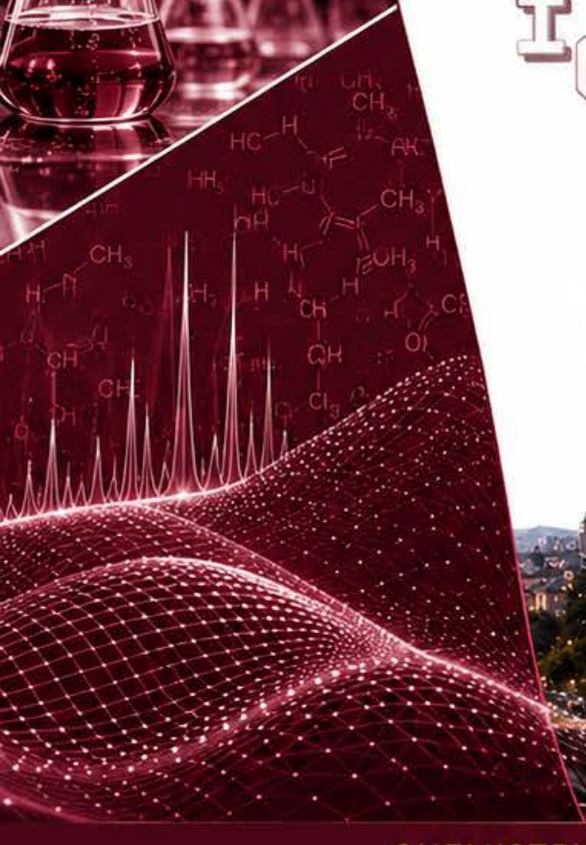

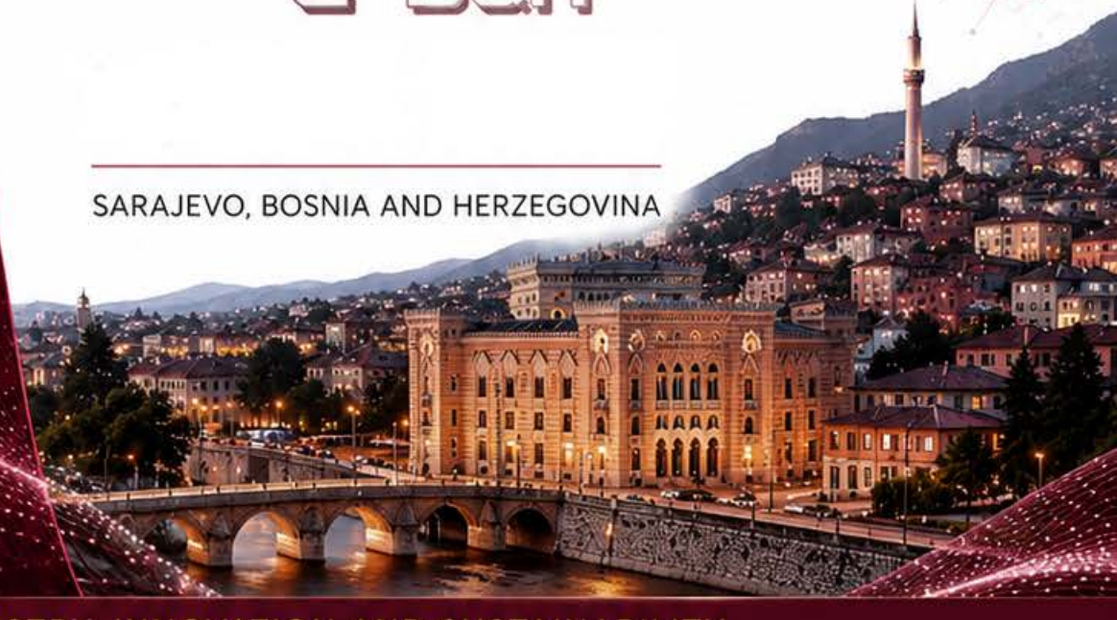

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CHEMISTRY, INNOVATION AND SUSTAINABILITY
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6th International Congress of Chemists and Chemical Engineers of Bosnia and Herzegovina organized by

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GENERAL INFORMATION

Congress dates
24 June-27 June 2026 / Sarajevo, B&H
Web: https://icccebih.dktks.ba/

Language
The official language of the ICCCEB&H 2026 is English

Venue and Registration
Hotel Radon Plaza, Džemala Bijedića 185, Sarajevo 71000
Registration desk will be open on Wednesday (24 June 2026) from 18:00 to 19:30;
Thursday (25 June 2026) from 8:30 to 09:30

Satelitte Event

Venue: University of Sarajevo – Faculty of Science, Zmaja od Bosne 33-35, 71000 Sarajevo
Date and Time: Thursday, 25 June 2026, 11:00 – 15:00

KEY TO ABSTRACT IDENTIFICATION

PL	Plenary Lectures
KL	Keynote Lectures
OP	Oral Presentations
PP-AER	Poster presentations - Analytical, Environmental & Radiochemistry
PP-OIMB	Poster presentations - Organic, Inorganic, Medicinal & Biochemistry
PP-MC	Poster presentations - Materials Chemistry
PP-CCEST	Poster presentations - Catalysis, Chemical Engineering & Sustainable Technologies
PP-PTAIC	Poster presentations- Physical, Theoretical & Artificial Intelligence Chemistry

WELCOME NOTE

On behalf of the Organizing and Scientific Committees, the Society of Chemists and Technologists of Canton Sarajevo, and the Department of Chemistry at the University of Sarajevo – Faculty of Science, it is my great pleasure and honor to welcome you to the 6th International Congress of Chemists and Chemical Engineers of Bosnia and Herzegovina (6th ICCCEB&H 2026).

Since its establishment, the Congress has grown into an important platform for bringing together researchers, educators, students, and professionals from academia and industry. It provides a unique opportunity to exchange scientific knowledge, discuss current challenges, and explore innovative solutions that contribute to the advancement of chemistry, chemical engineering, and related disciplines.

The scientific programme of the Congress reflects the diversity and interdisciplinary nature of contemporary chemical sciences. Through plenary and keynote lectures, oral presentations, poster sessions, and discussions, participants will share their latest research findings and establish valuable collaborations that may lead to future scientific achievements and joint initiatives. In addition, a satellite event for primary and secondary school chemistry teachers will be held as part of the Congress, fostering discussion on the growing role of artificial intelligence in chemistry education and its implications for teaching, learning, and pedagogical practice.

We are particularly proud to welcome participants from different countries and institutions, whose presence enriches the scientific and cultural dimensions of this event. Your contributions are essential to creating a dynamic environment that encourages creativity, critical thinking, and the exchange of ideas.

All accepted abstracts will be published in a special issue of the Bulletin of Chemists and Technologists of Bosnia and Herzegovina, while selected papers will be considered for publication in the journal following the peer-review process.

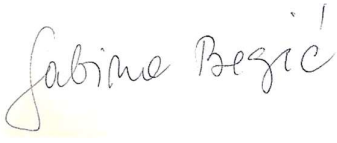
I would like to express my sincere gratitude to the members of the Organizing Committee, International Scientific and Advisory Committee, and Scientific Committee for their dedication and hard work. I also extend my appreciation to all authors, speakers, participants, sponsors, and partners whose support and commitment have made this Congress possible.

I warmly welcome you to Sarajevo and wish you a productive, inspiring, and enjoyable Congress. May the discussions, ideas, and collaborations initiated here contribute to scientific excellence and strengthen the connections within our international scientific community.

With my best wishes for a successful Congress,

Congress Chair

Dr. Sabina Begić



PLENARY LECTURER

Dr. Debbie C. Crans

Department of Chemistry and Cell & Molecular Biology Program

Colorado State University

United States of America

PLENARY LECTURER

Dr. Stefan Wuttke

Department of Nanoscience, Academic Centre for Materials and Nanotechnology

AGH Krakow

Poland

PLENARY LECTURER

Dr. Adisa Azapagić

Department of Chemical Engineering

The University of Manchester

England

PLENARY LECTURER

Dr. Blaž Likozar

Department of Catalysis and Chemical Reaction Engineering

National Institute of Chemistry Ljubljana

Slovenia

PLENARY LECTURER

Dr. Damir Brđanović

IHE Delft (formerly UNESCO-IHE) Institute for Water Education and Endowed Professor at Delft University of Technology

Netherlands

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Dr. Tarita Biver

Department of Chemistry and Industrial Chemistry

University of Pisa

Italy

KEYNOTE LECTURER

Dr. Ivana Škugor Rončević

Faculty of Chemistry and Technology

University of Split

Croatia

KEYNOTE LECTURER

Dr. Tamara Terzić

VINČA – Institute of Nuclear Sciences

University of Belgrade

Serbia

PLENARY LECTURER – Satellite Event

Dr. Silvija Markić

Ludwig-Maximilians-University Munich

Germany

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Coordination Chemistry, Metal Speciation, and Intracellular Reactivity in Vanadium-Based Therapeutics

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Keywords: Oxovanadium Complexes; Schiff Base Ligands; Protein Tyrosine Phosphatases (PTSs); PTP1B; Intracellular Speciation; Vanadium-Based Therapeutics; Coordination Chemistry; Nanoparticle-Assisted Delivery

Abstract: Vanadium, a first-row transition metal and naturally occurring trace element, forms a wide range of coordination complexes with emerging therapeutic potential. Our work has focused on the development and characterization of novel vanadium compounds, including several classes of oxovanadium Schiff base complexes, as potent inhibitors of regulatory protein tyrosine phosphatases (PTPs) (1–2). PTPs are versatile signaling enzymes implicated in numerous disease processes; in particular, protein tyrosine phosphatase 1B (PTP1B) is closely associated with glucose dysregulation in diabetes, whereas dual-specificity phosphatase 5 (DUSP5) has recently emerged as a potential modulator of cocaine addiction pathways (3). PTPs catalyze phosphate ester hydrolysis which is inhibited by five-coordinate vanadium complexes mimicking transition states and high-energy intermediates (1,4). However, vanadium complexes exhibiting a wide range of coordination geometries are effective PTP inhibitors, suggesting that coordination environment, ligand architecture, redox behavior, and, importantly, intracellular speciation contribute to the observed biological activity in both cellular and animal model systems. Emphasis must therefore be placed on the speciation chemistry and intracellular processing of vanadium complexes, as these factors critically influence pharmacological efficacy. Strategies to improve therapeutic performance include ligand modification, method of administration, co-administration approaches, and nanoparticle-assisted delivery systems, several of which have resulted in substantial enhancements in compound activity (6). Collectively, these studies highlight the central importance of coordination chemistry, metal speciation, and intracellular reactivity in the development of vanadium-based therapeutics.

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Metal–Organic Frameworks: From Discovery to a Nobel Legacy

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Keywords: MOFs, Nobel Prize, Pore Chemistry, Aerogels, Life Cycle Assessment

Abstract: Metal-organic frameworks (MOFs) reticular pore chemistry addresses the precise control over the position and spatial arrangement of the installed functionalities guided by the framework scaffold. Its chemistry operates in an infinite space of composition, structure, property, application and hence has given us an infinite freedom to build an enormous variety of new porous materials – but also placed upon us a profound responsibility to use it wisely. The responsibility – especially after winning the Nobel Prize in Chemistry – lies in identifying:

1. What are the key scientific questions that still need to be answered?
2. What are the societal challenges that reticular science can address?
3. How can reticular chemistry can provide real and sustainable solutions?

In this talk, we will explore these questions and reflect on our role in shaping the future of high-performance MOF materials enabling sustainable technologies. We will outline a general strategy using MOFs as molecular scaffolds to systematically construct and probe noncovalent interactions by positioning selective chemical groups and measuring associated electric fields as a universal, physics-based metric. That approach reveals a range of interaction strengths and guides design rules for functionality. We also present MOF-derived aerogels engineered for practical applications such as atmospheric water harvesting and removal of persistent contaminants like PFAS from water, illustrating translational pathways from molecular design to devices. Central to advancing MOF technologies is confronting the "sustainability paradox": many materials intended for sustainable use are produced via resource-intensive processes. We argue that qualitative green claims are inadequate and that quantitative tools—notably Life Cycle Assessment (LCA)—are essential to evaluate environmental impacts from *cradle to grave*. To link performance with environmental cost, we introduce a Performance–Sustainability Indicator (PSI) that balances functional benefit against footprint, enabling objective comparisons and design tradeoffs. Embedding sustainability metrics and principles into reticular chemistry will shift MOFs from academic curiosities toward responsible materials that contribute meaningfully to sustainable future.

Acknowledgment
I would like to deeply thank my collaborators and all of the former and current members of the "Wuttkegroup for Science".

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A Life Cycle Approach to Identifying Sustainable Technologies

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Keywords: Climate change; Life cycle assessment; Sustainable production; Sustainable technologies

Abstract: Unprecedented sustainability challenges we face today require novel, innovative responses. The implementation of innovative solutions is fundamental to addressing these challenges and scientists and engineers have a key role to play in delivering such solutions. However, the key question is: how do we identify sustainable solutions to ensure that we do not fix one sustainability issue while creating a number of other problems? This talk will argue that we can only do this by applying a whole systems approach and life cycle thinking to capture and address the complex interrelationships between different aspects of sustainability. This will be illustrated by considering real-life examples related to biofuels, plastics and negative emissions technologies.

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Beyond Sewers: Addressing the Hidden Challenge of Faecal Sludge in Cities

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Keywords: Septic Sludge, Faecal Sludge, Wastewater, Sewage, Co-treatment, Modelling

Abstract: In common sanitary engineering practice, it is often overlooked that faecal and septic sludge and municipal wastewater have distinctively different characteristics – the fact that can negatively influence performance as well as operational cost of wastewater treatment plants. This paper highlights the main differences in composition of faecal/septic sludge and sewage, and how these may influence the process engineering and design practice. It also presents the new Global Database of Faecal Sludge Analysis which reveals wealth of information on faecal and septic sludge characteristics, clearly supporting the motivation to write this paper. In addition, the results of the recent modelling study presented in this paper revealed interesting results in this respect. We have selected several full-scale wastewater treatment plants with different process configurations and run number of simulations describing the current plant operation receiving influent containing mostly municipal wastewater with limited contribution from septic/feacal sludge. We investigated hypothetical cases in which we applied an additional influent load to the plant originating from non-sewered sanitation. Three types of typical faecal/septic sludge compositions were used in the study: fresh faecal sludge, old septic sludge and a mixture of the two. In the model simulations, each plant was gradually loaded with the feacal sludge in addition to the original wastewater influent and individual process unit performances across the plant was monitored. When necessary, the operational mitigation measures were introduced in the model, until the overload point where one or more effluent quality parameters exceeded the regulatory limit. This was repeated for each plant and with three types of sludges. The results were compared between the treatment plants and conclusions are drawn about the capacity of different wastewater treatment processes to deal with septic/faecal sludge load.

Acknowledgment

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Chemical Engineering Challenges in Future Energy or Resource Optimisation

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Keywords: Multifunctional Catalyst Design, CO_2 Conversion, Ammonia Decomposition, Hydrogen Carriers, Biomass Valorization

Abstract: The design of a multifunctional catalyst can be optimized by modeling at multiple descriptive scales, allowing the tailoring of the catalyst composition, structure, and morphology for applications in CO_2 conversion, nitrogen utilization, and biomass valorization. Examples will present the methodology in catalytic carbon, nitrogen and hydrogen cycles outlined. During the methanol synthesis from CO_2, the hierarchical structure of heterogeneous $Cu/ZnO/Al_2O_3$ catalysts evolves under reaction conditions, which makes process optimization difficult and often leads to suboptimal performance. An extensive literature review shows that catalytic activity is strongly related to Cu–Zn interactions. To investigate this behavior, experimental data from catalytic reactor studies using an activated commercial catalyst exposed to different aging conditions were obtained. In addition to CO_2 conversion, nitrogen reduction and ammonia decomposition are also very important catalytic challenges. As the storage and transportation of compressed or liquefied hydrogen remains expensive and hazardous, alternative hydrogen carriers such as ammonia are attracting increasing attention. However, achieving instant start-up of conventionally heated ammonia decomposition reactors remains challenging. This presentation will therefore highlight the electrified, dynamically responsive ammonia decomposition. The principles of catalyst design can also be extended to biomass valorization, especially lignin upgrading, which is challenging due to the structural diversity of lignin compared to sugar-derived feedstocks. The kinetics of hydrodeoxygenation (HDO) of eugenol, a model compound of lignin, have been systematically investigated with commercially available hydrotreating catalysts. Previous studies have investigated the influence of noble metals (Pt, Pd, Rh, Ru) and non-noble metals (Ni, Cu) supported on carbon/supports.

Acknowledgment

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AI in Chemistry Education: Between Innovation and Pedagogical Responsibility

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Keywords: AI, Chemistry Education, Pedagogical Approaches

Abstract: This session critically examines the integration of Artificial Intelligence (AI) into contemporary chemistry education and reflects on the opportunities and challenges that arise from rapid technological developments. Rather than focusing exclusively on the use of new digital tools, the seminar emphasizes the changing role of educators in increasingly digital learning environments. Teachers are viewed not merely as users of technology, but as moderators and facilitators who guide meaningful and scientifically grounded learning processes. A central focus of the seminar is the pedagogical and ethical responsibility connected to the implementation of AI in science education. Participants will discuss how AI can be integrated in ways that support authentic learning, Scientific Literacy, and student engagement without undermining critical thinking or reflective inquiry. Special attention will be given to the risks of overreliance on algorithmically generated information and the importance of maintaining methodological rigor in chemistry education. The seminar further explores how AI can contribute to inclusive and adaptive teaching practices while preserving the integrity of scientific learning. Through critical discussion and reflection, participants will be encouraged to evaluate the educational value, limitations, and implications of AI-supported teaching approaches. The overall aim is to empower educators to engage with AI confidently, responsibly, and critically, ensuring that technological innovation remains a meaningful tool for fostering deep understanding of chemistry and preparing students for future scientific and societal challenges.

KEYNOTE LECTURES

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Spectroscopic Challenges in Dye–Nucleic Acid Binding Equilibria Analysis

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Keywords: Binding Mechanism, Thermodynamics, Metal Complexes, Nucleic Acids, Spectroscopy

Abstract: The mechanistic investigation of the interaction between a target molecule (frequently a metal complex considered for medicinal applications) and a biomolecule (nucleic acids, proteins) can be carried out through absorbance and fluorescence titrations, often combined with complementary methods and melting experiments. Although titrations may appear to be rather classical approaches, they are far from outdated. In fact, despite their apparent simplicity, they remain highly powerful techniques and may sometimes lead to unexpected or misleading interpretations. Careful experimental design and data analysis are therefore essential to obtain reliable mechanistic information on the interaction processes involved. This contribution will discuss recent results concerning the different binding modes promoted by both metal centres and ligands towards several bio-targets. These include proteins, natural DNA and RNA polynucleotides, as well as more peculiar oligonucleotide structures such as G-quadruplexes and four-way junctions. Emphasis will be placed on some critical and less straightforward aspects related to the spectroscopic analysis of these complex systems, highlighting possible pitfalls in the interpretation of titration and fluorescence data and discussing strategies to improve the reliability of the obtained results.

Acknowledgment

This research was supported by funding through grant number 2022APCTNA for the Project PRIN2022 - "TRILLI" provided by MUR - Ministero dell'Università e della Ricerca (Italian Ministry for University and Research). The ISMeC Group (International Group for the Thermodynamics of Metal Complexes, www.ismecgroup.org) is also acknowledged for fruitful discussion, scientific exchanges and support.

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Transition Metal Coordination Compounds in Electrochemical Sensing and Catalysis: From Synthesis and Structure to Dopamine Determination

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Keywords: Coordination Compounds; Dopamine; Electrochemical Sensing; Cyclic Voltammetry; Impedance Spectroscopy

Abstract: Transition metal coordination compounds are increasingly recognised as adaptable platforms for electrochemical sensing, owing to their tunable redox behaviour, structural versatility, and capacity to mediate controlled electron transfer processes. This work provides a focused overview of cobalt(II) coordination compounds and their application in the electrochemical determination of dopamine as a representative biologically relevant analyte. Cobalt(II) complexes were synthesised under hydrothermal and mild solution conditions using pyridine- and nicotinate-based ligands. Structural characterisation shows that coordination geometry, ligand functionality, and supramolecular arrangement critically influence redox activity and interfacial charge transfer kinetics. Glassy carbon electrodes modified with cobalt(II) complexes display pronounced electrocatalytic enhancement for dopamine oxidation. Cyclic voltammetry and electrochemical impedance spectroscopy were used to investigate electron transfer rates, charge transfer resistance, and electrode surface properties. The Co(II)/Co(III) redox couple reduces the oxidation overpotential, accelerates electron transfer, and suppresses electrode fouling, enabling sensitive, selective, and rapid dopamine detection in pharmaceutical samples. These results establish dopamine as a robust benchmark analyte for assessing the electrochemical performance of coordination compounds. More broadly, the study highlights the importance of integrating synthetic chemistry, structural design, and electrochemical methodology as a coherent strategy for developing reliable, application-oriented sensors and electrocatalysts. This framework supports the rational design of next-generation cobalt-based materials tailored for the sensitive detection of biologically and industrially relevant analytes.

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When Waste Becomes a Weapon: Carbon Materials Fighting Contaminants in Water

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Keywords: Organophosphorus Pesticides, Dyes, Antibiotics, Remediation, Adsorption

Abstract: This keynote lecture explores how diverse bio-waste streams, ranging from spent coffee grounds and viscose fibers to walnut residues and mushroom substrate, can be transformed into high-performance carbon materials for water purification. Through controlled carbonization, chemical activation, and hydrothermal processing, these waste-derived materials acquire tailored porosity, surface chemistry, and adsorption selectivity. Their effectiveness is demonstrated across several contaminant classes, including organophosphorus pesticides, synthetic dyes, and antibiotics. Mechanistic analysis highlights the roles of micropores, mesopores, π–π interactions, electrostatics, and heteroatom functionalities in governing adsorption behavior. Many materials exhibit excellent reusability and achieve substantial reductions in toxicological endpoints, such as acetylcholinesterase inhibition. Importantly, selected carbons perform well under dynamic filtration conditions, underscoring their practical applicability. The "When Waste Becomes a Weapon" concept unites material science, environmental engineering, and circular-economy principles to offer sustainable, scalable solutions for modern water-quality challenges.

Acknowledgment

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ORAL PRESENTATIONS

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Synthesis and Characterization of Four Novel Cationic Ruthenium Arene Complexes Based on Cycloalkyl Aldimine Schiff Base Ligands

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Keywords: Cationic Ruthenium Arene Complexes, Iminopyridyl Schiff Base Ligands, Cycloalkyl Substituents, Synthesis, Characterization

Abstract: Organometallic ruthenium complexes coordinated with Schiff base ligands have gained significant attention in the systematic development of new metal-based drugs with dual anticancer and antimicrobial properties. Despite the promising results of ruthenium complexes, the search for novel structural motifs that may serve as models for the synthesis of new derivatives continues to receive scientific interest in the rational design of metal-based therapeutics. In this context, four novel organometallic assemblies were designed, featuring ruthenium(II) coordinated with *p*-cymene, one chloride ligand, and bidentate neutral cycloalkyl aldimine Schiff base ligands derived from 2-pyridinecarboxaldehyde and selected cycloalkyl amines containing cyclobutyl, cyclopentyl, cyclohexyl, and cycloheptyl rings. The compounds isolated as $BPh4^-$ salts were characterized both in the solid state and in solution employing single-crystal X-ray diffraction, nuclear magnetic resonance, infrared spectroscopy and ultraviolet–visible spectroscopy. The characterization confirmed the proposed structures, including the presence of imine functionalities and cycloalkyl moieties, which have been recognized as important structural motifs in medicinal chemistry due to their diverse pharmacological mechanism of action. Furthermore, this work provides a comprehensive investigation of the synthetic routes and reaction parameters affecting the formation of four cationic ruthenium arene complexes, with particular emphasis on the influence of solvents and precipitation conditions on obtaining stable compounds suitable for complete characterization. The obtained results establish a basis for future studies of their biological activity, particularly their interactions with DNA and their effects on cancer cell lines.

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Formulation and HPLC Analysis of Azelaic Acid Topical Emulsion

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Keywords: Azelaic Acid, Emulsion, FTIR, HPLC, Organoleptic Analysis

Abstract: In recent years, azelaic acid has gained significant popularity as a topical agent. This compound exhibits antimicrobial and anticomedonic properties, in addition to various anti-inflammatory effects. The aim of this study was to develop an effective and safe oil-in-water (O/W) emulsion formulation for the topical application of azelaic acid, which is characterized by its low solubility in most conventional solvents. It is essential to create a fully solubilized topical composition, as this form is less likely to induce irritation; the skin absorbs azelaic acid more readily when it is dissolved rather than in an undissolved state within dispersions. Ethoxydiglycol and butoxydiglycol are identified as the most suitable solvents for azelaic acid, facilitating the production of clear gels at high concentrations. However, their use in cosmetic formulations is restricted in Europe due to exceptional penetration capabilities. High-Performance Liquid Chromatography (HPLC) analysis was conducted to verify the stated azelaic acid content in the formulated product. To ensure the development of an effective and safe preparation, several evaluations were performed, including organoleptic analysis, identification of active substances via Fourier Transform Infrared (FTIR) spectroscopy, and pH testing. The formulation process aimed to create an emulsion containing azelaic acid while minimizing the side effects associated with undissolved azelaic acid and preventing crystallization, which could compromise its bioavailability. The appropriate pH of the emulsion was confirmed, aligning with the stability and activity range of azelaic acid. The declared content of azelaic acid was validated through a reliable HPLC method applied to the produced emulsion.

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Temperature-controlled aggregation in a double-square-well model of polymerizing hard spheres

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Keywords: hard spheres; association; polymerization; resummed thermodynamic perturbation theory

Abstract: A primitive model of associating hard spheres with two competing bonding distances was investigated using an extended resummed thermodynamic perturbation theory [1] and canonical Monte Carlo simulations. The system is an equimolar binary mixture of hard spheres in which unlike particles interact through a double shielded square-well potential located inside the hard-core diameter. The two bonding minima, positioned at a shorter distance (L_s) and a longer distance (L_l), generate distinct aggregation pathways. Depending on the bonding distances, well depths, density, and temperature, particles may form short-bond dimers, long-bond linear chains, or mixtures of both. Theoretical expressions were derived for the fractions of free, singly bonded, and doubly bonded particles, together with thermodynamic properties such as excess internal energy and pressure. Monte Carlo simulations were used to test the theory and to analyse the populations of bonding states. Particular attention was given to the regime in which the two bonding modes compete, because cooling can induce non-monotonic restructuring of the aggregates. For suitable potential parameters, the system first forms one type of aggregate (e.g., dimers) and then reorganizes into another (e.g., chains) upon further temperature decrease. The results show that a simple isotropic pair potential can produce controllable switching between dimer-rich and chain-rich states. This behaviour provides a minimal statistical-mechanical model for temperature-responsive self-assembly and may be useful for designing soft-matter systems with tunable morphology and liquid-crystal-like ordering.

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Enhancing Electrochemical Energy Conversion via Interface Engineering Between Pt-Free Metallic Nanoparticles and Graphene-Based Materials

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Keywords: Graphene Oxide, Reduced Graphene Oxide, SECM, Electrochemical Reduction, Hindered Diffusion

Abstract: The hydrogen evolution reaction (HER) is central to sustainable hydrogen production, yet the development of efficient non-noble metal catalysts for alkaline electrolysis remains challenging. Here, we examine whether engineering the catalyst–support interface can modify the HER volcano relationship and enhance catalytic activity through hydrogen spillover. Particular attention is devoted to interfacial hydrogen transfer from the catalyst to reduced graphene oxide (rGO) and its influence on HER kinetics. Our results reveal that the effect of spillover strongly depends on the hydrogen adsorption characteristics of the metal. Activity enhancement occurs only when the catalyst surface is highly covered with adsorbed hydrogen, a condition typically achieved at elevated overpotentials for strongly hydrogen-binding metals. Accordingly, rGO-supported Pt, Pd, Fe, Co, and Ni catalysts exhibit improved HER performance, effectively shifting the strong-binding branch of the volcano curve toward lower overpotentials. In contrast, weak hydrogen-binding metals, such as Ag, Au, and Zn, show negligible or even adverse support effects.Among the investigated systems, Ni@rGO, Pd@rGO, Co@rGO, and Fe@rGO display substantially enhanced activity compared with unsupported metals. These findings demonstrate that interface engineering via hydrogen spillover represents a general strategy for improving HER electrocatalysts, provided that the relevant thermodynamic and kinetic requirements are fulfilled.

POSTER PRESENTATIONS

Analytical, Environmental &

Radiochemistry

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A Novel SiO_2 Biosorbent Modified with Pomegranate Peel Extract for Methylene Blue Removal

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Keywords: Biosorption, Methylene blue, Modified silica gel, Pomegranate peel

Abstract: This study investigates a novel, low-cost, and environmentally friendly biosorbent based on silica gel (SiO_2) modified with an ethanol extract of pomegranate peel, an abundant agricultural waste, for the removal of methylene blue (MB) from aqueous solutions. To the best of our knowledge, this is the first study reporting the functional modification of SiO_2 using pomegranate peel extract for dye removal, contributing to the development of sustainable adsorption materials. The sorbent was characterized by SEM, EDS, and FTIR analyses, confirming successful surface modification and effective interaction with MB. The effects of key operational parameters were systematically evaluated, with optimal conditions determined at pH 5–7, sorbent dose 100 mg, contact time 90 min, initial dye concentration 20 mg/L, and temperature 25 °C. Under these conditions, the removal efficiency reached 98.4%, with an adsorption capacity of approximately 8.2 mg/g. Kinetic studies showed that the adsorption process follows a pseudo-second-order model, with an additional contribution of intraparticle diffusion, indicating a multi-step mechanism. Equilibrium data were well described by Langmuir, Freundlich, and Temkin isotherm models ($r^2 > 0.94$). The modified sorbent also demonstrated good reusability, retaining about 72% of its initial efficiency after four adsorption–desorption cycles. Compared to similar low-cost biosorbents reported in the literature, the developed material exhibits competitive adsorption performance. These findings highlight the potential of biomass-modified silica materials as scalable and sustainable solutions for wastewater treatment, supporting the transition toward circular and resource-efficient environmental technologies.

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Affinity of *Aloe* spp. for Selected Heavy Metals: Accumulation, Translocation, and Phytostabilization Potential

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Keywords: Heavy Metals, *Aloe* spp., Acumulation, Translocation, Phytostabilization

Abstract: This study investigates the accumulation and translocation of selected heavy metals (Cd, Cu, Ni and Pb) in *Aloe* spp., with the aim of evaluating its phytoremediation potential. The contribution of this work lies in linking metal bioavailability in spiked, organic-rich substrates with plant uptake patterns and organ-specific distribution, providing insight into phytostabilization processes. Simulated soil contamination was performed by metal spiking, followed by evaluation of pseudo-total and bioavailable (DTPA-extractable) fractions after 15-days. A significant fraction of the added metals remained in bioavailable form (Cd~50%, Cu 23-25%, Ni 6-10%, Pb 21-28%), indicating partial mobility and incomplete immobilization in the humus matrix. Experimental results showed that Aloe spp. accumulates metals predominantly in roots, with a clear metal-dependent affinity trend observed in root tissues (Pb>Cu>Ni>Cd). Root concentrations ranged from 0.85-1.19 mg/kg (Cd), 32.88-54.56 mg/kg (Cu), 9.42-13.07 mg/kg (Ni), to 9.22-16.18 mg/kg (Pb), while leaf concentrations were significantly lower. Translocation factors remained low, particularly for Cd (0.06-0.12) and Pb, indicating strong root retention, whereas Ni exhibited higher mobility (TF up to 0.43). These findings demonstrate that Aloe spp. primarily acts as a phytostabilizer, effectively limiting metal transfer to aerial parts and thereby reducing the risk of entry into the food chain. Overall, these findings highlight the potential of Aloe spp. for sustainable remediation strategies in metal-contaminated soils.

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Development of a Layered Biofiltration System for Heavy Metal Removal from Mine Wastewater

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Keywords: Mine Wastewater, Heavy Metals, Layered Biofiltration, Competitive Sorption, Sustainable Water Treatment

Abstract: Mine wastewater represents a significant environmental challenge due to elevated concentrations of dissolved heavy metals. This study investigated the development of a layered biofiltration system based on natural materials for the treatment of mine wastewater from the Rupice mine (Vareš, Bosnia and Herzegovina). The biofiltration system consisted of gravel, sand, humus and lemon peel arranged in successive layers within a laboratory aquarium. Physicochemical characterization of process water and pit water revealed substantial differences in water quality and metal composition between the investigated samples. The contribution of individual filtration layers was evaluated using single-metal and multimetal model solutions containing Mn, Cr, Cd, Pb, Cu and Ni. The addition of organic layers, particularly humus and lemon peel, significantly enhanced metal removal compared to mineral layers alone, confirming the importance of biosorption processes. Competitive sorption effects were observed in multimetal systems, with manganese showing the lowest removal efficiency (75.1%), while lead was removed with efficiencies up to 100%. Further improvement was achieved by introducing NaOH-modified lemon peel as the final filtration layer, resulting in removal efficiencies of 90.6–100% for all investigated metals at an initial concentration of 50 mg L^{-1}. The optimized system was subsequently applied to metal-enriched real mine wastewater samples. During four consecutive treatment cycles, high removal efficiencies were maintained, and after one day of retention all investigated metals were removed with efficiencies exceeding 91%. The results demonstrate that layered biofiltration combining mineral and organic materials represents an efficient, low-cost and sustainable approach for mine wastewater treatment, with strong potential for practical environmental applications.

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Voltammetric Techniques as an Alternative to Spectrophotometric Methods for Estimating Total Phenol Content

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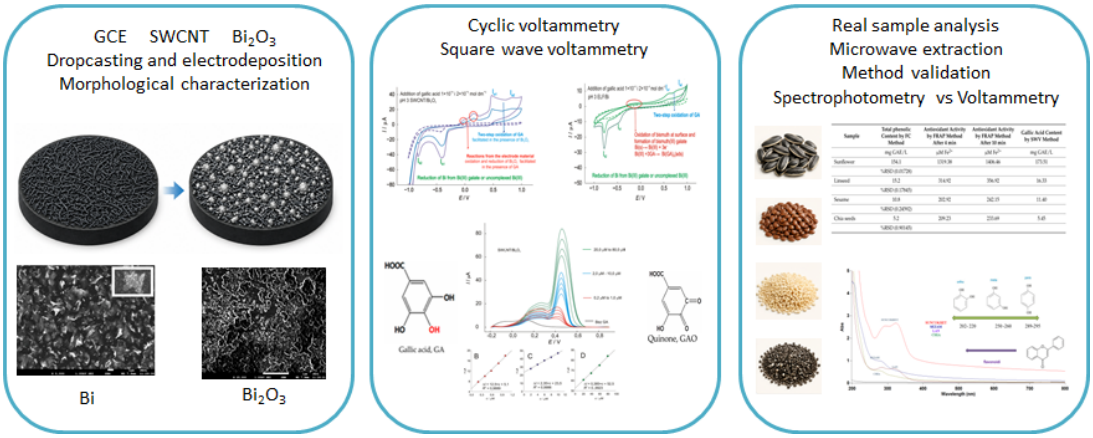
Keywords: Bismuth-film Electrodes; SWCNT; Sensing Purposes; Gallic Acid; Seeds

Abstract: Bismuth and its compounds have been known as environmentally friendly alternatives for electrochemical sensors applications for several decades. This work explored their potential for further improved in electroanalytical applications in combination with exceptional advantages of single-layer carbon nanotubes (SWCNTs). The focus of the research is the simple phenol, gallic acid (GA) and the possibilities of introducing this type of sensors and methods as standard for determining total phenols. Four different types of bismuth-based electrodes have been prepared: SWCNT with bismuth (SWCNT/Bi) or bismuth (III) oxide (SWCNT/Bi_2O_3) and bismuth or bismuth (III) oxide electrodeposited to a glassy-carbon electrode (ELF/Bi and ELF/Bi_2O_3). The prepared electrodes are characterized by scanning electron microscopy and cyclic voltammetry in phosphate electrolytes. SWCNT electrodes at pH 3 with the addition of Bi_2O_3 proved to be an optimal system for analytical determination of GA. SWCNTs facilitate adsorption and accumulation of GA and significantly enhance their oxidation signal. The addition of Bi_2O_3 improves electron transfer kinetics for oxidation reactions. Square wave voltammetry with the SWCNT/ Bi_2O_3 electrode provided reliable and accurate results and proved suitable for quantitative GA determination. The proposed method gives linear dependence over a wide range of concentrations (0.2–80 μM), with sensitivities of 12.5, 2.35 and 0.385 μA μmol^{-1} dm^3 respectively, for lower, middle and higher concentration ranges. The calculated detection limit was 0.06 μmol dm^{-3}. The electrochemical results were validated by spectrophotometric methods. The electrode has been successfully applied to determine gallic acid in aqueous extracts of flaxseed, sunflower, sesame and chia seeds.



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Determination of Simazine and Atrazine in Surface Water by HPLC Method with UV Detection

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Keywords: Simazine, Atrazine, Surface Water, Monitoring, HPLC, UV Detection

Abstract: Triazine pesticides, particularly simazine and atrazine, are widely used herbicides in agriculture for weed control in crops such as corn and sugar beet. Due to their chemical stability and low biodegradability, these compounds can persist in the environment and contaminate surface and groundwater, raising concerns regarding potential ecological and human health effects. Since simazine and atrazine are included in the List of Priority Substances of the European Water Framework Directive, their monitoring in surface waters of the Federation of Bosnia and Herzegovina is of significant importance. The determination of simazine and atrazine in surface water samples was performed according to ISO 11369:1997 using HPLC-UV detection following solid-phase extraction (SPE). Sample preparation was carried out using both SPE manifold systems and automated SPE extraction. Comparative measurements were performed using UV and PDA detectors. The aim of this study was to evaluate the suitability of the selected analytical method for monitoring compliance with legally prescribed concentration limits in surface waters. Method validation included the assessment of selectivity, linearity, working concentration range, accuracy, precision, reproducibility, and limit of quantification. Measurement uncertainty and interlaboratory comparison results were also evaluated to confirm method reliability. Monitoring was conducted over a two-year period at 111 measuring points in surface water bodies across FBiH. The obtained results indicated that simazine and atrazine concentrations were below levels that could pose significant risks to aquatic organisms and the ecosystem. The study confirms the applicability of the validated HPLC method for routine environmental monitoring of triazine pesticides in surface waters.

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Determination of Organohalogen Compounds in Drinking Water by GC-ECD

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Keywords: Chlorination, Drinking Water, Trihalomethanes, Organohalogen Compounds, GC-ECD

Abstract: This study investigated the occurrence of organohalogen compounds formed as disinfection by-products (DBPs) in the drinking water distribution system of *"Water supply and sewerage" LCC Sarajevo*. Chlorination is widely applied for effective microbiological disinfection; however, reactions between chlorine and natural organic matter may result in the formation of trihalomethanes (THMs), including chloroform, bromoform, bromodichloromethane (BDCM), and dibromochloromethane (DBCM). Since these compounds are considered potentially toxic and carcinogenic, their monitoring is essential for assessing drinking water safety. The presence of organohalogen compounds was determined using gas chromatography with electron capture detection (GC-ECD), a sensitive and reliable analytical method for halogenated compounds in water. The obtained results showed that concentrations of total THMs in all analyzed samples were below the maximum allowable concentration of 100 μg/L prescribed by the national Rulebook on the Health Safety of Drinking Water. Seasonal variations in THM concentrations were observed, with higher levels detected during summer months, likely due to increased biological activity and runoff from surrounding areas. Differences related to water source type were also identified, as groundwater samples contained lower THM concentrations compared to surface and karst water sources. The findings confirm the effectiveness of the applied disinfection process and emphasize the importance of continuous monitoring of DBPs in drinking water distribution systems to ensure public health protection and compliance with regulatory standards.

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Ecotoxicological Screening of Medlar Fruits (*Mespilus germanica* L.) in Bosnia and Herzegovina

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Keywords: *Mespilus germanica* L., potentially toxic elements, FAAS, food safety, Bosnia and Herzegovina.

Abstract: Although *Mespilus germanica* L. (medlar) is native to Southwest Asia and Southeast Europe and is widely cultivated across the European continent, it remains a largely neglected crop in Bosnia and Herzegovina, despite its exceptional nutritional potential which surpasses related species like apples in mineral and vitamin content. Furthermore, the specificity of its shallow root system and high affinity for element accumulation render these regional fruits ecotoxicologically sensitive. This study contributes to the fields of food safety and ecotoxicology by providing the first systematic assessment of the potentially toxic element profile in medlar fruits within Bosnia and Herzegovina, thereby addressing the lack of regional data regarding their health safety. Using flame atomic absorption spectrometry (FAAS), the content of selected metals was determined in unwashed fruits collected from five locations (Bugojno, Ilijaš, Konjic, Jajce, and Goražde). The concentrations of the determined elements ranged as follows: Cd (< LOD - 0.022 mg/kg), Co (< LOD - 0.099 mg/kg), Cr (0.129 - 0.367 mg/kg), Ni (0.593 - 1.97 mg/kg), and Pb (< LOD - 2.54 mg/kg). Comparative analysis indicates that chromium (Cr) contents are below the maximum permitted level of contaminants in fruit according to national regulations and international standards (FAO/WHO), whereas elevated lead (Pb) concentrations at certain locations exceed the maximum permitted level of contaminants in fruit. These findings underscore the necessity for regular monitoring and further research, particularly in industrial and agricultural areas, to safeguard consumer health.

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Geographical Variability of Phenolic Composition and Antioxidant Activity of *Mespilus germanica* L. Fruits in Bosnia and Herzegovina

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Keywords: *Mespilus germanica* L., Polyphenols, Flavonoids, Phenolic Acid, Antioxidant Activity, Geographical Variability, Bosnia and Herzegovina

Abstract: Mespilus germanica L., commonly known as medlar, is a traditional fruit species native to southwestern Asia and southeastern Europe. The nutritional properties of M. germanica fruits are attributed to their rich composition of carbohydrates, carotenoids, amino acids, organic acids, proteins, vitamins, and fatty acids. Furthermore, the fruits contain significant amounts of phenolic compounds, which contribute to their antioxidant and antidiabetic potential. The aim of this study was to evaluate the content of bioactive compounds in urban medlar fruits collected from different locations in Bosnia and Herzegovina. Total phenolic content (TPC), total flavonoid content (TFC), total phenolic acid content (TPAC), and antioxidant activity using the DMPD assay were determined. The results revealed that samples III (Bugojno), IV (Ilijaš), and V (Goražde) exhibited the highest levels of total phenolics and phenolic acids. Sample III showed 20.997 mg GAE/g extract and 13.93 mg CAE/g extract, sample IV contained 20.61 mg GAE/ g extract and 17.30 mg CAE/ g extract, while sample V contained 19.20 mg GAE/g extract and 14.49 mg CAE/ g extract, respectively. The highest total flavonoid content was also recorded in sample III (3.43 mg QE/g extract). Although samples I (Jajce) and II (Konjic) exhibited the lowest concentrations of phenolic compounds, sample II demonstrated the strongest antioxidant activity, with an IC_{50} value of 0.265 mg/mL. These findings indicate significant variability in the phytochemical composition and antioxidant potential of urban medlar fruits from different regions of Bosnia and Herzegovina, highlighting the influence of geographical location on the accumulation of bioactive compounds.

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Partial Microbial Profile of Cultivable Moonmilk Bacteria from Selected Dinaric Caves with Potential Biotechnological Applications

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Keywords: Moonmilk, Cave Microbiology, Cultivable Bacteria, Biotechnological Potential, Bioremediation

Abstract: Moonmilk is a secondary cave deposit primarily composed of calcium carbonate and characterized by diverse microbial communities. Due to their adaptation to extreme and nutrient-limited subterranean environments, cave microorganisms represent a promising source of novel bioactive compounds with potential applications in biotechnology, medicine, and bioremediation. This preliminary study aimed to investigate the diversity of cultivable bacterial communities isolated from moonmilk samples collected from seven speleological sites in the Duvanjsko Polje region, Dinara, and Bjelašnica Mountains, with particular focus on the genus *Pseudomonas*. Selective and non-selective cultivation media were used for bacterial isolation, while preliminary identification was performed using the automated VITEK® 2 COMPACT system. The obtained results indicated the presence of bacterial genera *Pseudomonas*, *Aerococcus*, *Sphingomonas*, and *Serratia*. Several identified genera are known for metabolic versatility, production of secondary metabolites, and degradation of organic pollutants, highlighting their potential application in bioremediation processes and discovery of novel bioactive molecules. Although additional molecular analyses, including 16S rRNA sequencing and metagenomics, are required for more precise characterization of cave microbial communities, these preliminary findings indicate that the VITEK® 2 COMPACT system can represent a useful tool for rapid profiling of cultivable moonmilk bacteria and may help direct future research toward cave microhabitats with increased potential for targeted isolation of microorganisms of biotechnological interest.

Acknowledgment
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From Ingestion to Alteration: How Synthetic Microfibers Induce Morphological Changes in Brine Shrimp

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Keywords: *Artemia salina,* Microplastics and Microfibers, Ecotoxicology

Abstract: Micro-waste, particularly microplastics and microfibers, represents one of the major pollutants of aquatic ecosystems due to its persistence and easy distribution in water and sediments. Numerous studies have shown that exposure to micro-waste can impair growth, development, reproduction, and survival of aquatic organisms. In this study, *Artemia salina* was used as a model organism because of its short life cycle, simple cultivation, and high sensitivity to pollutants. Nauplii were exposed to polyamide (white) and polyester (black) microfibers at concentrations of 1 and 10 mg/L. The fibers were produced by mechanical blending to simulate microfiber formation during household laundry drying in tumble dryers. Prior to incubation, cysts were decapsulated using 10% sodium hypochlorite and cultured in artificial seawater at 28 ± 0.5°C under aeration. Fiber dimensions ranged from 105.37–237.67 µm for polyamide and 77.34–162.40 µm for polyester. FTIR analysis confirmed the chemical identity of both microfiber types. At lower concentrations (1 mg/L), only mild effects were observed, including slight body deformities and reduced transparency. However, exposure to 10 mg/L caused severe morphological and tissue alterations, including antenna deformities, carapace damage, tissue degeneration, and mortality. After 72 h, the most pronounced effects were recorded in nauplii larvae exposed to polyamide at 10 mg/L, while polyester caused milder abnormalities. Overall, the results demonstrate that microfibers significantly affect the survival, morphology, and development of *A. salina*, highlighting their ecological risk and supporting the use of this organism in ecotoxicological assessment of micro-waste pollution.

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Preliminary Identification of Bacterial Isolates from Ice Caves with Potential Biotechnological Applications

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Keywords: Cold Cave Environments, Bacterial Isolation, *Pseudomonas* Spp., VITEK Identification, Environmental Microbiology, Biotechnological Potential

Abstract: Cold cave environments represent understudied subterranean habitats characterized by stable low temperatures and oligotrophic conditions and are considered potential reservoirs of microorganisms with biotechnological and antimicrobial relevance. This preliminary study investigated bacterial communities isolated from samples collected in Resanovačka Ledenica Cave and Ledenica Cave on Mount Grmeč in order to identify cultivable taxa adapted to cold subterranean environments. Following sample processing, mixed microbial cultures were established, and individual bacterial colonies were isolated using standard cultivation techniques on Pseudomonas and Mueller–Hinton agar, accompanied by colony morphology assessment. Bacterial characterization included Gram staining and biochemical identification using the VITEK system. The analysis identified *Pseudomonas fluorescens* and *Pseudomonas putida*, species recognized for their metabolic versatility and production of bioactive compounds with potential applications in bioremediation and antimicrobial discovery. Phenotypic testing confirmed oxidase positivity of the isolates, while *Pseudomonas fluorescens* exhibited UV-induced fluorescence and growth at low temperatures, consistent with its psychrotrophic characteristics. Additionally, a high-probability identification of *Rothia kristinae* was obtained, a species widely distributed in environmental and host-associated niches. Isolates were also tentatively assigned to *Kocuria rosea*, a ubiquitous environmental bacterium associated with soil, indicating its possible presence as part of the background environmental flora of subterranean ecosystems. The obtained results demonstrate the microbial diversity of cold subterranean environments and highlight their potential as sources of metabolically active bacteria of interest for pharmaceutical, medical, and industrial applications. Further studies should include molecular confirmation of taxonomic assignments and evaluation of antimicrobial activity and bioactive metabolite production in the isolated strains.

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Monitoring and Removal of Pharmaceutical Residues in Cross-border Surface Watercourses with an Emphasis on Optimization of Wastewater Treatment

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Keywords: Wastewater, Surface Water, Pharmaceutical Active Substances

Abstract: Pharmaceutical active substances constitute a significant category of micropollutants that are increasingly present in all water bodies, attributable to their rising usage and the limited efficacy of removal processes in municipal wastewater treatment plants. The Pharmwater project, involving the National Laboratory for Health, Environment and Food, Pannon University (Hungary), and the Slovenian Environment Agency, aims to assess the prevalence of these substances, evaluate their removal efficiency in existing wastewater treatment facilities in alignment with the newly established Urban Wastewater Treatment Directive (UWWTD), and investigate their effects on surface water quality. Following six months of wastewater monitoring, a total of 49 pharmaceutical active substances were identified from a targeted analysis of 66 compounds. The predominant groups detected include antibiotics, analgesics, antidepressants, beta-blockers, hormones, and antimicrobial agents. Analytical methods included LC/HRMS for qualitative results and compound identification and LC/MS/MS for quantitative results of presented pharmaceutical active substances. The observed removal efficiency of these pharmaceutical substances in wastewater treatment plants varies between 45% and 58%. Notably, enhanced removal performance tends to occur during warmer months, likely due to the positive influence of temperature on microbial activity. This seasonal variation is evidenced by a trend of increasing concentrations of pharmaceuticals in receiving water bodies downstream of the treatment facilities.

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Indoor Air Metal Pollution Assessment using Lichens as Bioindicators

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Keywords: Indoor Air Quality, Metals, Relative Accumulative Factor, Bioindicators, Lichens

Abstract: Indoor air quality (IAQ) has attracted increasing attention because of its impact on human health and workplace conditions, particularly in environments influenced by tobacco smoke as a source of toxic metals associated with particulate matter. This study contributes to analytical and environmental chemistry by evaluating lichens as bioindicators of indoor metal pollution under different smoking conditions. Lichens were collected in Bokšići, Bosnia and Herzegovina, cleaned from mechanical impurities. The samples were placed in perforated bags and exposed for 40 days in smoking-permitted and non-smoking indoor areas. After exposure, acid digestion was performed, and concentrations of Cr, Co, Cd, Pb, and Fe were determined by flame atomic absorption spectrometry (FAAS). Metal accumulation was assessed using the relative accumulation factor (RAF). The highest RAF values in the smoking-permitted area were recorded for Pb (3.08), Co (2.32), and Cd (1.85), while in the non-smoking area the highest RAF was found for Co (4.52), followed by Pb (0.58) and Cd (0.52). The lowest RAF value in both areas was recorded for Cr (-1.00), whereas Fe showed a slightly negative value in the permitted smoking area (-0.09) and a low positive value in the non-smoking area (0.24). The results indicate accumulation of Co, Cd, and Pb in lichen samples, while Cr showed no accumulation. Overall, lichens reflected differences in indoor metal contamination and may be considered suitable bioindicators of indoor air pollution.

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Lichen Biomonitoring for Air Pollution Assessment with Metals

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Keywords: Trace Elements, *Hypogimnia*, Air Quality, FAAS, Sarajevo

Abstract: A wide range of pollutants is present in outdoor air, making air pollution one of the major health risks today. Biomonitoring, which applies living organisms as indicators of environmental changes across space and time, enables direct assessment of the ecosystem status. The aim of this research is to collect quantitative data on the presence of metals using lichen (*Hypogimnia*) as biomonitors. Samples were collected from five locations in a mountainous area near Sarajevo, Bosnia and Herzegovina (BiH), in December 2025. Metal concentrations were determined using flame atomic absorption spectrometry. In order to differentiate whether metals had come from natural or anthropogenic sources at selected sites, soil samples were also analyzed to calculate the enrichment factor (EF). High concentrations were found for metals like Pb, and Ni, while Cd revealed low concentrations in lichen samples. The sequence of the mean metals concentrations in lichen were Fe > Mn > Zn > Pb > Ni > Cu > Co > Cd > Cr. EF for all metals revealed moderate enrichment in the location 2 (Trebević) indicating a slight human impact or specific natural processes. The EF for Cd showed moderate enrichment at locations 4 and 5 (Nahorevska brda). According to EF for other metals the sites have no to very little enrichment, which likely means there is no anthropogenic pollution. Lichen biomonitoring is an effective and low-cost alternative method for air pollution assessment with metals. This study contributes to a better understanding of atmospheric pollution and supports efforts toward sustainable environmental management.

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This research was supported by the BiH and Slovenia Bilateral scientific research projects "Air Quality Assessment Using Selected Biomonitors" and "Physicochemical characterization of atmospheric aerosol particles; biomonitoring and new particle formation" grant number(s) [0101-12710-16/25 and 0101-13380-3/23; 0101-13378-3/24] provided by [Federal Ministry of Education and Science (FMON) and Slovenian Agency for Scientific Research and Innovation (ARIS)].

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Gamma Spectrometric Determination of Radionuclides in Lichens and Mosses from Bosnia and Herzegovina

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Keywords: Gamma Spectrometry, Lichens; Mosses, Bioindicators, Radionuclides, Environmental Radioactivity

Abstract: Lichens and mosses are widely recognized as valuable bioindicators of environmental quality because of their ability to accumulate radionuclides from atmospheric deposition and surrounding ecosystems. Gamma spectrometric analysis of these organisms is commonly applied for monitoring both naturally occurring radionuclides including ^{226}Ra, ^{232}Th, and ^{40}K, and anthropogenic radionuclides such as ^{137}Cs, which persists in the environment as a result of nuclear accidents and atmospheric nuclear weapons testing. The aim of this study was to determine the activity concentrations of selected radionuclides in lichens and mosses collected in Bosnia and Herzegovina and to assess their suitability as bioindicators of environmental radioactive contamination. A total of 30 samples (15 lichens and 15 mosses) were collected from three locations: the foothills of Ivan Mountain, Bjelašnica Mountain, and Ranče Mountain. After collection, samples were air-dried, homogenized, placed in plastic counting containers, and stored for 30 days to establish secular equilibrium between radionuclides and their progeny. The activity concentrations of radionuclides were determined using a Baltic Scientific Instruments gamma spectrometer equipped with a coaxial HPGe detector with a relative efficiency of 30% and an energy resolution of 1.80 keV. The activity concentrations of ^{137}Cs, ^{226}Ra, ^{232}Th, and ^{40}K were measured. The obtained activity concentrations ranged from <LOD to 4.40±0.06 Bq kg^{-1} for ^{137}Cs, from 11.20±0.27 to 21.30±0.54 Bq kg^{-1} for ^{226}Ra, from 11.40±0.32 to 16.20±0.89 Bq kg^{-1} for ^{232}Th, and from 344.20±37.90 to 421.80±37.67 Bq kg^{-1} for ^{40}K for mosses and <LOD to 3.10±0.07 Bq kg^{-1} for ^{137}Cs, from 9.65±1,25 to 22.30±1,02 Bq kg^{-1} for ^{226}Ra, from 10.15±1.52 to 17.10±1.75 Bq kg^{-1} for ^{232}Th, and from 320.60±20.08 to 441.60±39.01 Bq kg^{-1} for ^{40}K for lichens. Differences observed among sampling locations and between the two types of bioindicators indicate their significant potential for assessing the spatial distribution of radionuclides and for long-term environmental radioactivity monitoring in Bosnia and Herzegovina

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Microplastics in Coastal Waters and Beach Sand: Analytical Approaches and Environmental Significance

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Keywords: Microplastics ,Coastal Waters, Beach Sand; Environmental Monitoring, FTIR Spectroscopy, Raman Spectroscopy, Polymer Identification, Marine Pollution

Abstract: Microplastic pollution has emerged as one of the most significant environmental challenges of the 21st century due to its widespread distribution, persistence, and potential impacts on ecosystems and human health. Coastal waters and beach sand represent important environmental compartments that act as both sinks and transport pathways for microplastics originating from terrestrial and marine sources. Consequently, the identification and quantification of microplastics in these matrices have become essential components of environmental monitoring programmes. This paper provides an overview of the current approaches used for the determination of microplastics in coastal water and beach sand samples. The analytical workflow generally includes sample collection, filtration or sieving, density separation, removal of organic matter, visual characterization, and polymer identification. Particular attention is given to spectroscopic techniques, such as Fourier Transform Infrared Spectroscopy (FTIR) and Raman spectroscopy, which enable reliable identification of polymer composition and differentiation of plastic particles from natural materials. The advantages and limitations of these techniques, as well as challenges related to contamination control, particle size determination, and method standardization, are discussed. Recent studies have demonstrated the widespread occurrence of microplastics in coastal waters and beach sediments worldwide, highlighting the need for harmonized analytical protocols and long-term monitoring programmes. The implementation of standardized monitoring strategies is crucial for assessing the spatial distribution, sources, transport pathways, and environmental fate of microplastics. Improved analytical methodologies and international cooperation will contribute to a better understanding of microplastic contamination and support the development of effective mitigation measures for the protection of aquatic and coastal ecosystems

Acknowledgment

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POSTER PRESENTATIONS

Organic, Inorganic, Medicinal

& Biochemistry

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Exploring the Inhibitory Effects of Cabernet Sauvignon Wine Concentrates on Elastase Activity *in vitro*

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Keywords: Elastase, Polyphenols, Cabernet Sauvignon Wine Concentrates

Abstract: Elastase is a serine protease responsible for the degradation of elastin, a key structural protein of the extracellular matrix. Excessive elastase activity contributes to skin aging and loss of elasticity. Natural elastase inhibitors are therefore of considerable interest, particularly in the context of functional foods and cosmetic applications. The aim of this study was to investigate the *in vitro* elastase inhibitory potential of selected Cabernet Sauvignon (CS) wine concentrates and to examine the relationship between their chemical composition and biological activity. Nine commercially available CS wines originating from Serbia, France, Italy, Spain and North Macedonia were analyzed. Spectrophotometric methods were used to determine the content of total polyphenols, tannins, monomeric anthocyanins and flavonoids. Elastase inhibition was evaluated *in vitro* by spectrophotometric method based on hydrolysis of N-succinyl-Ala-Ala-Ala-*p*-nitroanilide. The results demonstrated notable differences in polyphenolic composition among the analyzed samples (e.g. the content of total polyphenols ranged from 62.55 to 93.90 μg gallic acid equivalents/mg of dry mass), which were reflected in their elastase inhibitory capacity. At a concentration of 100 mg/L, CS wine concentrates inhibited elastase activity by 35.95–84.59%, which was comparable to the activity of the standard compound epigallocatechin-3-gallate (1500 mg/L, 98.99% of inhibition). These findings highlight CS wine concentrates as a potential source of natural elastase inhibitors. The study provides a scientific basis for further research into their possible applications in dermatology and cosmetic formulations aimed at preventing premature skin aging.

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High-Fat and High-Carbohydrate Diets Affect Serum Levels of Selected Liver Enzymes in Male Wistar Rats

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Keywords: High-Fat Diet, High-Carbohydrate Diet, Alanine Aminotransferase, Aspartate Aminotransferase, Male Wistar Rats

Abstract: Liver enzymes such as alanine aminotransferase (ALT) and aspartate aminotransferase (AST) are commonly used biomarkers of liver injury that may be associated with high-fat and high-carbohydrate diets (HFD and HCD, respectively). The objective of this study was to assess the effects of HFD and HCD on serum ALT and AST levels in Wistar rats (*Rattus norvegicus*). Six adult male Wistar rats, previously fed standard chow until reaching 200 g body weight, were randomly divided into two experimental groups (n=3 per group). One group received an HFD, while the other received an HCD, and both treatments lasted over a period of 12 weeks. Blood samples were collected from the rats' tails at three-week intervals over four sampling sessions. Thereafter, serum was obtained by centrifugation of whole blood, followed by measurement of ALT and AST levels. The data underwent statistical analysis, using $p<0.05$ as the threshold for significance. Variance equality was assessed with F-test. According to the calculated p-values, Student's t-test or Welch's t-test was performed, independently comparing groups and sampling sessions. Based on the Student's t-test, the HCD group showed significantly higher ($p<0.05$) serum ALT and AST levels (40.58±7.19 U/L and 110.78±9.20 U/L, respectively) in comparison to the HFD group (19.62±5.40 U/L and 93.59±12.94 U/L, respectively) across all four sampling sessions. Additionally, the appropriate t-test analysis generally showed no significant variation between sampling sessions for either parameter across both groups. To conclude, the results suggest that the HCD contributed more to the increase in serum ALT and AST levels.

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Synthesis and Biological Evaluation of D-Secosteroid Hydrazones

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Keywords: Steroids, D-Secosteroids, Hydrazone, Steroid Hormone Receptors, AKR1C3, AKR1C4

Abstract: Secosteroids are steroidal compounds formed by cleavage of a bond within the tetracyclic steroid nucleus, yielding structures with distinct biological properties. Among these modifications, D-ring opening has attracted particular interest because it often reduces or eliminates intrinsic estrogenic activity, a desirable feature for targeting hormone-dependent breast cancer. Many D-secosteroid derivatives can interact with steroid hormone receptors and inhibit key enzymes involved in steroid biosynthesis and metabolism, highlighting their potential as modulators of receptor- and enzyme-mediated pathways. Building on this framework, we synthesized a series of, 17-hydrazones, a thiosemicarbazone, and a semicarbazone, of the 16,17-seco derivative of dehydroepiandrosterone. Their relative binding affinities for the ligand-binding domains of estrogen receptors α and β (ERα and ERβ), androgen receptor (AR), and glucocorticoid receptor (GR), as well as inhibitory activity against the steroid-metabolizing enzymes AKR1C3 and AKR1C4, were evaluated *in vitro*. All compounds displayed selective binding to GR, with negligible affinity for ERα, ERβ, and AR. Several derivatives exhibited inhibitory activity against AKR1C3, whereas others were active against AKR1C4. Overall, the obtained results suggest that 16,17-secoandrosten-5-en-17-hydrazone derivatives may serve as useful structural motifs for further development of selective GR ligands and inhibitors of steroid-metabolizing enzymes relevant to hormone-dependent cancers and other steroid-related disorders.

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Antioxidant Potential of *Sambucus nigra* L. from Bosnia and Herzegovina Determined by DPPH and CUPRAC Methods

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Keywords: *Sambucus nigra* L., DPPH, CUPRAC, Antioxidant, Bosnia and Herzegovina

Abstract: Black elderberry (*Sambucus nigra* L.) is a medicinal plant whose biological properties are primarily ascribed to phenolic compounds with strong antioxidant activity**.** Antioxidants have a major role in reducing oxidative stress related to various chronic diseases, including cardiovascular and metabolic problems. Earlier research has indicated that plant organs, such as fruits, flowers, and leaves, show considerable antioxidant potential. The aim of this study was to evaluate the antioxidant activity of black elderberry flowers, leaves, and fruits harvested from different areas in Bosnia and Herzegovina. The DPPH and CUPRAC methods were used to assess antioxidant activity based on different reaction mechanisms providing evaluation of antioxidant capacity. The findings of both methods consistently demonstrated that flowers and leaves possess stronger antioxidant activity than fruits. The DPPH assay revealed lowest IC_{50} values in flower extracts from Bileća (0.041 mg/mL) and Tuzla (0.046 mg/mL), as well as in leaf extracts from Bijeljina (0.048 mg/mL), whereas fruit extracts showed higher IC_{50} values, reflecting lower activity. A similar trend was confirmed by the CUPRAC assay, exhibiting the strongest activity in flower extracts from Sarajevo (15.13 mg/mL) and leaf extracts from Mostar (16.39 mg/mL), while fruit extracts showed the lowest activity, mostly in Tuzla (284.40 mg/mL) and Bijeljina (256.67 mg/mL). This study adds to existing literature by providing relative data on antioxidant activity across different plant organs and geographical origins in Bosnia and Herzegovina. The findings support the antioxidant potential of *Sambucus nigra* L. and suggest its use as a natural source of antioxidants in the pharmaceutical and food industries.

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Phenolic and Flavonoid Profiles in Different Organs of *Sambucus nigra* L. Collected in Bosnia and Herzegovina

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Keywords: *Sambucus nigra L.*, Total Phenolics, Total Flavonoids, Folin–Ciocalteu, $AlCl_3$ Method, Bosnia and Herzegovina

Abstract: Black elderberry (*Sambucus nigra* L.) belongs to the family Adoxaceae and is found throughout Europe, North America, and Western Asia. It is a medicinal plant used in traditional and modern phytotherapy due to its pronounced antioxidant, antibacterial, antitumor, antiviral, and immunomodulatory properties. These activities are mostly a result of phenolic compounds and flavonoids with antioxidant activity, which play an important role in neutralizing free radicals and reducing oxidative stress. This study aimed to determine the total phenolic content (TPC) and total flavonoid content (TFC) in flowers, leaves, and fruits of *Sambucus nigra* L. collected from five locations in Bosnia and Herzegovina (Sarajevo, Tuzla, Mostar, Bijeljina and, Bileća). Ethanolic extracts were prepared from air-dried plant material and analyzed spectrophotometrically. TPC was determined by the Folin-Ciocalteu method while TFC was obtained using the aluminium chloride colorimetric method. TPC was expressed as mg GAE/g dry weight, while TFC was expressed as mg QE/g dry weight. Significant differences among plant organs were observed. TPC ranged from 4.76 to 26.55 mg GAE/g, with the highest values in flowers, followed by leaves, whereas fruits showed a lower amount. Similarly, TFC ranged from 3.64 to 21.84 mg QE/g, with flowers richest in flavonoids, indicating organ-specific accumulation of phenolics. These results suggest that elderberry flowers are the richest source of phenolic antioxidants, explaining their pronounced biological activity and potential application in pharmaceutical, nutraceutica, and functional food products. This study contributes to a better understanding of the phytochemical potential of *Sambucus nigra* L. in Bosnia and Herzegovina.

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Impact of Alcohol and Benzodiazepines on Hypothermia and Postmortem Biomarkers: Implications for Forensic Interpretation

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Keywords: Hypothermia, Benzodiazepines, Alcohol, HIF-1α, Forensic toxicology

Abstract: Hypothermia is a life-threatening condition associated with environmental exposure and substance use. Alcohol and benzodiazepines impair thermoregulation through different mechanisms, affecting heat loss, survival, and physiological responses. Hypothermia may also alter biomarkers such as hypoxia-inducible factor 1-alpha (HIF-1α) and cortisol, but their behavior under combined hypothermic and toxicological conditions remains unclear. This study evaluated the effects of alcohol and benzodiazepines on hypothermia progression, survival time, and changes in HIF-1α and cortisol levels in kidney and adipose tissue. A randomized experimental study was conducted on 21 male rats divided into three groups (alcohol, benzodiazepines, control; n=7). Hypothermia was induced by immersion in water at 7°C. Core temperature and survival time were recorded. Postmortem tissue samples were analyzed using ELISA. Statistical analysis included the Kruskal–Wallis test, Dunn's test, and Spearman correlation ($p < 0.05$). Significant differences were observed for hypothermia temperature ($p = 0.00176$) and temperature at death ($p = 0.00239$), with lower values in the benzodiazepine group. Temperature change during hypothermia progression also differed significantly ($p = 0.0045$). Temperature positively correlated with survival time ($\rho = 0.620$; $p < 0.01$) and HIF-1α in adipose tissue ($\rho = 0.434$; $p < 0.05$), while no significant associations were found in kidney tissue. Benzodiazepines accelerate hypothermia more than alcohol, likely due to central thermoregulatory suppression. Temperature is a key determinant of survival, while biomarker responses appear tissue-specific. These findings provide insight into substance related modulation of hypothermia and may improve forensic interpretation of hypothermia related deaths.

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Antimicrobial Potential of Dithienylideneacetone Derivatives

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Keywords: Dithienylideneacetone Derivatives; Antimicrobial Activity; Agar Diffusion Method; *Candida albicans*; Gram-positive Bacteria; Gram-negative Bacteria

Abstract: Antimicrobial resistance (AMR) is a serious global problem that threatens the effective treatment of various infections. One of the ways to combat AMR is to design and synthesize new drugs. The aim of this research was to investigate the antimicrobial activity of four newly synthesized dithienylideneacetone derivatives (2,2'-dithienylideneacetone (**1**), 3,3'-dibromo-2,2'-dithienylideneacetone (**2**), 2,2'-dibenzothienylideneacetone (**3**), and, 3,3'-dibenzothienylideneacetone (**4**)), whose structures were analyzed by IR and NMR. The agar diffusion method was used to test the antimicrobial potential against Gram-positive (*Bacillus subtilis* ATCC 3366, *Staphylococcus aureus* ATCC 6538) and Gram-negative (*Escherichia coli* ATCC 8739, *Pseudomonas aeruginosa* ATCC 27853) bacterial strains, and against the fungus *Candida albicans* ATCC 10231. Antibiotics (ampicillin, colistin, and streptomycin) and the antimycotic nystatin were used as positive controls while the solvent dimethyl sulfoxide was used as a negative control. The largest zones of inhibition were achieved on the fungus *C. albicans* for all four investigated derivatives. When it comes to bacteria, the overall results indicate that the tested compounds achieved a stronger inhibition of the growth of Gram-negative bacteria. In *E. coli*, compound **4** (18.33±2.08 mm) had the strongest effect, while compound **3** (18.00±1.00 mm) had the strongest effect in *P. aeruginosa*. In Gram-positive bacteria, the strongest activity of the tested compounds was observed in the case of compound **4** (17.33±0.58 mm) in *S. aureus*. These findings show the promising antimicrobial potential of the investigated derivatives especially against *C. albicans* and Gram-negative bacteria highlighting their potential as candidates for the development of new antimicrobial agents to combat AMR.

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Docking Study of Dithienylideneacetone Derivatives with 5-Lipoxygenase Enzyme

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Keywords: Dithienylideneacetone Derivatives; Molecular Docking Study; 5-Lipooxigenase; Anti-inflammatory Activity

Abstract: Inflammatory diseases associated with 5-lipoxygenase (5-LOX) activity are marked by the excessive production of leukotrienes, potent lipid mediators that drive inflammation, promote immune cell recruitment, and contribute to tissue damage. This pathway plays a central role in a range of conditions, including bronchial asthma, chronic obstructive pulmonary disease (COPD), atherosclerosis, rheumatoid arthritis, and neurodegenerative disorders such as Alzheimer's disease. By facilitating the recruitment and activation of neutrophils and macrophages, the 5-LOX pathway sustains chronic inflammation and disease progression, highlighting the enzyme as an important target for therapeutic intervention and the development of novel antagonists. The aim of this study was to investigate, by *in silico* approaches, the anti-inflammatory potential of four synthesized dithienylideneacetone derivatives (2,2′-dithienylideneacetone (**1**), 3,3′-dibromo-2,2′-dithienylideneacetone (**2**), 2,2′-dibenzothienylideneacetone (**3**), and 3,3′-dibenzothienylideneacetone (**4**)) against the 5-LOX enzyme. Molecular docking simulations were performed using YASARA Structure software. The calculated binding energies ranged from −10.89 to −7.38 kcal/mol, and dissociation constant values ranged from 0.01 to 3.89 μM. Compounds **3** and **4**, which incorporate benzothiophene heterocycles, exhibited higher binding affinity toward 5-LOX, suggesting the formation of more stable enzyme–ligand complexes. The investigated derivatives interacted with the enzyme at an allosteric site, forming predominantly hydrophobic interactions. Overall, these findings indicate a promising anti-inflammatory potential for the investigated derivatives, supporting their further consideration as candidates for the development of therapies targeting chronic inflammatory diseases.

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Ru(II)-catalyzed C–H Activation and Further Functionalization of *N*-protected 2-Phenylimidazoles

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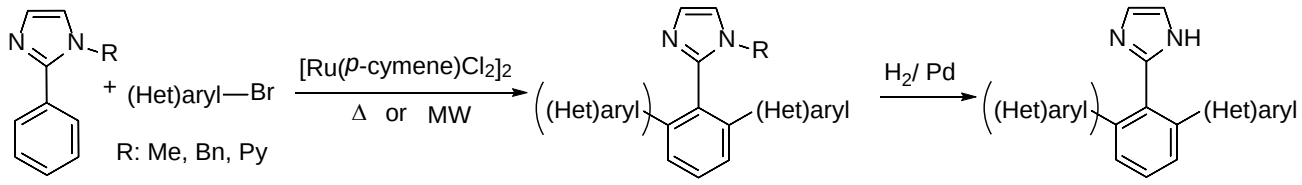
Keywords: Ruthenium Catalysis, Direct Arylation, Heterocycles

Abstract: Direct catalytic C–H functionalization has emerged as an efficient strategy for constructing carbon–carbon bonds, particularly in the synthesis of biaryl motifs relevant to pharmaceuticals, agrochemicals, and materials science. Compared to traditional cross-coupling reactions, these methods offer improved atom and step economy with reduced waste. While palladium catalysts have dominated this field, ruthenium systems provide a cost-effective and air-stable alternative with complementary reactivity. However, challenges such as limited regioselectivity, dependence on directing groups, and harsh reaction conditions remain. In this work, we investigated the influence of *N*-substitution on 2-phenylimidazole in ruthenium-catalyzed direct C–H (hetero)arylation. *N*-functionalized 2-phenylimidazoles bearing methyl, benzyl and pyridyl groups were subjected to *ortho*-functionalization with a series of (hetero)aryl bromides as arylating reagents using [Ru(*p*-cymene)Cl_2]$_2$ as the catalyst precursor. We were able to prepare a series of mono- and di-arylated products with *N*-methyl and *N*-benzyl groups using conventional heating in toluene and KOPiv as a ligand, affording high yields and selectivity. *N*-benzylimidazole products were subsequently deprotected by catalytic hydrogenation. Microwaves proved to be crucial in the preparation of *ortho*-heteroarylated products. Investigations on arylation of *N*-pyridyl protected 2-phenlyimidazole are in progress.



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Ruthenium-Catalyzed Transformation of 2-Haloazines and Their Fused Analogues Towards Heteroarylated Azinones

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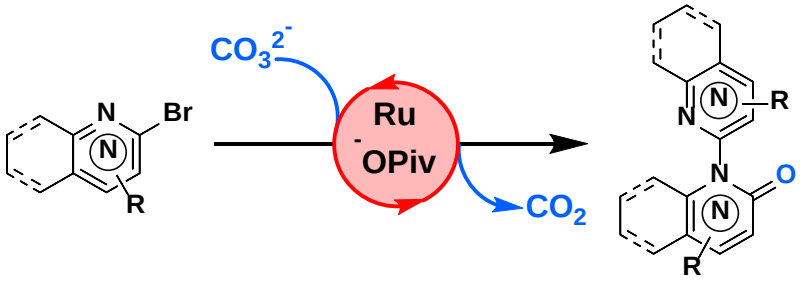
Keywords: Haloazines, Azinone, C–H Activation, Ruthenium Catalysis

Abstract: Reactions that enable the straightforward formation of hetero(aryl)-hetero(aryl) systems are of interest from a synthetic perspective, as such systems are found in many biologically active compounds and natural products. A novel strategy for synthesising azinones decorated with hetaryl groups is presented, starting from substituted halopyridines, haloquinolines, halopyrazines, halopyridazines, and halopyrimidines, using a simple Ru(II)–pivalate–carbonate catalyst system. Unsubstituted 2-bromopyridine afforded penta-heteroarylated 2-pyridone, while other haloazines yielded at most di-substituted 2-azinone products. The range of substitution on the 2-azinone ring was controlled by selecting appropriate starting 2-haloazines. Preliminary mechanistic studies revealed a possible synthetic pathway to the heteroarylated azinone products, involving consecutive oxygen incorporation, a Buchwald–Hartwig-type reaction, and C–H bond activation.



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Integrated *in silico* Approach in the Evaluation of Goniofufurone Analogues: Target Prediction, Molecular Docking, and ADME-Tox Analysis

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Keywords: Goniofufurone, Lactones, Molecular Docking, ADME-Tox

Abstract: Goniofufurone and its analogues have attracted considerable attention due to their potential biological activity and structural relevance in drug design. *In silico* approaches provide efficient tools for the early evaluation of such compounds, enabling the prediction of biological targets, binding affinity, and pharmacokinetic properties. This study investigated three structurally simplified goniofufurone analogues with modified stereochemistry using an integrated i*n silico* approach, including target prediction, molecular docking, and ADME-Tox analysis. Computational predictions indicated potential interactions with kinases involved in cytotoxic activity, in agreement with the known biological profile of the lead compound. Molecular docking revealed acceptable binding energy within the active site of the selected enzyme, suggesting stable ligand–enzyme interaction. ADME-Tox analysis showed favorable physicochemical properties, including good membrane permeability and predicted oral bioavailability, with no significant toxicity risks. Overall, these findings highlight goniofufurone analogues as promising candidates for further investigation and support their potential for future experimental validation.

Acknowledgment

This research was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grant Nos. 451-03-33/2026-03/200125 and 451-03-34/2026-03/200125) and the Serbian Academy of Sciences and Arts (Grant No. F-130).

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Biological Evaluation of Ring-Expanded Bile Acid Lactones

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Keywords: Bile Acid Lactones, Antiproliferative Activity, AKR1C, Steroid Hormone Receptors

Abstract: Bile acids are attractive steroidal scaffolds for the development of biologically active molecules because of their rigid structure, defined stereochemistry, and amphiphilic character. Structural modifications of the bile acid framework, such as ring expansion and insertion of a heteroatom, can substantially influence their physicochemical properties and biological activity. In this study, a series of synthesized B- and C-ring-expanded bile acid lactones were evaluated for cytotoxicity against six cancer cell lines and one non-malignant cell line, as well as for their inhibitory effects against human recombinant aldo-keto reductases 1C3 (AKR1C3) and 1C4 (AKR1C4). In addition, their receptor-binding properties toward steroid hormone receptors were evaluated using a fluorescence-based yeast assay. Several derivatives exhibited strong inhibition of AKR1C enzymes, reaching 60–90% inhibition under the assay conditions, as well as moderate cytotoxicity. Receptor-binding studies revealed no affinity toward the estrogen receptor β (ERβ) and androgen receptor (AR), whereas moderate binding was observed toward estrogen receptor α (ERα) and the glucocorticoid receptor for the selected compounds. These findings highlight ring-expanded bile acid lactones as promising steroid-derived scaffolds for the development of novel AKR1C modulators and steroid receptor ligands.

Acknowledgment

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Structural and Bioactivity Studies of Novel 5′-Substituted Benzo[*d*][1,3]dioxol-5-yl Chalcone Derivatives

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Keywords: Chalcones; Benzo[*d*]dioxole; Antioxidant Activity; Acetylcholinesterase Inhibition.

Abstract: Chalcones represent an important class of naturally occurring and synthetic compounds with a wide range of biological activities, making them valuable scaffolds in medicinal and pharmaceutical chemistry. In this study, the design and synthesis of a series of 5′-substituted benzo[*d*][1,3]dioxol-5-yl chalcones were performed with the aim of obtaining new derivatives with potential biological relevance. The presence of the benzo[*d*][1,3]dioxole moiety, together with various substituents on the chalcone framework, was expected to influence both the physicochemical and biological properties of the prepared compounds. The synthesized compounds were characterized in detail in order to confirm their structures and purity. Instrumental characterization was based on CHN elemental analysis, as well as on the ATR-FTIR spectra and NMR spectra of ^{19}F, ^{1}H and ^{13}C nuclei ($^{13}C\{^{1}H\}$ and ^{13}C-APT). After structural characterization, all compounds were subjected to biological evaluation, including the assessment of antioxidant activity and acetylcholinesterase inhibitory potential. These investigations were carried out to examine the possible pharmacological importance of the newly synthesized chalcone derivatives, particularly in relation to oxidative stress and enzyme inhibition. The obtained results provide insight into the influence of different substituents on the properties of benzo[*d*][1,3]dioxole-based chalcones. This study may serve as a useful basis for further synthesis, optimization, and biological investigation of structurally related chalcone derivatives with potential applications in medicinal chemistry.

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Bioactivity-Oriented Design and Synthesis of Fluoro-Substituted Benzo[*d*][1,3]dioxol-5-yl Chalcones

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Keywords: Fluoro-substituted Chalcones; Benzo[*d*]dioxole; Antioxidant Activity; Enzyme Inhibition.

Abstract: Fluorine-containing chalcones have attracted considerable attention in medicinal chemistry due to the unique ability of fluorine atoms to modulate molecular stability, lipophilicity, electronic distribution, and interactions with biological targets. In this study, a bioactivity-oriented approach was applied to the design and synthesis of fluoro-substituted benzo[*d*][1,3]dioxol-5-yl chalcones, with the aim of developing structurally defined compounds with potential pharmacological relevance. The chalcone scaffold was selected as a privileged structural motif, while the benzo[*d*][1,3]dioxole fragment was incorporated due to its frequent occurrence in bioactive molecules. The target fluoro-substituted chalcone derivatives were synthesized through an appropriate condensation reaction and subsequently subjected to detailed structural characterization. The proposed molecular structures were confirmed by CHN elemental analysis, ATR-FTIR spectroscopy, and multinuclear NMR techniques, including ^{1}H-, ^{13}C-, and ^{19}F-NMR spectroscopy. Particular attention was given to ^{19}F-NMR analysis, as it provided direct evidence of fluorine incorporation and valuable information regarding the chemical environment of the fluorinated aromatic moiety. Following structural confirmation, the synthesized compounds were evaluated for their biological activity, with emphasis on antioxidant potential, acetylcholinesterase and tyrosinase inhibitory activity. These assays were selected to assess the possible relevance of the compounds in relation to oxidative stress and enzyme inhibition, both of which are important targets in the development of bioactive small molecules. The obtained results provide insight into the role of fluorine substitution in benzo[*d*][1,3]dioxole-based chalcones and may serve as a foundation for further optimization of fluorinated chalcone derivatives as promising bioactive molecular scaffolds.

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Application of GC–MS and ADME/T Profiling in the Forensic Evaluation of Emerging Phenethylamine Derivatives

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Keywords: ADME/T profile, *N*-benzyl phenethylamines, forensic identification, GC-MS, new psychoactive substances

The continuous emergence of structurally diverse new psychoactive substances represents a significant challenge for forensic and analytical chemistry, particularly in the development of reliable detection and identification methods. Among these, phenethylamine derivatives are particularly significant due to their ease of chemical modification, which leads to extensive structural diversity and varied pharmacological effects, ultimately contributing to their frequent emergence on the illicit drug market. In this work, two novel N-benzyl phenethylamine derivatives were synthesized via reductive amination of substituted benzaldehydes, followed by $NaBH_4$-mediated reduction, affording the corresponding secondary amines in moderate to good yields (65–78%). Structural elucidation was performed using gas chromatography–mass spectrometry (GC-MS), where distinct molecular ions and reproducible fragmentation pathways enabled confident compound identification. The obtained mass spectral data contribute to the expansion of existing analytical libraries and provide valuable reference markers for the detection of emerging psychoactive substances. In silico ADME/T profiling revealed notable differences in pharmacokinetic behavior between the synthesized compounds. The 2-chloro-substituted derivative exhibited increased lipophilicity (logP > 3) and a higher predicted ability to cross the blood–brain barrier, suggesting enhanced central nervous system activity. In contrast, the 4-methoxy analogue showed lower lipophilicity, reduced predicted toxicity, and decreased bioavailability. These findings highlight the critical role of aromatic substitution in modulating physicochemical properties and biological potential. Overall, this study presents an integrated approach combining synthetic chemistry, instrumental analysis, and computational toxicology, providing a systematic framework for improved early detection, characterization, and risk assessment of novel psychoactive substances.

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N,O-Coordinated Schiff Base Pt(II) Complexes: Synthesis, Spectroscopy, and Early Biological Insights

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Keywords: Pt(II) Complexes; Schiff Base; Benzophenone Derivatives, Cristal Structure, p*K*a Values

Abstract: In the study, three Schiff base ligands were synthesized: **L1** (propylamine-5-chloro-2-hydroxybenzophenone), **L2** (butylamine-5-chloro-2-hydroxybenzophenone), and **L3** (propylamine-2,2''-dihydroxy-4-methoxybenzophenone). The crystal structure of ligand **L2** was determined to verify molecular configuration. These ligands were subsequently coordinated to platinum(II), yielding three novel complexes with the general formula $K[PtCl_2(L)]$. Single crystals of ligand **L2** suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution at room temperature. The molecular structure reveals that the **L2** adopts the enol–imine tautomeric form typical for ortho-hydroxy Schiff bases, stabilized by a strong intramolecular O–H···N hydrogen bond between the phenolic oxygen atom and the azomethine nitrogen atom. This interaction enforces a nearly planar arrangement of the chelate fragment. The acidity constants (p*K*a values) of the diaqua platinum(II) complexes **1a**–**3a** were determined by UV–Vis spectrophotometric titration. The pH-dependent UV–Vis spectra of complexes **1–3** reveal gradual spectral changes in the 230–300 nm region, indicating the presence of two protonation–deprotonation equilibria. These transitions reflect stepwise ionization of the proton-active donor sites within the ligand framework. The pK_a values were calculated from absorbance–pH plots at selected wavelengths. The obtained results contribute to a better understanding of structure–property relationships in Pt(II) Schiff base complexes, particularly in terms of protonation behavior and structural features relevant to biomolecular interactions.

Aknowledgment

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para-Phenylenediamine (PPD) Content in Commercially Available Henna Preparations in Bosnia and Herzegovina

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Keywords: *para*-Phenylenediamine (PPD), Henna, HPLC analysis, Natural dyes.

para-Phenylenediamine (PPD) is a synthetic compound commonly found as an undeclared additive in commercial henna preparations, posing significant health risks to henna consumers. This study contributes to the existing literature by providing quantitative data on PPD content in henna products available on the market of the Bosnia and Herzegovina (BiH), a region where such systematic analysis has not previously been reported. Twelve henna samples of different origin and developed color (black, brown, red, and burgundy) were analyzed. Samples were prepared by ultrasound-assisted extraction using methanol as solvent, followed by quantification using high-performance liquid chromatography (HPLC). The results revealed that darker henna preparations, particularly black and dark brown, contained significantly higher content of PPD. Furthermore, PPD was not detected in samples declared as "natural henna" of red shades. The PPD content ranged from 98.06 to 233.14 mg/kg across all positive samples. The lowest concentration was detected in sample H11 (burgundy henna), while the highest was detected in sample H2 (black henna). These findings highlight the need for improved quality control of cosmetic products containing henna, particularly regarding exact and transparent ingredient labeling. Stronger regulatory measures would contribute to better protection of consumers from potential adverse health effects linked to PPD exposure from henna and other cosmetic products, including allergic contact dermatitis and sensitization.

Acknowledgment

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Health Risk Assessment of Dermal Exposure to Heavy Metals in Natural Hair Dyes

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Keywords: Heavy Metals, Henna, Health Risk Characterization, Natural Dyes

Due to growing concerns about the health risks associated with artificial hair dyes, more and more consumers are turning to plant-based alternatives that are considered safer. Natural dyes are of increasing economic importance, and most are obtained by extracting the leaves of *Lawsonia inermis* or its pure dye called Lawsone (2-hydroxy-1,4-naphthoquinone). However, despite being classified as natural products, many natural dyes contain traces of heavy metals. The aim of this study was to assess the health risk to consumers of natural hair dyes based on the content of heavy metals (Cu, Fe, Mn and Zn). The mentioned metals were analyzed by inductively coupled plasma – optical emission spectroscopy (ICP-OES) in hair dye samples, and the following parameters were calculated: Systemic Exposure Dose (SED), Margin of Safety (MoS), Hazard Coefficient (HQ) and the overall hazard index (HI). The concentrations of all analyzed metals in the examined samples were found to be low, well within the regulatory acceptable limits, not posing a significant health risk. The SED values were minimal, reflecting negligible systemic absorption. The MoS values exceeded 100 for all metals (MoS ≥ 100), confirming the high safety of the product. The HQ and HI remained below 1, indicating the absence of a non-carcinogenic risk. The study highlights the need for regular quality control of natural hair dyes and raising consumer awareness about the use of proven and safe cosmetic products.

Acknowledgment

This research was supported by funding through grant number(s) [05-35-3626-1/25, dated December 9, 2025] provided by Federal Ministry of Education and Science, FB&H.

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"Weight-Loss" Teas as Inhibitors of Lipid Peroxidation *in vitro*

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Keywords: Herbal "weight-loss" Teas, Polyphenols, Tannins, Flavonoids, Lipid Peroxidation Inhibition

Abstract: "Weight-loss"teas represent a widespread and easily accessible category of beverages that has gained significant popularity. These herbal products are commonly used for their potential effects on body weight reduction and metabolic regulation. They often contain bioactive compounds such as polyphenols, which are known for their antioxidant properties. Lipid peroxidation is a key process of oxidative damage to cell membranes and is associated with the development of various chronic diseases. Therefore, evaluating the ability of these teas to inhibit lipid peroxidation is important for assessing some of their potential health benefits. As a part of a broader research, the aim of this study was to investigate the ability of 12 teas to inhibit lipid peroxidation. Moreover, total polyphenol, tannin and flavonoid contents were evaluated spectrophotometrically. The analyzed samples showed variability in polyphenol (6.37 – 143.9 mg gallic acid equivalents/tea cup), tannin (4.17 – 107.9 mg gallic acid equivalents/tea cup), and flavonoid (1.60 – 24.07 mg quercetin equivalents/tea cup) contents. All samples demonstrated the potential to inhibit lipid peroxidation, ranging from 0.688 to 20.45 mg Trolox equivalents per tea cup. A moderate correlation was observed between the lipid peroxidation inhibition and total polyphenol, tannin and flavonoid contents. These findings represent preliminary results that provide an initial insight into the antioxidant properties of commercially available herbal "weight-loss" teas. The study contributes to a better understanding of the relationship between phytochemical composition and lipid peroxidation inhibition, and may serve as a basis for further, more detailed investigations.

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"Weight-loss" Teas as Potential α-Glucosidase Inhibitors *in vitro*

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Keywords: "Weight-loss" Teas, Polyphenols, Tannins, Flavonoids, Inhibitors of α-Glucosidase

Herbal teas are often consumed as part of dietary strategies aimed at body weight control and the maintenance of metabolic balance. Their potential health effects are largely associated with the presence of polyphenolic compounds, which are known to influence various metabolic pathways. The aim of this study was to evaluate the ability of 12 different slimming teas available on the Serbian market to inhibit α-glucosidase, a key enzyme involved in carbohydrate digestion in the gastrointestinal tract. Inhibition of α-glucosidase may reduce postprandial glucose levels, and potentially contribute to the prevention and reduction of obesity. The α-glucosidase inhibitory potential was evaluated using a spectrophotometric method based on the hydrolysis of the substrate 4-nitrophenyl α-D-glucopyranoside, where the released *p*-nitrophenol was quantified by measuring absorbance at 400 nm. Acarbose was used as a reference inhibitor. In addition, the total contents of polyphenols, tannins, and flavonoids were determined spectrophotometrically using a method adapted for microtiter plates. The analyzed teas showed considerable variation in the content of the investigated bioactive compounds. Ten out of twelve analysed teas exhibited the ability to inhibit α-glucosidase activity, ranging from 154.28 to 2963.2 mg acarbose equivalents. A moderate correlation was observed between the contents of total polyphenols, tannins and flavonoids and the inhibitory capacity of the investigated teas against α-glucosidase These findings may provide a basis for further studies investigating the mechanisms of action of slimming teas, particularly regarding their potential role in obesity prevention.

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Interaction of Salicin Derivatives with Bovine Serum Albumin: A Spectroscopic and In Silico Approach

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Keywords: Bovine Albumin Serum, Salicin Derivatives, Fluorescence Spectroscopy, Molecular Docking

In this study, fluorescence spectroscopy was used to examine the interactions between selected salicin derivatives—methyl salicylate (Me-SA), salicyl hydrazide (SA-H), helicin (Hel), and Hel-SA-H—and bovine serum albumin (BSA) under physiological conditions. The experiments were conducted at three temperatures, and key parameters, including Stern-Volmer constants (K_{sv}), bimolecular quenching constants (k_q), binding constants (K_b), and the number of binding sites (n), were determined. The results indicate that fluorescence quenching of BSA occurs predominantly via a static mechanism, with the Hel-SA-H complex showing the highest quenching efficiency (k_q 35.0 × 10^{12} M^{-1} s^{-1}). Binding affinities varied notably among the compounds, with Hel-SA-H and Hel exhibiting the strongest interactions, while Me-SA showed the weakest. Negative $\Delta G°$ values confirmed the spontaneity of binding, with thermodynamic data suggesting different contributions of enthalpic and entropic factors depending on the ligand. Synchronous fluorescence spectra revealed minor changes in the microenvironment of tyrosine residues, whereas tryptophan residues remained largely unaffected, indicating localized conformational changes. Three-dimensional fluorescence spectra further confirmed structural alterations in BSA upon ligand binding. Förster Resonance Energy Transfer (FRET) analysis showed donor–acceptor distances of 2.4–3.3 nm, supporting complex formation, with Hel-SA-H demonstrating the highest energy transfer efficiency. Molecular docking results were consistent with experimental findings, highlighting strong binding affinity for Hel-SA-H (−7.655 kcal mol^{-1}) and emphasizing the role of hydrogen bonding, hydrophobic, and π-interactions. Overall, the results demonstrate that structural differences among salicin derivatives significantly influence their interaction with BSA.

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Triple Polymorphism in a New Oxidovanadium(V) Aroylhydrazone Complex

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Keywords: vanadium aroylhydrazone complex, crystal structures, polymorphism

Abstract: A new oxidovanadium(V) complex incorporating a tridentate dianionic ONO aroylhydrazone ligand, derived from 2'-hydroxy-5'-methylacetophenone and benzhydrazide, and a co-coordinated methoxide ion was synthesized and structurally characterized. Interestingly, the synthesis yielded crystals of varying morphologies, which single-crystal X-ray diffraction identified as three distinct polymorphic forms. Among these, two polymorphs crystallize in the monoclinic crystal system (space group $P2_1/c$), while the third belongs to the triclinic system ($P\text{-}1$). While all three polymorphs share an identical coordination environment around the vanadium(V) center, they exhibit unique crystal packing modes and intermolecular interaction networks. The structural diversity in the solid state was further correlated with differences observed in their infrared spectra. These findings expand the structural chemistry of oxidovanadium(V) aroylhydrazones and highlight the subtle role of non-covalent interactions in directing polymorphism.

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Salicylaldehyde-derived 8-aminoquinoline Amines: Synthesis and Biological Evaluation

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Keywords: Secondary amines; 8-Aminoquinoline; Antimicrobial activity; *Artemia salina* toxicity; DNA/BSA interactions.

Abstract: Three novel secondary amines derived from salicylaldehyde and its 5-halogenated analogues with 8-aminoquinoline, (1) (R = H), (2) (R = Cl), and (3) (R = Br), were synthesized through Schiff-base formation followed by $NaBH_4$ reduction. The products were obtained in good yields (64–86%) and characterized by IR, UV–Vis, $^1H/^{13}C$ NMR and 2D NMR spectroscopy, confirming successful C=N reduction to C–NH and formation of the target amines. The compounds were further evaluated for antimicrobial activity, *Artemia salina* toxicity, and interactions with calf thymus-DNA (CT-DNA) and bovine serum albumin (BSA). All compounds showed antimicrobial activity against selected Gram-positive and Gram-negative bacteria and *Candida albicans*. The strongest antibacterial effect was observed against *Bacillus subtilis* for the halogenated derivatives (2) and (3), with MIC values of 0.039 mM, while all three compounds displayed pronounced antifungal activity against *C. albicans* (MIC = 0.009 mM). In the *Artemia salina* assay, mortality increased with concentration and exposure time; the highest mortality was recorded for (3) at 100 μM after 72 h (40%), suggesting LC_{50} values above the tested range. Sublethal morphological and developmental alterations were most evident for halogenated derivatives. Fluorescence studies showed efficient BSA quenching, moderate binding affinities (K_b = 0.99–13.03 × 10^3 M^{-1}), and thermodynamic parameters consistent with spontaneous binding mainly driven by hydrogen bonding and van der Waals interactions. Ethidium bromide displacement experiments indicated interaction with CT-DNA, with apparent binding constants up to 2.24 × 10^5 M^{-1}.

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Effect of Different Extraction Methods on the Phenolic Compound Concentration and Antioxidant Capacity of *Achillea millefolium* L. Aerial Parts

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Keywords: *Achillea millefolium* L., Antioxidant Capacity, ABTS, CUPRAC, FRAP, Phenolic Compounds

Abstract: *Achillea millefolium* L. is widely used in traditional medicine for wound healing, anti-inflammatory treatment, and gastrointestinal disorders, but comparative studies on phenolic extraction methods and their effects on antioxidant capacity remain limited. This study aimed to compare the effects of different extraction methods of phenolic compounds on the antioxidant capacity of *A. millefolium*. The ability of ethanol extracts to scavenge ABTS (2,2′-azino-bis(3-ethylbenzothiazoline-6-sulfonate)) radicals, as well as to reduce Cu^{2+} and Fe^{3+} ions using CUPRAC (Cupric Ion Reducing Antioxidant Capacity) and FRAP (Ferric Reducing Antioxidant Power) assays, was evaluated. Concentrations of total phenolic compounds, flavonols, flavonoids, and phenolic acids were also determined. Extracts from dried leaves (L) and flowering aerial parts (FAP) were prepared using 80% ethanol by two extraction procedures: sonication (5 min) followed by stirring (30 min) (E1), and Soxhlet extraction (E2). Antioxidant assays showed higher activity in leaf extracts than in FAP extracts for both extraction methods. In the ABTS assay, the E2 leaf extract exhibited the strongest antioxidant activity, with the lowest IC_{50} value (3.72 ± 0.03 μg/mL). Similarly, CUPRAC and FRAP assays demonstrated higher antioxidant capacity in leaf extracts, with the highest values recorded for the E1 leaf extract. The E2 leaf extract contained the highest levels of total phenolic compounds, flavonols, and phenolic acids, while the E1 leaf extract showed the highest flavonoid content. In general, leaf extracts demonstrated stronger antioxidant potential than FAP extracts, while antioxidant activity varied depending on the extraction procedure and assay applied.

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Antiproliferative activity and *in Silico* Assessment of Essential Oils of Two Genotypes of Cultivated Mentha Species

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Keywords: *Mentha spicata*, Essential Oil, Antiproliferative Activity, Docking Study

Abstract: Mentha species essential oils (EOs), obtained by steam distillation of leaves and flowering tops, are widely used in the perfumery, cosmetic, pharmaceutical, and aromatherapy industries due to their rich content of bioactive compounds. Major constituents, including carvone, limonene, menthol, and menthone, contribute to their characteristic cooling effect and diverse biological activities, including cytotoxicity. The antiproliferative activity of two Mentha genotypes (Spica and Lemon) cultivated in Isparta Province, Türkiye, was evaluated using the MTT assay against non-small cell lung carcinoma (A549) and normal human fetal lung fibroblasts (MRC-5). Results were expressed as IC_{50} values. To complement the biological evaluation, molecular docking was performed against three cancer-related protein targets involved in cell survival and proliferation: BCL-2 (PDB: 6O0K), ERK2 (PDB: 4ZXT), and MLK1 (PDB: 3DTC). The examined EOs exhibited strong cytotoxic activity, with IC_{50} values ranging from 1.50 µL/mL (Spica) to 3.21 µL/mL (Lemon), while showing excellent selectivity toward normal MRC-5 fibroblasts. Constituents associated with the most active oils, particularly carvone-rich genotypes, demonstrated the most favorable binding affinities, especially toward MLK1 and ERK2. This trend was consistent with the high antiproliferative activity of genotype Spica (*Mentha citrata*). In contrast, genotype Lemon (*Mentha gentilis*) displayed strong experimental activity despite less favorable docking of its major constituents, suggesting possible synergistic or multitarget effects. These findings provide mechanistic support for the observed antiproliferative differences among chemically distinct Mentha genotypes.

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Cytotoxic activity of Essential Oil of *Helichrysum italicum* from the Continental and sub-Mediterranean Regions

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Keywords: *Helichrysum italicum* (Roth) G. Don; Anticancer Activity; Genotoxicity; Comet Assay

Introduction: *Helichrysum italicum (Roth) G. Don* (immortelle) is highly valued for its essential oil (EO) rich in volatile compounds, such as sesquiterpenes, flavonoids, and phloroglucinols, which contribute to its diverse biological activities. The antiproliferative activity of helichrysum EO has gained increasing scientific attention due to its potential application in cancer research. EOs were obtained from dried plant material by 2 h hydrodistillation. GC–MS analysis identified nerol acetate as the major constituent of EO from continental populations, whereas italidone predominated in EO from sub-Mediterranean populations of Bosnia and Herzegovina. Cytotoxic activity was evaluated against human myelogenous leukemia (K562), prostate cancer (PC-3), and normal fetal lung fibroblast (MRC-5) cell lines. Cell viability was assessed using a modified MTT assay, and IC_{50} values were determined. The EO from the sub-Mediterranean population exhibited IC_{50} values ranging from 0.220 µL/mL (K562) to 2.03 µL/mL (PC-3). The continental EO showed stronger activity, with IC_{50} values ranging from 0.039 to 0.295 µL/mL against the same cell lines. Both EOs demonstrated substantial cytotoxic effects on K562, PC-3, and MRC-5 cells. Comet assay results indicated relatively low genotoxicity toward healthy MRC-5 cells, suggesting a favorable safety profile. The investigated immortelle EOs exhibited promising antiproliferative activity and potential for further biomedical applications. However, these findings are limited to in vitro conditions. Additional studies, including in silico analyses, in vivo validation, and clinical investigations, are required to confirm their efficacy and safety for human use.

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Pharmacogenomics of Apixaban: Bridging Biochemistry and Clinical Outcomes

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Keywords: Apixaban, Pharmacogenomics, CYP3A4/5, ABCB1, ABCG2, Variability, Metabolism, Transporters, Anticoagulation

Abstract: Apixaban, an oral factor Xa inhibitor, has predictable pharmacokinetics, but variability is partly driven by genetic factors affecting metabolism and transport. Biochemically, apixaban undergoes hepatic oxidative metabolism primarily via CYP3A4/5, and the parent compound remains the main active form. In parallel, drug transporters play a key role: apixaban is a substrate of P-glycoprotein (*ABCB1*) and breast cancer resistance protein (BCRP, *ABCG2*), which regulate intestinal absorption and elimination pathways. This review synthesizes recent data related to apixaban pharmacokinetics and pharmacogenomics, linking Metabolism, Transport, and Clinical Variability drawing from databases including PubMed, Embase, Medline, and ScienceDirect. Few pharmacokinetic studies have demonstrated associations between polymorphisms in the *CYP3A5*, *ABCG2*, and *ABCB1* genes and the pharmacokinetics of apixaban. An intronic polymorphism in the *ABCB1* gene associated with lower apixaban concentrations, was also linked to a lower risk of bleeding in one study. Although a recent study found an association between *CYP3A5* and *ABCG2* polymorphisms and bleeding risk with apixaban, two other studies failed to confirm the impact of pharmacokinetic polymorphisms on clinical outcomes such as bleeding risk and thromboembolic events. Genetic determinants alone appear insufficient to fully explain interpatient variability, as clinical factors including age, renal function, comorbidities and concomitant medications may also play an important role. Although pharmacogenomics has potential to explain variability in apixaban response, current evidence does not support genotype-guided dosing, highlighting the need for further research in personalised anticoagulation therapy.

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Biological Potential of *Sanguisorba minor* L. in Terms of Antidiabetic Activity

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Keywords: *Sanguisorba minor* L., Antioxidant Activity, Biogenic Elements, *A*-Amylase, *A*-Glucosidase

Abstract: *Sanguisorba minor* L. (Rosaceae), known as small burnet is a wild edible plant usually consumed in the form of salads. As a medicinal plant it is used in traditional medicine in various countries. Due to its hemostatic effect, small burnet has been used as an astringent. Its infusions and tinctures are known for their diuretic, digestive, and appetite-stimulant activity. The aim of this study was to evaluate the total phenolic and flavonoid content, content of biogenic elements (K, Na, Mg, Ca, Cr, Mn, Fe, Co, Ni, Cu, and Zn), as well as antioxidant and antidiabetic potential of *S. minor*. The ethanol, methanol, and water extracts were characterized by total phenolic (64.18±1.02, 58.4±1.05, and 49.29±1.02 mg/g of extract) and flavonoid content (41.27±0.04, 15.43±0.08, and 28.58±0.07 mg/g of extract, respectively). The results obtained by the FRAP method ranged from 363.95±2.11 for the water extract to 650.91±1.74 μM $FeSO_4$/g of extract for the ethanolic extract. IC_{50} values, obtained by the DPPH method, were 2.5, 2.7, and 2.9 mg/mL for the ethanol, water, and methanol extracts, respectively. All tested extracts show good *α*-amylase inhibition potential, ranging from 30.38±1.98% for the water extract to 57.4±1.19% for the ethanol extract, and excellent *α*-glucosidase inhibition potential, ranging from 87.29±2.43% for the water extract to 97.28±1.33% for the ethanol extract (1 mg/mL). The results for *α*-amylase and *α*-glucosidase inhibition, antioxidant activity, and significant content of biogenic elements indicate the potential of using the plant *S. minor* in the treatment of diabetes and as a functional food, suggesting the need for further research.

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Potential of *Arctium lappa* L. Root Extracts in Protection of Lipids from Oxidation

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Keywords: *Arctium lappa* L., Phenols, Flavonoids, Antioxidant Activity, Lipid Oxidation

Abstract: *Arctium lappa* L. (Asteraceae), known as burdock, is a perennial herb with a rich historical background in the traditional medicine of numerous countries. Its roots, fruits, seeds, and leaves are rich in bioactive metabolites and are utilized in a diverse array of medicinal applications. Burdock root has nutritional and therapeutic value. The main goal in this work was to examine the antioxidant potential of ethanol extract, methanol extract, water macerate, and infusion of *Arctium lappa* L. root in terms of protection of lipids from oxidation. Antioxidant potential was also tested by DPPH and FRAP methods. By determining the content of total phenols and flavonoids, and by statistical analysis, their correlation with the antioxidant activity was tested. Regarding total phenol content, results ranged from 34.09±0.09 for the macerate to 255.9±0.02 mg/g for the methanol extract. Methanol root extract showed the highest content of total flavonoids (106.3±0.05 mg/g of extract), and also the highest results tested by the DPPH (IC_{50} = 0.55±0.04 mg/mL), and FRAP methods (1.89±0.5 mM $FeSO_4$/g of extract). Results for testing potential in protecting lipids from oxidation were highest for water macerate 35.53±1.31%, and infusion 32.89±1.02% (1 mg/mL of root extracts). The results of statistical analysis showed a very strong positive correlation between the content of phenols, flavonoids, and antioxidant activity (DPPH and FRAP) (Pearson's test, $r = 0.990–1.000$; $p < 0.01$), while lipid protection from oxidation showed a significant negative correlation with the examined parameters. Thus, additional research is needed that would point to compounds with a lipid-protective effect.

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Sage Extract as a Potent Inhibitor of Tyrosinase: Mechanisms and Therapeutic Implications

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Keywords: *Salvia officinalis* L., Tyrosinase, Hyperpigmentation

Abstract: *Salvia officinalis* L. extract has been widely used in skin care applications due to its significant biological and functional properties. However, its effects and mechanisms in regulating skin (de)pigmentation remain insufficiently understood. Therefore, the present study investigated the inhibitory potential of sage ethanol extract (SEE) and sage glycerol extract (SGE) toward tyrosinase activity. The extracts were prepared by finely grinding sage leaves followed by extraction using 70% ethanol and 70% glycerol in a 1:5 ratio. A combination of heat- and cold-assisted extraction procedures was applied to improve the isolation of bioactive compounds, and the obtained extracts were further evaluated for anti-tyrosinase activity. Tyrosinase activity was determined spectrophotometrically using mushroom tyrosinase and L-DOPA as substrate in phosphate buffer (pH 7.4). The reaction mixtures contained varying concentrations of L-DOPA (1–8 mM), enzyme solution, and either SEE or SGE, while the total reaction volume was adjusted to 320 µL. Both extracts reduced tyrosinase activity compared to the control samples without inhibitors. SEE showed the highest inhibitory activity at lower substrate concentrations, reaching approximately 51% inhibition at 1 mM L-DOPA. In contrast, SGE exhibited a more stable inhibitory effect across the investigated concentration range, with a maximum inhibition of approximately 48% at 2 mM L-DOPA. The results indicate that sage extracts possess significant anti-tyrosinase potential, likely due to the presence of phenolic compounds and flavonoids with known antioxidant and enzyme-inhibitory properties. Differences observed between SEE and SGE may be associated with variations in solvent polarity and extraction efficiency of bioactive constituents. These findings suggest that sage extracts could represent promising natural agents for cosmetic and dermatological applications related to hyperpigmentation control.

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Evaluation of Antioxidant and Anti-Inflammatory Activity of *Hypericum perforatum* L. Extract and Topical Formulations

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Keywords: *Hypericum perforatum*, Antioxidant Activity, Anti-Inflammatory Activity, DPPH, DMPD, Topical Formulations, Gels, Creams

Abstract: *Hypericum perforatum* L. is a medicinal plant widely recognized for its antioxidant, anti-inflammatory, and wound-healing properties, making it a promising ingredient in cosmetic and pharmaceutical formulations. The aim of this study was to evaluate the antioxidant and anti-inflammatory activities of *H. perforatum* extract and topical formulations containing this plant. Ten samples were analyzed, including an ethanolic extract of *H. perforatum*, oil macerates, creams, and gels with and without *H. perforatum*. Eight formulations were prepared in the laboratory. Antioxidant activity was determined spectrophotometrically using DPPH and DMPD assays, while anti-inflammatory activity was evaluated by the protein denaturation method. The ethanolic extract *H. perforatum* demonstrated pronounced biological activity, with the highest antioxidant activity observed using the DPPH assay (85.39%). The DMPD method also confirmed antioxidant potential, although to a lesser extent. Oil-based formulations exhibited varying antioxidant capacities, with olive and sunflower oils showing higher activity than *H. perforatum*-enriched oils. Cream formulations displayed notable antioxidant activity, with values of 43.38% and 42.60%, indicating the contribution of both *H. perforatum* and additional active ingredients. However, comparison with individual components suggested an antagonistic effect within the cream formulations. Anti-inflammatory testing revealed significant activity in several formulations, particularly gels and sunflower oil. The highest anti-inflammatory activity was recorded for the *H. perforatum* gel (43.88%), highlighting its potential for topical treatment of inflammatory skin conditions. Overall, the results confirm that *H. perforatum* is a valuable raw material for the development of cosmetic and pharmaceutical products with local therapeutic effects. The findings provide a basis for further optimization of formulations intended for the treatment of damaged and inflamed skin.

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Validation of the Method for Determination of Levetiracetam Content in Levetiracetam 250 mg, 500 mg, and 1000 mg Film-Coated Tablets

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Keywords: Levetiracetam, HPLC, Method Validation, Assay, Film-Coated Tablets, Pharmaceutical Analysis, USP, Quality Control

Abstract: This study presents levetiracetam assay validation. The content assay of levetiracetam in 250 mg, 500 mg, and 1000 mg film-coated tablets was performed using an HPLC method developed as a modification of a USP dissolution procedure, in accordance with HSE requirements. The analysis was performed using an HPLC system equipped with a C18 column (150×4.6 mm, 5 µm). The mobile phase consisted of acetonitrile: phosphate buffer pH 5.6 (15:85, v/v). Conditions: flow rate- 1.2 mL/min, detection: 220 nm, injection volume: 10 µL. The retention time of levetiracetam: 2.5 minutes, total run time: 4 minutes. Selectivity testing confirmed no interference from placebo components. Forced degradation studies (thermal, photolytic, oxidative, acidic, and alkaline) demonstrated that the method is stability-indicating. Linearity was established over the range 50–120% with a correlation coefficient: r = 1.0000, slope: 1.01, CV of response factor: 0.7%, meeting acceptance criteria (r≥ 0.995; CV≤ 3.0%; intercept ±2.0%). Accuracy studies showed mean recovery of 100.8% with bias between 0.1% and 2.0%, within the acceptance range of 97.0–103.0% and bias ≤3.0%. System and method precision were confirmed with CV values of 0.05% and 0.3%, respectively (acceptance criterion ≤ 2.0%). Robustness testing recovery: 99.4%-101.7% with CV 0.1–0.9%, with no significant effect on retention time. All validation parameters complied with predefined acceptance criteria. The method is selective, reproducible, linear, accurate, precise, and robust, and is suitable for routine quality control and assay of levetiracetam in film-coated tablets of different strengths.

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Verification of the Karl Fischer Titration Method for Determination of Water Content in Nifuroxazide 200 mg Hard Capsules

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Keywords: Karl Fischer Titration, Water Content, Method Verification, Pharmaceutical Analysis, Hard Capsules, Ph. Eur. 2.5.12, Quality Control

Abstract: Verification of the Karl Fischer titration method for determination of water content in Nifuroxazide 200 mg hard capsules was performed according to Ph. Eur. 2.5.12. Water: semi-micro determination. According to Ph. Eur. 2.5.12., verification of the Karl Fischer method for finished pharmaceutical products requires evaluation of accuracy, linearity, and percentage error parameters in order to confirm suitability of the method for routine quality control. Accuracy was evaluated through recovery studies by cumulative addition of water (five additions). The obtained mean recovery was 100.6%, which complied with the acceptance criterion of 97.5–102.5%. Linearity was assessed using linear regression analysis of added versus determined water content. The obtained slope was 1.005, meeting the acceptance criterion of 0.975–1.025 (±2.5%). Percentage errors for intercept values were determined as |e1| = 0.08% and |e2| = 0.43%, both complying with the acceptance criterion of <2.5%. System suitability testing gave an average water equivalent of 5.2026 mg/mL with RSD of 0.96%, fulfilling the criterion of RSD<1.5%. All evaluated parameters fulfilled the acceptance criteria defined by Ph. Eur. 2.5.12. The obtained results confirmed that the Karl Fischer titration method is suitable for determination of water content in Nifuroxazide 200 mg hard capsules.

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Comparative GC–MS Analysis of the Perfume Headspace, the Perfume, and Aroma Compounds Used in Its Formulation

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Keywords: Perfumes, Headspace, GC-MS

Abstract: Perfume composition represents a complex mixture of natural and synthetic volatile compounds that in sinergy determine fragrance character and stability. The chemical composition of the commercial fragrance for man, its corresponding headspace, selected essential oils, and synthetic fragrance materials used in perfume formulation was analysed by gas chromatography–mass spectrometry (GC/MS). Compounds identification was performed by comparison of mass spectra and retention indices with reference in Adams library and Essentaial Oil4 in MassFinder software. The perfume was dominated by cis-methyl diydrojasmonate (29.5%), followed by trans-methyl diydrojasmonate (9.8%) and linalyl acetate (8.4%). A similar profile was observed in the headspace, where cis-methyl diydrojasmonate (23.4%), linalyl acetate (8.1%), and trans-methyl diydrojasmonate (7.7%) were the major constituents. The slightly lower proportions of cis- and trans-jasmonate in the headspace indicate differences between the liquid composition and the volatile fraction released into the air, whereas linalyl acetate showed comparable abundances in both samples. Synthetic Hedione, hidrodestiled rosemary essential oil and commercial reconstracted jasmine oil, selected due to their correspondence with the declared top and middle fragrance notes of selected parfume, were additionally analyzed. Rosemary oil was characterized by α-terpineol (32.3%) and borneol (27.5%), whereas jasmine oil contained amyl cinnamaldexide (38.8%) and benzyl acetate (21.2%) as dominant constituents. None of these compounds were detected in the perfume sample, suggesting that the characteristic jasmine and aromatic accords were recreated predominantly through synthetic fragrance materials rather than direct incorporation of the analyzed oils. The detected ambroxide and cedryl methyl ketone correspond well with the declared amber and cedar base notes of the perfume.

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Effect of Brewing Temperature and Infusion Time on the Antioxidant and Anti-Inflammatory Activity of Commercial Tea Samples

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Keywords: Tea infusions; Antioxidant Activity; Anti-inflammatory Activity; DMPD assay; Brewing Temperature

Abstract: Tea is one of the most widely consumed beverages worldwide and is recognized as a valuable source of bioactive compounds with antioxidant and anti-inflammatory properties. Since brewing conditions may significantly influence its biological activity, this study investigated the effects of temperature and infusion time on the antioxidant and anti-inflammatory potential of commercial tea samples. Twelve commercially available tea samples (black tea, green tea, chamomile, thyme, nettle, St. John's wort, mint, and marigold tea) were prepared at two temperatures (20 °C and 80 °C) and five infusion times (3, 5, 15, 30, and 60 min). Antioxidant activity was determined using the DMPD radical scavenging assay, while anti-inflammatory activity was evaluated by the protein denaturation inhibition method. All tested samples exhibited antioxidant activity. At 20 °C, the highest antioxidant activity was recorded for St. John's wort tea after 30 min of infusion (64.01%), whereas the lowest activity was observed for loose-leaf green tea after 5 min (4.45%). At 80 °C, St. John's wort tea also showed the highest antioxidant activity (57.38%), while bagged green tea exhibited the lowest value (0.095%). Regarding anti-inflammatory activity, black tea and bagged chamomile tea demonstrated the highest activities at 20 °C, reaching 76.77% and 75.20%, respectively. At 80 °C, black tea showed the strongest anti-inflammatory effect (89.74%). The lowest activities were observed for St. John's wort tea and bagged mint tea, while loose-leaf nettle tea showed no detectable anti-inflammatory activity under the tested conditions. The results demonstrate that both temperature and infusion time significantly affect the biological activity of tea infusions, highlighting the importance of optimizing brewing conditions to maximize their potential health benefits.

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Investigation of the Adsorption Potential of Herbicides on Selected Metal-Organic Adsorbents

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Keywords: Glyphosate, Adsorption, Green Synthesis, Fe–Tannin Adsorbent, FTIR

Abstract: The presence of herbicides in aquatic systems represents an environmental concern due to their persistence, mobility, and adverse effects on ecosystems and human health. This study investigated glyphosate removal using a Fe–tannin adsorbent synthesized via a green approach, employing concentrated black tea infusion as a natural source of polyphenolic ligands and iron (III) chloride as the metal precursor. FTIR analysis confirmed the formation of Fe–polyphenol coordination structures. Optimization of the adsorption process included determination of the point of zero charge (pHpzc), adsorbent mass, solution pH, and contact time. The pHpzc value was approximately 4, while the highest glyphosate removal efficiency was achieved using 0.250 g of adsorbent (66.76%). The optimal pH was 4, whereas strongly alkaline conditions (pH 10–12) resulted in negative adsorption capacity values. Contact time studies showed rapid initial adsorption, with removal increasing from approximately 34% after 15 min to 66.78% after 3 h, with only minor improvement after prolonged contact (24–48 h), indicating near-equilibrium conditions after 3 h. Kinetic analysis revealed that glyphosate adsorption followed the pseudo-second-order model (R^2 = 0.9973), while the pseudo-first-order model showed poor agreement (R^2 = 0.4682), suggesting a significant contribution of chemisorption. Adsorption isotherm analysis indicated that the Freundlich model better described the adsorption process than the Langmuir model, suggesting adsorption on a heterogeneous surface, while the Langmuir model yielded non-physical parameter values. These findings demonstrate that the green-synthesized Fe–tannin adsorbent represents a simple, environmentally friendly, cost-effective, and promising material for glyphosate removal from aqueous systems.

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Effect of Brewing Conditions on Caffeine Content in Green and Black Tea Infusions

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Keywords: Caffeine; Tea Infusions; Brewing Temperature; Infusion Time; Green Tea; Black Tea

Abstract: Caffeine is a naturally occurring alkaloid widely distributed in plants such as Camellia sinensis, Coffea arabica, and Theobroma cacao. Due to its stimulant properties and widespread consumption through tea, coffee, soft drinks, and pharmaceutical products, caffeine remains a subject of considerable scientific interest. The aim of this study was to investigate the influence of brewing temperature and infusion time on caffeine extraction from commercially available tea samples. Green and black teas, both in tea bags and bulk form, were prepared under different brewing conditions. Infusions were prepared at 20, 50, 75, and 100 °C, with brewing times of 2.5, 5, 10, and 30 minutes, as well as 24 hours. Caffeine content was determined and compared across the different preparation conditions. The results revealed a general trend of maximum caffeine extraction at 75 °C after 2.5 minutes of brewing. An exception was observed for bagged green tea, where the highest caffeine content was obtained after 10 minutes of infusion (2.28 mg/g). At 100 °C, caffeine concentrations ranged from 1.63 to 2.28 mg/g for green tea and from 1.01 to 2.71 mg/g for black tea. In most cases, tea bag samples exhibited higher caffeine concentrations than their loose-leaf counterparts. For black tea, higher caffeine levels were observed in tea bags in approximately 75% of the analyzed samples. These differences may be attributed to variations in plant material, processing methods, particle size, and tea quality. The findings demonstrate that brewing conditions significantly affect caffeine extraction and should be considered when preparing tea to achieve the desired caffeine content.

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Initial Comparative Assessing of New Imidazole Derivatives by on-line ADMET and QSAR-prediction Services

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Keywords: Imidazole Derivatives, ADME Properties, Prediction of Biological Activity

Abstract: The derivatives of imidazoles show a wide range of biological activities such as antibacterial, antimycobacterial, anti-inflammatory, and antitumor. Many drugs contain an imidazole ring, such as certain antifungal drugs, the nitroimidazole series of antibiotics, and the sedative midazolam. Histamine, an almost ubiquitous substance in the human body, is characterised by an imidazole ring and is a natural organic chemical that acts as a neurotransmitter in the brain and an inflammatory mediator in the immune system. Recently, we have synthesised novel arylamide imidazole derivatives that can be structurally classified in two groups: carboxamides and acetamides. In silico absorption, distribution, metabolism, excretion (ADME) and drug-likeness parameters were calculated by AdmetLab 3.0 (https://admetlab3.scbdd.com/), an online tool. According to the Lipinski rule of 5', which predicts good absorption or permeation if a molecule has: all molecules satisfy drug likeness criteria. Also, all compounds satisfy criteria: total polar surface area (TPSA) between 20 and 130 Å^2, solubility in water, log S, not lower than -6, and flexibility; the molecule should not have more than 9 rotatable bonds. The only criterion for a drug's effectiveness is saturation: the ratio of sp^3-hybridised carbons in the molecule, which should be at least 0.25. Introducing more alkyl groups into the structure will satisfy the drug likeness criteria completely. Prediction of biological activity, including pharmacological effects was obtained using PASS program on Way2Drug predictive online service (https://way2drug.com/passonline/). The highest probability (P_a = 0.862) was calculated for the derivate 1A (*N*-phenyl-1*H*-imidazole-4-carboxamide) to be a mannotetraose 2-alpha-*N*-acetylglucosaminyltransferase inhibitor. The studied compounds have potential as future drug candidates since their pharmacokinetic properties are appropriate.

Acknowledgment

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Determination of the Content of Metoprolol Oral Suspension

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Keywords: Cold Chain, HPLC, Metoprolol, Ora-Sweet, Ora-plus, Suspension

Abstract: Metoprolol is primarily prescribed for the management of hypertension, angina pectoris, heart failure, and arrhythmias. In the past decade, significant efforts have been undertaken to create pediatric-friendly oral dosage forms to ensure the safe and effective administration of this medication. This study aims to assess the stability and drug content of metoprolol oral suspensions, which are frequently recommended for use in liquid oral dosage forms but are not commercially available. A metoprolol tartrate solution at a concentration of 10 mg/ml was prepared using a 1:1 mixture of Ora-Sweet and Ora-Plus and stored in a 50 ml dark glass bottle. The source of the medication was tablets. Three bottles of the oral suspension were prepared; one was maintained at room temperature (25°C), while the other two were kept in a cold chain at temperatures between 2°C and 8°C, all stored in a dark environment. Samples were collected from each bottle after 30, 60, 75, and 90 days, and the drug concentration was analyzed using high-performance liquid chromatography (HPLC). The average concentration of metoprolol in the oral suspension stored at room temperature was found to be 100.26%, while the suspension stored in the cold chain exhibited a concentration of 101.75%. Both results met the quality standards, indicating that the content should not fall below 90% or exceed 110%. At least 96.55% of the initial drug concentration was preserved in all oral suspensions for up to 90 days, with no observable changes in appearance, odor, or pH values of the liquids.

POSTER PRESENTATIONS

Materials Chemistry

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Adsorption of Malachite Green from Aqueous Solutions Using Waste *Sorghum*

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Keywords: *Sorghum*, Adsorption, Malachite Green

Abstract: Synthetic dyes are extensively utilized in manufacturing industries to color a variety of finished products. Among these, malachite green (MG) is commonly applied in the dyeing of cotton, leather, wool, silk and paper. The discharge of dye-containing wastewater without adequate purification leads to significant environmental challenges. Consequently, various methods are under investigation for the treatment of dye-contaminated water. Adsorption has proven to be an effective, cost-efficient, and environmentally sustainable method, particularly when employing natural lignocellulosic adsorbents. This study investigates the adsorption of MG onto *sorghum* (SR) from aqueous solutions under batch conditions. The *sorghum* surface was characterized using Fourier-transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM). Adsorption experiments were conducted at an initial solution pH of 6.5, a temperature of 25 °C, and an adsorbent mass of 90 mg, with varying initial adsorbate concentrations. The adsorption process is better described by the Freundlich model than by the Langmuir model, indicating multilayer adsorption with a heterogeneous distribution of active sites on the *sorghum* surface. The kinetics of MG adsorption on SR align more closely with the pseudo-second-order model than with the pseudo-first-order, suggesting the predominance of chemical interactions between the adsorbate and available sites on the adsorbent. It is proposed that MG adsorption on SR results from the combined effects of electrostatic interactions between deprotonated carboxyl groups from hemicellulose and the cationic dye and π–π interactions between lignin aromatic structures and dye aromatic rings. The experimental findings and comparison with related studies suggest that *sorghum* has potential as an adsorbent for the removal of malachite green dye from aqueous solutions.

Acknowledgment

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Synthesis and Characterization of a 1-D Nickel(II) Coordination Polymer with Mixed 2-Bromonicotinate and 4,4'-Bipyridine Ligands

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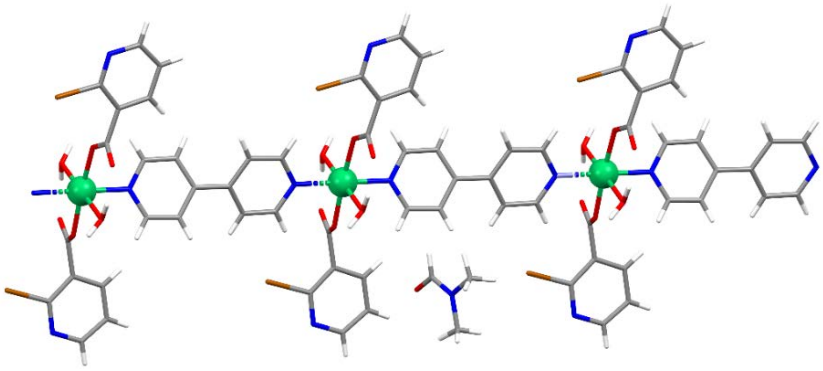
Keywords: Coordination polymer, Nickel(II), 2-Bromonicotinate, 4,4'-Bipyridine, Crystal structure

Abstract: The synthesis of halonicotinate-based coordination polymers (CPs) has attracted considerable research interest due to their diverse properties and wide range of applications. In our earlier work, we obtained 1-D nickel(II) coordination polymers with mixed ligands such as 6-fluoronicotinate or 6-chloronicotinate and 4,4'-bipyridine, in a mixture of water and ethanol [1, 2]. This time, in the reaction of nickel(II) sulfate heptahydrate, 2-bromonicotinic acid (2-BrnicH) and 4,4'-bipyridine (4,4'-bpy), performed in a mixture of water and *N,N'*-dimethylformamide (DMF), the compound $\{[Ni(H_2O)_2(4,4'\text{-bpy})(2\text{-Brnic})_2]\cdot 3DMF\}_n$ (1) was prepared and its crystal structure determined by single-crystal X-ray crystallography. The nickel(II) ion in 1 is octahedrally coordinated by two O atoms of two water molecules, two O atoms from *O*-monodentate 2-bromonicotinate ligands, and by two N atoms from bridging 4,4′-bipyridine ligands, forming a *trans* isomer (Figure 1). Nickel(II) ions are connected by bridging 4,4′-bipyridine ligands into a polymeric chain extending along the [010] direction. There are three lattice DMF molecules in the asymmetric unit. The compound 1 was also studied by IR spectroscopy and TGA/DSC methods.



The 1-D polymeric chain of $\{[Ni(H_2O)_2(4,4'\text{-bpy})(2\text{-Brnic})_2]\cdot 3DMF\}_n$.

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Sage Essential Oil as a Green Corrosion Inhibitor for Carbon Steel in Acidic Media

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Keywords: Corrosion, Steel, Green Inhibitor, Plants

Abstract: The development of sustainable corrosion inhibitors is critical for mitigating steel degradation in aggressive acidic environments. Here, we report the performance of sage essential oil as an efficient, environmentally benign corrosion inhibitor for carbon steel in 1 M HCl. The oil was extracted from fresh and dried leaves of sage by hydrodistillation using a Clevenger-type apparatus and evaluated over a range of concentrations and immersion times. Inhibition efficiency was quantified using potentiodynamic polarization and electrochemical impedance spectroscopy (EIS). Electrochemical analyses reveal a maximum inhibition efficiency at an optimal concentration of 150 ppm, with protection improving progressively over immersion periods from 1 to 4 h. The inhibitor behaves as a mixed-type system with a dominant suppression of the cathodic reaction. To elucidate the inhibition mechanism, surface and interfacial characterizations were performed. Scanning electron microscopy (SEM) shows a markedly smoother steel surface in the presence of the oil, indicating effective surface coverage. Contact angle measurements demonstrate enhanced hydrophobicity due to inhibitor adsorption. These findings establish sage essential oil as a high-performance green inhibitor and highlight its promise for sustainable corrosion control of steel in acidic media.

Acknowledgment

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POSTER PRESENTATIONS

Catalysis, Chemical Engineering &

Sustainable Chemistry

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Synthesis of 2-Methyl-3-substituted-quinazolin-4(3*H*)-ones – A Mechanochemical Approach

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Keywords: Quinazolinone, Mechanochemistry, Green Chemistry, Thiosemicarbazide

Abstract: Quinazolinones are a class of heterocyclic compounds whose design and synthesis are often studied due to their potential biological activity. Many different marketed drugs contain a quinazolinone core in their structure. As small structural modifications can influence biological activity greatly, novel quinazolinone derivatives are studied and synthesized daily. In order to diminish the environmental impact of such processes, many researchers try to design such synthetic paths to comply with green chemistry principles. Among other green chemistry methods, mechanochemistry was found to be very effective in the synthesis of different organic compounds. This work describes the synthesis of thiosemicarbazides with quinazolinone core in a solvent-free mechanochemical reaction. First, 2-methylquinazolin-4(3*H*)-one was synthesized from anthranilic acid and ammonium acetate using acetic anhydride, which, in reaction with bromomethyl acetate yielded the corresponding ester, methyl 2-(2-methyl-4-oxoquinazolin-3(4*H*)-yl)acetate, namely. A reaction with hydrazine hydrate yielded 2-(2-methyl-4-oxoquinazolin-3(4*H*)-yl)acetohydrazide, which served as a starting compound for thiosemicarbazide synthesis. A series of thisemicarbazides was synthesized in the reaction of corresponding hydrazide and isothiocyanates. Products were obtained in 10 min, in high yields with minimal demands for purification. This method was shown to be more effective than the conventional one, which was much more time consuming, used reflux conditions at higher temperatures and lower yields were obtained.

Acknowledgment

This research was funded by the European Union – NextGenerationEU, Institutional Research Project "Environmentally friendly methods for the synthesis and extraction of organic compounds with potential biological activity" (581-UNIOS-92).

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Real-Time Control of Crystallisation Processes through In-Line Monitoring and Adaptive Nucleation Control

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Keywords: Crystallisation, Process Analytical Technology (PAT), In-Line Monitoring, Direct Nucleation Control (DNC), Image Processing, Machine Learning

Abstract: Batch processing remains the dominant approach in the manufacture of fine chemicals and active pharmaceutical ingredients due to the relatively low production volumes and diversity of active compounds. In such processes, crystallisation is a critical step that directly influences final product properties. Conventional quality assessment is typically performed after processing, which can result in material rejection or the need for additional downstream treatment when specifications are not met. This study focuses on designing and validating a prototype system for improved control of crystallisation through active direct nucleation control. The approach integrates a modified crystalliser configuration with an external dissolution module, enabling dynamic control of the crystal population during operation. A key feature of the system is continuous process monitoring achieved through in-line microscopy combined with advanced image analysis supported by machine learning techniques. These tools provide real-time insight into crystal size distribution and system behaviour, forming the basis for feedback control. The developed control strategy employs process analytical technology (PAT) with an advanced algorithm to adjust operating conditions in response to observed process states. This allows immediate corrective actions, improving consistency and reducing the likelihood of off-spec material. The resulting prototype is a compact and adaptable unit suitable for use at various scales, from laboratory experiments to pilot and potential industrial implementation. The paper presents the system architecture and discusses experimental results that demonstrate its performance.

Acknowledgment

This research was conducted within the Prototype system for optimal process control of crystallisation with the upgraded DNC method (NPOO C 3 2 R 3 I 1 06 0102) project and partially the Dig-ChemEng-Lab (112113) project, funded by the European Union's NextGenerationEU fund from source 581, the Recovery and Resilience Mechanism, under the Programme for Financing Public Higher Education Institutions and Public Scientific Institutes.

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Electrochemical Nickel Deposition in The Hindered Diffusion Conditions

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Keywords: Scanning Electrochemical Microscopy (SECM), Nickel Electrodeposition, Ultramicroelectrode, Diffusion-Limited Mass Transport, Reduced Graphene Oxide, Electrocatalytic Properties

Abstract: This study investigates the electrodeposition of nickel under diffusion-limited mass transport conditions using Scanning Electrochemical Microscopy (AC SECM). Local control of diffusion conditions was achieved through the application of an ultramicroelectrode, enabling the investigation of electrochemical processes with high spatial resolution. Nickel electrodeposition was performed from an aqueous nickel sulfate solution with a concentration of 50 g/L, while the electrochemical changes induced by deposit formation at precisely defined coordinates were monitored in a 30 g/L sodium sulfate solution. The research encompassed both the reduction and deposition of nickel on a copper substrate and the deposition of nickel on reduced graphene oxide, with the aim of evaluating the influence of substrate nature on the nucleation and growth mechanisms of the deposits. The SECM technique enabled spatially resolved detection of electrochemical reduction products and monitoring of local electrochemical activity through the analysis of recorded response signals. The obtained results demonstrate the capability of SECM for precise mapping of electrochemically active regions and highlight its importance in the investigation of localized processes occurring at the electrode–electrolyte interface. Such an approach provides valuable insights into electrodeposition mechanisms and contributes to the evaluation of the electrocatalytic properties of advanced functional materials.

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Local Electrochemical Modification and AC-SECM Mapping of Graphene Oxide Films

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Keywords: Graphene Oxide, Reduced Graphene Oxide, SECM, Electrochemical Reduction, Hindered Diffusion

Abstract: Graphene oxide (GO) and reduced graphene oxide (rGO) are promising materials for applications in electrochemical energy storage and sensing, owing to their tunable electrical and surface properties. This study investigates the electrochemical reduction of GO under hindered diffusion conditions, as well as the resulting changes in local electrochemical behavior using scanning electrochemical microscopy (SECM), cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), and chronopotentiometry. GO films were deposited onto conductive substrates and examined in inert electrolytes to isolate non-Faradaic processes associated with double-layer formation and ion adsorption. Electrochemical reduction led to partial restoration of the sp^2carbon network, resulting in increased conductivity and reduced impedance. SECM mapping revealed significant surface heterogeneity and differences in local reactivity between GO and rGO domains. The results demonstrate that diffusion limitations strongly influence the reduction process and the electrochemical performance of graphene-based materials, providing insights relevant to the development of advanced electrodes, sensors, and energy storage systems.

Acknowledgment

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POSTER PRESENTATIONS

Physical, Theoretical & Artificial

Intelligence Chemistry

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Molecular Dynamics of Surfactant-Free Water/Ethanol/*n*-Hexanol Microemulsions

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Keywords: Molecular Dynamics, Surfactant-Free Microemulsions, n-Hexanol

Abstract: Surfactant-free microemulsions based on ternary alcohol systems have attracted significant attention due to their unique structural properties and potential applications. In this work, molecular dynamics (MD) simulations were employed to investigate the microscopic organization of the water/ethanol/n-hexanol system. All simulations were performed using the GROMACS software package. Water molecules were modeled using the SPC/E model, while alcohols were described by the OPLS-UA force field, ensuring a balance between computational efficiency and structural accuracy. Initial configurations consisting of 16,000 molecules were generated according to experimentally relevant compositions. Following energy minimization, systems were equilibrated at 300 K and 1 bar, and production runs of 5 ns were conducted. Visualization of final configurations revealed no macroscopic phase separation, in agreement with experimental phase diagrams. However, pronounced microheterogeneity was observed, characterized by the formation of nanodomains enriched in longer-chain alcohols. Radial distribution functions provided insight into short- and long-range molecular ordering. Strong correlations between n-hexanol oxygen atoms indicate significant self-association, while ethanol exhibits weaker, composition-independent correlations. Water retains a relatively stable hydrogen-bonded network, although its medium-range structure is less pronounced compared to systems with longer alcohols. Coordination number analysis further supports these findings. Water–water interactions remain dominant, whereas water–n-hexanol interactions are minimal, indicating limited miscibility. Ethanol acts as an amphiphilic mediator, facilitating interactions between hydrophilic and hydrophobic components. Overall, the results confirm that surfactant-free microemulsions exhibit significant nanoscale structuring driven by molecular interactions, highlighting the crucial role of alcohol chain length and amphiphilicity in determining system organization.

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The Effect of Statins on Lactate Dehydrogenase Activity

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Keywords: Statin, Inhibition, Kinetic, LDH

Abstract: Statins, HMG-CoA reductase inhibitors, are the most commonly prescribed hypolipidemic agents due to their efficacy in lowering LDL cholesterol and preventing cardiovascular disease. However, their use can be accompanied by adverse effects, especially in skeletal muscle. Lactate dehydrogenase (LDH) is an enzyme involved in anaerobic glucose metabolism and is often used as a marker of tissue damage. Increased serum LDH values may indicate cytotoxic effects of statins, especially in the context of myopathy and rhabdomyolysis. Studies show that statins can indirectly affect LDH activity through the induction of oxidative stress, disruption of mitochondrial function, and destabilization of cell membranes. Although the clinical significance of these changes varies, monitoring LDH together with creatine kinase (CK) may contribute to the early detection of muscle adverse effects of statin therapy. The kinetics of statin (atorvastatin) binding to LDH were monitored spectrophotometrically at 37°C. The kinetic constants obtained indicate an uncompetitive type of inhibition, and for the tested concentrations of atorvastatin, the IC_{50} value is 52%. Further studies are needed to clarify the exact mechanistic relationship between statins and LDH activity, as well as the potential biomarker status of LDH in assessing the safety of statin therapy.

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Computational Study of Benzodioxole-Based Chalcone Derivatives: DFT, ADME, and Albumin Binding Analysis

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Keywords: Benzodioxole-based Chalcone, DFT, ADME, Albumin Serum Binding

Abstract: A series of benzodioxole-based chalcone derivatives and their corresponding acetophenone precursors were investigated using an in silico approach to evaluate their electronic, structural, and pharmacokinetic properties. Molecular structures were designed and optimized using ChemDraw and Avogadro, while quantum chemical calculations were performed at the DFT/B3LYP level using ORCA. Key descriptors, including HOMO–LUMO energies, energy gaps, electronegativity, chemical hardness, and electrophilicity, were calculated to assess molecular reactivity and stability. Pharmacokinetic properties were predicted using SwissADME, indicating high gastrointestinal absorption and generally favorable drug-likeness profiles for most compounds. Chalcone derivatives exhibited higher lipophilicity and lower aqueous solubility compared to their precursors, suggesting improved membrane permeability. Molecular docking studies, performed using AutoDock Vina via the SwissDock platform, examined interactions with bovine serum albumin (BSA) and human serum albumin (HSA). Chalcone derivatives showed significantly stronger binding affinities (up to −9.37 kcal/mol) compared to acetophenone analogues. These interactions were primarily governed by hydrophobic contacts and hydrogen bonding within the protein binding sites. Target prediction analysis suggested potential biological activities, with several compounds showing affinity toward enzymes such as monoamine oxidase B, aldose reductase, and cyclooxygenase-2. Overall, the results highlight benzodioxole-based chalcone derivatives as promising candidates for further pharmacological investigation due to their favorable electronic properties, drug-likeness, and strong protein-binding potential.

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Determination of Selected Physicochemical Parameters and Heavy Metal Content in Honey Samples

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Keywords: Honey Quality, Physicochemical Properties, HMF Determination, Heavy Metals, Food Quality Control

Abstract: There are approximately 300 different types of honey worldwide, differing in aroma, color, taste, and chemical composition. Honey is a complex natural mixture predominantly composed of carbohydrates (>80%), mainly fructose and glucose, while water content typically ranges from 15% to 20%. It also contains organic acids, vitamins, and minerals, which contribute to its nutritional and physicochemical properties. In this study, 14 honey samples collected from different regions of Bosnia and Herzegovina (Banja Luka, Čelinac, Kupres, Mostar, Novi Grad, and Bosanski Petrovac) were analyzed. The investigated samples included meadow, acacia, forest, chestnut, and linden honey. Organoleptic analysis and physicochemical characterization were performed, including determination of water content, pH value, electrical conductivity, specific optical rotation, hydroxymethylfurfural (HMF) content, and lead concentration. The obtained results were compared with the Regulation on Honey and Other Bee Products of Bosnia and Herzegovina. Water content ranged from 17.8% to 20.8%, while pH values varied between 3.5 and 5. The HMF content complied with the prescribed maximum limit of 40 mg/kg in all samples except one. Lead concentrations were below the maximum permitted value of 0.1 mg/kg. Electrical conductivity values ranged from 460 to 813 μS/cm, whereas one chestnut honey sample exhibited a significantly higher value of 1977 μS/cm. The results indicate that most analyzed honey samples meet the physicochemical quality requirements prescribed by national legislation. Furthermore, the observed variations among different botanical types of honey confirm the strong influence of floral origin on the physicochemical properties and overall quality of honey produced in Bosnia and Herzegovina.

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The Influence of Ascorbic Acid on the Catalytic Activity of Tyrosinase

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Keywords: Vitamin C, Inhibition, Kinetic, Tirosinase

Abstract: Vitamin C (ascorbic acid) is a known inhibitor of the enzyme tyrosinase, a key catalyst in the biosynthesis of melanin. In this paper, the influence of vitamin C as an inhibitor on the activity of the tyrosinase enzyme was analyzed using the Lineweaver–Burk (LB) diagram. The obtained results show a mixed type of inhibition, i.e. that the presence of vitamin C leads to a change in both the maximum rate of the reaction and the Michaelis-Menten constant. Specifically, in the presence of an inhibitor, a lower V_{max} value and a higher K_m are observed compared to the reaction without the presence of an inhibitor, which indicates a reduced catalytic efficiency and a reduced affinity of the enzyme towards the substrate. This behavior indicates that vitamin C binds to both the free enzyme (E) and the enzyme-substrate complex (ES), whereby different affinities for these forms cause simultaneous changes in kinetic parameters. Apart from the direct influence on enzyme kinetics, vitamin C additionally acts on reaction intermediates, by reducing dopaquinone back to DOPA, which further slows down the synthesis of melanin. The combination of these effects confirms that the mechanism of vitamin C inhibition is complex and multifaceted. In conclusion, the experimental data and the corresponding LB diagrams confirm that vitamin C acts as a mixed tyrosinase inhibitor, which explains its effectiveness in inhibiting melanogenesis and its wide application in dermatology and the cosmetic industry.

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