Book of Abstracts

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27 June-30 June 2024 / Sarajevo, B&H
Web: https://icccebih.dktks.ba/

Language

The official language of the ICCCEB&H 2024 is English

Venue and Registration

Hotel Radon Plaza, Džemala Bijedića 185, Sarajevo 71000
Registration desk will be open on Thursday (27 June 2024) from 18:30 to 20:00; Friday (28 June 2024) from 8:00 to 09:00

KEY TO ABSTRACT IDENTIFICATION

PL	Plenary Lectures
KL	Keynote Lectures
OP	Oral Presentations
PP-AC	Poster presentations- Analytical Chemistry
PP-BB	Poster presentations- Biochemistry and Biotechnology
PP-CAM	Poster presentations- Chemistry of Advanced Materials
PP-CE	Poster presentations- Chemical Engineering
PP-CNP	Poster presentations- Chemistry of Natural Products
PP-EDC	Poster presentations- Education in Chemistry
PP-ENC	Poster presentations- Environmental Chemistry
PP-FC	Poster presentations- Food Chemistry
PP-IC	Poster presentations- Inorganic Chemistry
PP-MC	Poster presentations- Medicinal Chemistry
PP-OC	Poster presentations- Organic Chemistry
PP-PTC	Poster presentations- Physical and Theoretical Chemistry
PP-RC	Poster presentations- Radiochemistry
PP-TRC	Poster presentations- Topics Related to Chemistry

OPENING CEREMONY LECTURER

We are honored to announce that Dr. Emira Kahrović, a distinguished scientist, professor emeritus and the only member of our department who is also a member of the Academy of Science and Arts of Bosnia and Herzegovina, will deliver a lecture at the grand opening of the Congress. Dr. Kahrović is recognized as one of the leading experts in the field of chemistry in general, and particularly inorganic chemistry, with a long-standing career and numerous significant contributions to science.

Throughout her illustrious career, Dr. Kahrović has published a series of studies that have greatly advanced our understanding of chemical processes in the field of Inorganic Chemistry. Her passion for science and dedication to research have inspired many young scientists to follow in her footsteps.

Dr. Kahrović's lecture at this congress represents a unique opportunity for all participants to hear firsthand about the latest advancements in chemistry, as well as her own experiences and challenges in scientific work. Her presentation will be rich with valuable insights and motivation, which will undoubtedly enhance the congress program.

Dr. Emira Kahrović

Faculty of Science, University of Sarajevo, Bosnia and Herzegovina

Academy of Sciences and Arts of Bosnia and Herzegovina

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On behalf of the Organizing and Scientific Committee, the Society of Chemists and Technologists of Canton Sarajevo, and the University of Sarajevo - Faculty of Science, it is my great pleasure to welcome you to the 5th International Congress of Chemists and Chemical Engineers of Bosnia and Herzegovina (5th ICCCEB&H 2024) in Sarajevo.

I am thrilled to host this gathering of brilliant minds and passionate professionals from around the world, all united by a common goal: to advance the field of chemistry and harness its potential for the betterment of society. This congress marks a significant milestone in our ongoing journey of discovery and innovation. Over the next few days, we will have the opportunity to share groundbreaking research, exchange ideas, and foster collaborations that will shape the future of chemistry. Our diverse program includes plenary lectures, keynote lectures, oral and poster sessions, all designed to stimulate intellectual curiosity and inspire new avenues of thought.

All submitted abstracts will be published in a special issue of the Bulletin of Chemists and Technologists of Bosnia and Herzegovina, and selected papers will be published in an issue of the Bulletin of Chemists and Technologists of Bosnia and Herzegovina after the peer-review process.

Thank you for being here and contributing to the 5th International Congress of Chemists and Chemical Engineers of Bosnia and Herzegovina. We look forward to engaging with you and witnessing the remarkable progress that will emerge from our collective efforts. We thank the members of the Organizing Committee, International Scientific and Advisory Committee, Scientific Committee, and last but not least, all the participants for organizing, supporting, and contributing to the quality of this Congress. We are grateful for their hard work and commitment to making this congress a success. This event would also not be possible without the generous support of our sponsors.

We welcome all of you once again to the 5th ICCCEB&H 2024 and wish you an interactive, inspiring, and joyful scientific gathering and a pleasant stay in Sarajevo, Bosnia and Herzegovina.

Sabina Begić

Congress Chair

Dr. Sabina Begić

CONTENT

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Abstract

Tumor Selective Ru(III) Schiff Bases Complexes, Discrimination of Ru(III)/Ru(II) Complexes in Solution: A DFT Study

Kahrović, E.[a,b]

[a]*Faculty of Science, University of Sarajevo, Bosnia and Herzegovina*
[b]*Academy of Sciences and Arts of Bosnia and Herzegovina*

Article info
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Abstract: We recently reported a new Ru(III) complex (C1) with two Schiff bases and two chlorides that showed higher efficacy and improved cytotoxicity toward the triple-negative breast cancer cell line MDA-MB-231 compared to traditional antineoplastic drugs in use. In order to investigate hydrolysis as a possible activation step DFT method of electronic structure calculation was used to obtain a preliminary insight for C1 under the conditions of the predicted atomic/ionic/molecular environment. The presence of both Na(+) and Mg(2+) counterions and reducing agents in every cell plasma, give rise to several scenarios of C1 complexes interaction with living cell media. The DFT calculations showed the following: (i) the absolute energies of the complexes depend on the ruthenium oxidation state and the nature and type of association with the counter ion(s) (ii) the pairing of the C1-complex with the metal ion lowers the energy for solvated Mg(2+) compared to Na(+) (iii) the C1-Ru(II)/EtOH is more stable than the C1-Ru(III)/EtOH, and (iv) overall, the substitution of a chloride ligand by a water molecule is a thermodynamically unfavorable process. The proton from all Ru(III)Cl-OH2 species is more acidic compared to free water, consequently, under physiological conditions Ru(III)-ClOH2 does not exist. For Ru(II)-ClOH2 associated with Mg(2+) proton loss is a slightly favored process. Simulated substitution of Ru(III)-ClCl to Ru(III)-ClOH2 and the corresponding Ru(II) species suggest the following trend: from the *a prori* thermodynamic point of view hydrolysis of the C1 complex ranges from unfavorable to significantly prohibitive. Based on these calculations, hydrolysis does not appear to be a significant activation step of C1 as a potential drug.

Acknowledgment

This research was supported through the project: Ilich, P., Kahrović, E. „Electronic structure correlates in a Rutenium-complex Solvolysis" by National Science Foundation (NSF), USA. Charge number CHE230093.

PLENARY LECTURES

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Abstract

2024

Special Issue

PL-01

Reticular Nanoscience: Bottom-Up Assembly Nanotechnology

Wuttke, S.[a, b]

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Keywords:
MOFs
COFs
Nanoparticles
Nanoscience
Reticular
Materials

Abstract: The chemistry of metal-organic and covalent organic frameworks (MOFs and COFs) is perhaps the most diverse and inclusive among the chemical sciences, and yet it can be radically expanded by blending it with nanotechnology. The result is reticular nanoscience, an area of reticular chemistry that has an immense potential in virtually any technological field. In this talk, we explore the extension of such an interdisciplinary reach by surveying the explored and unexplored possibilities that framework nanoparticles can offer. We localize these unique nanosized reticular materials at the juncture between the molecular and the macroscopic worlds, and describe the resulting synthetic and analytical chemistry, which is fundamentally different from conventional frameworks. Such differences are mirrored in the properties that reticular nanoparticles exhibit, which we described while referring to the present state-of-the-art and future promising applications in medicine, catalysis, energy- related applications, and sensors. Finally, the bottom-up approach of reticular nanoscience, inspired by nature, is brought to its full extension by introducing the concept of augmented reticular chemistry. Its approach departs from a single-particle scale to reach higher mesoscopic and even macroscopic dimensions, where framework nanoparticles become building units themselves and the resulting super-materials approach new levels of sophistication of structures and properties.

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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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Abstract

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PL-02

Element Accumulation in Mushrooms

Goessler, W.

Analytical Chemistry for Health and Environment, Institute of Chemistry, University of Graz, Austria

Keywords:
Fungi
Arsenic
Speciation
Elements
Accumulation

Abstract: Mushrooms are important in ecosystems as symbionts, saprotrophs, and parasites. The roles of fungi involve element cycling, rock and mineral transformations, bioweathering, fungal-clay interactions, and metal-fungal interactions. Therefore, fungi can also liberate elements from soil, effectively transform halogens, metals, metalloids, and organometallic compounds by reduction, methylation, and dealkylation. These processes are very important for our ecosystems since transformations of metal(loid)s modify their mobility and toxicity.

As it is really difficult to remove soil or rotted wood from the mycelium fruit bodies are mainly investigated for the transformed elements from soil. Moreover fruit-bodies serve as important nutrient source for parasites, wild animals, and also humans. It is not commonly known that fruit bodies may accumulate remarkable concentrations of (trace) elements. The well-known *King Bolete* (Boletus edulis) is known to accumulate the essential trace element selenium but on the other hand this fungus also accumulates significant amounts of mercury. This heavy metal is well known for its toxic properties. *The Fly Agaric* (Amanita muscaria) is a selective vanadium accumulator. Several 100s of mg V/kg dry mass have been determined during our studies. Thelephora penicillata was found to be a cadmium accumulating mushroom (more than 1000 mg Cd/kg). Additionally, this mushroom accumulated high concentrations of arsenic. The *Violet Crown Cup* (Sarcosphaera coronaria), a mushroom considered edible in previous days, has been reported as an arsenic accumulator. We have determined close to 1 % of arsenic on a dry mass basis. Such concentrations are hardly ever reported for any natural living organism. The edible *Ink Stain Bolete* (Cyanoboletus pulverulentus) is also capable to accumulate up to 1300 mg As/kg. The *False Chantarelle* (Hygrophoropsis aurantiaca) was discovered to be an iron accumulating mushroom. Up to 5000 mg Fe/kg were found frequently in this species. As not all arsenic compounds have the same toxic properties it is necessary to determine the arsenic speciation. Our research provided new results with respect to the arsenic speciation in mushrooms. During our research we discovered several new arsenicals for the first time in living organisms. The presentation covers analytical aspects as well as the results for the total element determinations and the elemental speciation in different mushroom species.

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Abstract

PL-03

Ruthenium Complexes as Antitumor Agents – Current Status and Perspective

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Abstract: The unique characteristics of metal-based compounds make them attractive as therapeutic and imaging agents. In the treatment of cancer, metal complexes have occupied an important place, helping to cure or prolong millions of lives. The most famous complex, cisplatin (cis-diamminedichloridoplatinum(II)), used alone or in combination therapy, is one of the most successful therapeutic metallodrugs discovered so far. Its limitations, such as drug resistance, limited spectrum of activity, and worsening side effects, have initiated efforts to critically consider other metal-based complexes with cytotoxic properties. Anticancer Ru complexes gained significant interest after two iconic Ru(III) complexes - NAMI-A ((ImH)[trans-RuCl4(dmso-S)(Im)], Im = imidazole) and KP1339 (later renamed as IT-139 and BOLD-100, Na[trans-RuCl4(Ind)2], Ind = indazole) - entered their first human clinical trials at the beginning of the 21st century. The successful completion of phase I and entry into phase II clinical trials of the phototherapeutic TLD1433 has further enhanced the role of Ru as a metal of choice for the design of new anticancer agents. Besides, the ruthenium(II)-arene motif, modifiable through mono- or bidentate ligands, and halide coordination also provide complexes with excellent antiproliferative activity. For instance, a variety of ruthenium(II)-arene complexes with dppz (dipyrido[3,2-a:2’,3’-c]phenazine-based ligands) also provides a promising strategy for developing potent antitumor agents. To conclude, ruthenium compounds hold significant promise due to their diverse structures, mechanism of action, and potential to overcome limitations associated with traditional anticancer agents.

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KEYNOTE LECTURES

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Abstract
KL-01

A Chemical Biology Toolkit to Understand and Target Biomolecular Condensates

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Abstract: Cells organize functional processes into compartments to survive. Biomolecular condensates are unique compartments in that they can locally concentrate components to execute specific functions while lacking a surrounding membrane. As such, condensates dynamically respond to changes caused by stress, disease states, cell cycle stages, and drug treatments. These responses are reflected in microscopically-visible changes in condensate morphology; however, the link between a condensate's (dys)function and its morphology change is not well understood.

The aim of this work was to understand the structure-function relationship of the nucleolus, the cell's largest condensate and center of ribosome biogenesis. Specifically, we used a set of small molecule drugs to selectively inhibit different steps of ribosome assembly and observed distinct changes in nucleolar architecture by fluorescence microscopy. We then utilized this data as a training set to build a first-in-class deep neural network that accurately classifies drug-induced nucleolar morphology changes. Importantly, we demonstrated that the extent of nucleolar morphology disruption caused by these drugs can be quantified and used to predict the degree to which they perturb specific nucleolar processes. Next, we conducted a pilot drug screen to identify novel nucleolar phenotypes and nucleolar interaction networks. Given that nucleolar morphology and ribosome production are dysregulated in disease, current efforts are focused on clinically relevant applications of this technology. Together, this work demonstrates that automated imaging and deep learning-assisted analysis of condensate perturbations by small molecules can be used as a powerful discovery platform for new biology as well as for novel diagnostic and therapeutic development.

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Abstract

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KL-02

Understanding the Activity and Stability of Electrocatalytic Materials

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Abstract: Climate change and environmental degradation, which are among the greatest concerns of the modern world, are directly linked to the ever-increasing use of fossil fuels. Electrochemistry and electrocatalysis have proven to be key factors in the transition to sustainable energy and clean chemical production. For example, the implementation of the hydrogen economy concept largely depends on the efficiency of water electrolyzers and fuel cells, which are used to produce green hydrogen and convert it into electricity without carbon emissions. In addition, electrochemical conversion processes offer promising opportunities to extract value-added chemicals from abundant CO_2 and to produce ammonia through the electro-reduction of nitrogen. The efficiency of these electrochemical devices depends on the performance of the catalytic materials used to carry out the reactions.

This talk will focus on investigating the stability and activity of electrocatalytic composites as two key factors for their applicability. I will present the approaches developed in our group for the in-depth investigation of the degradation processes of electrocatalytic materials based on the coupling of electrochemistry with advanced techniques such as electron microscopy and ICP-MS. The necessity of using these methods to evaluate the stability of some practical materials will be illustrated. The second part of my presentation will focus on metal-support interaction (MSI) as an effective tool for tailoring advanced electrocatalytic composites. In contrast to carbon, advanced support materials (such as in-house developed titanium oxynitride) can induce MSI, which can enhance the activity and also the stability of supported metal nanoparticles for water-splitting reactions.

Acknowledgment

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KL-03

The "Pure Water" Model, a New/Old Approach for the Medium and Ionic Strength Dependence of Formation Constants

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Abstract: Several models and theories exist for the medium, ionic strength and temperature dependence of stability constants and activity coefficients, all with their pros and cons. Between the '80s and '90s, the group of Prof. Silvio Sammartano from the University of Messina proposed, with the precious support of other colleagues, a model for the ionic strength (and temperature) dependence of formation constants, based on three assumptions:

[H1]: It is possible to express the dependence on ionic strength of formation constants by a simple equation, independently of the type of reactants and products, and only dependent on the type of reaction.

[H2]: All the deviations from the predicted behavior are ascribed to weak complex formation between components and/or species under study and the background ions (e.g., the ionic medium). This implies that "pure water" is considered as reference state, and some ions as non-interacting with the reactants and/or products involved in the studied equilibrium.

[H3]: Perchlorate does not interact with cationic species, tetraethylammonium cations (and higher tetraalkylammonium analogues) do not with O-donor ligands, and Na^+ and K^+ do not with N-donor ligands.

Evidences collected during more than half a century demonstrated the validity of this "pure water model", showing its potential to model the speciation of several multicomponent complex systems in a simple way. This contribution describes the main features of the model through some examples, highlighting the theoretical and practical aspects of this approach in the speciation modeling of systems of different complexity, including real systems.

Acknowledgment
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Abstract

KL-04

Characterization of Silver(I) Complexes with Halo-Substituted Pyridine Derivatives in Solution and in the Solid State

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Abstract: The coordination chemistry of silver(I) complexes has attracted significant attention due to their antimicrobial and antitumor properties. The flexibility of the silver(I) coordination sphere along with the versatile role of the nitrate ion (bridging, monodentate, bidentate ligand) offers the possibility to create structurally diverse compounds. Moreover, halogen (Cl, Br, I) substitution of the pyridine ring further modulates the properties and behavior of such compounds through halogen and hydrogen bonds.

Herein we highlight the importance of structure-property relationships in the development of bioactive compounds. The new silver complexes were prepared by the reaction of $AgNO_3$ and the corresponding pyridine derivative, yielding compounds with the general formula $[Ag(NO_3)(X_n py)_2]$, X = Cl, Br, I; n = 1-2. The isolated products were characterized by multinuclear NMR spectroscopy (^1H, ^{13}C, ^{15}N, ^{109}Ag), mass spectrometry and single crystal X-ray diffraction data. The bioactivity of the compounds was also tested.

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Abstract

KL-05

Anti-inflammatory Effects of Onion Bulb Extract in the Murine DSS-Colitis Model

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Inflammation

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Abstract: The research is conducted as **a** contribution to existing literature to determine if onion bulb extract (OBE) reduces colitis severity in mice using treatment, prophylactic, and preventative approaches and the mechanism(s) responsible for these effects. Colitis was induced in mice by dextran sulfate sodium (DSS) daily administration in drinking water. For the treatment approach, mice received DSS for 4 days followed by daily i.p injections of OBE/vehicle administration for 3 days (without DSS administration). For the prophylactic approach, mice received daily i.p injections of OBE/vehicle along with DSS administration for 5 days. For the preventative approach, mice initially received daily i.p injections of OBE/vehicle for 7 days, followed by DSS administration for 5 days (without OBE/vehicle treatment). Colitis severity was determined at the gross and histological levels. The colonic level/activity of various cytokines and chemokines were measured using proteome profiling-based assays, western blotting, and immunofluorescence techniques. In vitro neutrophil superoxide release and survival were assessed by chemiluminescence and Annexin-V/7AAD assays, respectively. DSS-induced colitis was significantly reduced by OBE treatment using the three approaches at both gross and histological levels. OBE was also shown to reduce the colonic expression and activity of several pro-inflammatory molecules and signaling pathways, various cytokines and chemokines, and molecules involved in the apoptotic machinery. In addition, OBE inhibited superoxide release and increased the spontaneous apoptosis of neutrophils. OBE showed anti-inflammatory actions, which are attributed, in part, to the modulation of the expression and activity of important pro-inflammatory molecules and signaling pathways involved in the inflammatory response.

Acknowledgment

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ORAL PRESENTATIONS

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Abstract

OP-01

Influence of TNT Melting Methods from Waste Munition on the Quality of Pink Wastewater

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TNT
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Explosive
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Abstract: The explosives in many conventional munitions are cast. These munitions can be demilitarized by heating the charge until it melts and leaks out of the projectile.

This research examined the efficiency of two methods of melting trinitrotoluene (TNT), direct (MDH) and indirect (MIH) heating with water vapor, and examined their impact on the environment through the production of pink wastewater. Samples of 60 and 82 mm projectiles were used for the research. The MIH compared to the MDH for the 60 mm (82 mm) projectile has: an increased capacity of working and melting TNT in one cycle by 55.6% (69%); increased charging, melting, cooling and discharging time of one cycle by 37.6% (35.8%); reduced water condensate by 63.2% (74.4%); reduced TNT drying time by 100% (100%); equal time of projectile preparation, crystallization and packing of TNT. The time of effective work, calculated according to one 60 mm (82 mm) projectile, was reduced by 28.7% (51.7%).

Pink wastewater produced from 60 mm projectiles MIH compared to MDH has: reduced content of TNT, RDX, 1,3-dinitrobenzene, 2,6-dinitrotoluene, 2,4-dinitrotoluene by 100% for samples taken at the outlet into the atmosphere, from the floor of the autoclave, and at the exit from the precipitator and autoclave. Pink wastewater from the 82 mm projectile is contaminated with the mentioned agents due to the human factor during the melting process. Increasing the caliber of the projectile increases the value of the factor that evaluates the efficiency of the melting method. MIH does not produce pink wastewater.

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Hofmeister Effects on the Phase Stability of Aqueous BSA Solutions with Added PEG

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Abstract: Research on the impact of co-solutes on protein aggregation is of crucial importance both for the life sciences and for industrial applications, particularly in the pharmaceutical sector. Measuring the cloud-point temperatures, we investigated the phase stability of bovine serum albumin (BSA) solutions mixed with polyethylene glycol (PEG) and salt in acetate buffer at a pH of 4.6, which is close to the isoionic point of BSA (pH ≈ pI), and at a pH of 4.0, at which the protein has a net positive charge (pH < pI).

Our results show that:

1) PEG induces BSA aggregation both in the presence and absence of added salt. These results are consistent with previous studies on protein solutions and can be explained by depletion forces.

(2) The addition of NaCl to BSA-PEG solutions has different effects depending on the pH: At pH ≈ pI, the salt stabilizes the solution against phase separation, while at pH < pI salt reduces the colloidal stability of the solution.

3) Ion-specific trends depend on the pH: At pH ≈ pI, the phase stability of the solution increases towards separation from NaF (least stable) to NaI (most stable) and from LiCl to CsCl. The opposite trend is observed at pH < pI.

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Abstract

OP-03

Plant's Secret Life: Biochemistry behind the Stress Memory

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Abstract: Plants, as sessile organisms, face various daily stressors that impact their growth, metabolism, and yield. In crop plants, understanding their responses to stressors and the transgenerational effects is crucial. We examined chickpea, tomato, and the model plant Arabidopsis to evaluate stress memory, its transfer to progeny, and resulting biochemical changes under optimal and stress conditions.

In Arabidopsis, we found that memory responses and biochemical changes correlate with stress severity, with more severe stress prompting memory reset. In tomato, both moderate and severe stress had transgenerational effects, altering hormone and polyamine levels, and metal uptake dynamics. Notably, the F1 and F2 generations retained altered polyamine profiles, such as elevated cadaverine and putrescine levels, indicating a persistent transgenerational response.

Furthermore, we explored how priming crops can leverage these biochemical changes for enhanced tolerance. Arabidopsis F2 seeds tested under different stressors showed that previous exposure to hexavalent chromium (Cr) induced increased tolerance to salt and cadmium (Cd) stress, attributed to elevated antioxidant enzyme activity and proline content.

Plant memory is a complex process, and evidence of transgenerational memory transfer is still emerging. Our studies demonstrate memory effects up to the F2 generation, providing proof of transgenerational memory and associated biochemical profile alterations.

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Abstract

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OP-04

Experimental and Computational Studies of Liquid-Liquid Phase Separation of Some Globular Proteins

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Abstract: Proteins are complex biomolecules that are involved in everything that enables the normal functioning of all living organisms. Consequently, even their minor change or instability can have devastating consequences for life itself. Over the last decade liquid-liquid phase separation (LLPS) of proteins has been associated with the onset of numerous diseases, therefore gained knowledge in this field is of vital importance for disease prevention and treatment. Despite thorough research work on LLPS of proteins, many open questions remain to be resolved. In recent years, our studies on LLPS of globular proteins were carried out as an interplay of various experimental techniques, theoretical approach as well as computer simulations. Buffer identity is often neglected, but our results indicate it is nonnegligible when discussing the phase stability of protein solutions. At the same time, we managed to extend our coarse-grained protein model to incorporate buffer-specific effects into LLPS theoretical predictions. Through experiments, supported by molecular dynamics simulations, we have demonstrated that arginine can affect the phase stability of protein solutions as a double-edged sword. It can reduce protein self-association when added as free arginine molecules in solution and enhance it when being protein-bound as residues on protein surface. By means of mutations of ARG with LYS on protein surface, we have shed light on the importance of hydrophobic interactions for the protein self-assembly.

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Abstract
OP-05

Comparison of the Extraction Methods for Iron Content Assay in St. John’s Wort

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St. John’s Worth
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Abstract: St. John's wort is a medicinal plant that has been proven to have neurological benefits, antiviral, antibacterial, anti-inflammatory and antidepressant properties in various pharmaceutical formulations such as infusions, decoctions and extracts, owing its effects mainly to hypericin, hyperforin, tannins, and xanthones. Iron is one of the most important microelements and is essential for photosynthesis, respiration and chlorophyll synthesis. It has been shown to be an effective elicitation factor for hypericin and hyperforin production. There are several methods for the extraction of iron from plant material, including dry, wet and microwave digestion, that were described for St. John’s wort. However, the extraction methods were not previously compared for their efficacy. The main goal of the research was to compare the extraction methods, namely wet and dry digestion, for the iron content assay of St. John's wort tea samples available in the Bosnian-Herzegovinian market. Three products were taken and analyzed using the thiocyanate spectrophotometric method for the determination of iron in triplicate. Both methods are practical in routine work and showed adequate sensitivity. The iron content found in samples prepared by dry digestion was 93.37 ± 17.89 mg/kg on average, while after wet digestion the iron content in the same samples was 75.7 ± 29.43 mg/kg. This is probably due to the fact that wet digestion is performed in an open system and at lower temperatures where the solubility of substances is lower. The level of iron content in St. John’s wort was comparable to the literature results.

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OP-06

Antioxidant Power of Tomato Seeds Measured by ESR Spectroscopy

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Abstract: Tomatoes are rich in several nutritionally valuable components, such as lycopene, *β*-carotene and polyphenols. During the industrial processing of tomatoes, a large amount of seeds is left behind, which is treated as biowaste. The aim of the research was to examine the antioxidant power (AP) of the seeds of two types of tomatoes "cherry" and "apple" tomato. The measurements were carried out using the electron spin resonance (ESR) method, using the DPPH radical. This spectroscopic technique enables precise measurement of the concentration of radicals in the sample. It was monitored how the concentration of DPPH radicals decreases over time after the addition of the ethanolic extract of the seeds to the DPPH solution. The influence of seed storage temperature on AP was examined. One part of the seeds was stored at room temperature, and the other in a refrigerator at +4 °C. The impact of freezing seeds at −18 °C, was also tested. The extracts were prepared by grinding the seeds, and then the active components were extracted from them by stirring in ethanol for 5 min. The samples were then centrifuged, and the liquid part was separated. Extracts were added to the ethanol solution of DPPH of known concentration and the signal loss was measured for 30 min. The results showed an approximately equal AP value of both types of tomatoes before storage. During storage at different temperatures and by freezing, there was a significant change in antioxidant activity and antioxidant capacity, which affected the change in AP value.

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Abstract

OP-07

Electron Spin Resonance Study of Pumpkin Seeds, Oil and Cake Antioxidant Power

Blečić, A-M.[a], Antonić Jelić, T.[b], Merunka, D.[b], Jurec, J., Ladan, I.[c], Pollak, L .[c], Tota, M.[a], Majetić Germek, V.[a], Koprivnjak, O.[a], Valić, S.[a,b,*]

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Pumpkin Seeds Flour
Pumpkin Seeds Cake

Abstract: Pumpkin (*Cucurbita pepo*) seed products, oil and flour, but also pumpkin seed cake as a by-product, are an important source of natural antioxidants. Antioxidants neutralize free radicals that harm human health. Radicals are products of the human metabolism, are ingested with food, smoke inhalation, and can be produced by the body's exposure to high-energy radiation (UV, X and γ). The electron spin resonance (ESR), known as an extremely sensitive spectroscopic technique in measuring the concentration of free unpaired electrons, was applied to measure the antioxidant power (AP) of pumpkin seed oil, flour and cake. 2,2-diphenyl-1-picrylhydrazyl (DPPH) radical, dissolved in ethanol, was used as a scavenging object. It was measured how the concentration of DPPH radicals decreases over time after the addition of an antioxidant (ethanol extract of oil, flour or cake. The influence of the proceeding temperature (40 °C and 122°C) as well as of samples storage temperature (4 °C and 22 °C) on AP was investigated in details. It was found that pumpkin seeds cake, as a by-product, shows a significant AP. Therefore, this result additionally supports the use of the cake in the food industry in order to improve the nutritional value of products. Moreover, an indication that the oil production temperature and the storage temperature of oil as the final product, but also the seeds as the raw material, might have an important influence on the AP values.

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Abstract

OP-08

Interplay between alloying and tramp element effects on temper embrittlement in bcc iron: DFT and thermodynamic insights

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DFT
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Abstract: The details of the temper embrittlement mechanism in steels caused by impurities are unknown. Especially from an atomistic point of view, there are still open questions regarding their interactions with alloying elements such as Ni, Cr, and Mo. Therefore, we used density functional theory to investigate the segregation and co-segregation behavior and the resulting influence on the cohesion of three representative tilt grain boundaries in iron. The results are implemented in a multi-site and multi-component kinetic and thermodynamic model for grain boundary segregation, to gain insights into the temporal and final grain boundary coverage. Our results show that the segregation tendency of As, Sb, and Sn is stronger than that of the alloying elements and significantly mitigates the grain boundary cohesion. Depending on the grain boundary type, interactions between Sb and Sn vary from negligible to strongly attractive, which increases the likelihood of co-segregation. The cohesion-weakening effect is further amplified when elements such as Sb, Sn, and As co-segregate, compared to their individual segregation. In contrast, the co-segregation of Ni and Cr does not significantly increase the enrichment of impurities at grain boundaries, and their impact on cohesion is found to be negligible. The ability of Mo to mitigate reversible temper embrittlement is primarily attributed to its cohesion-enhancing effect and its capability to repel tramp elements from grain boundaries, rather than scavenging them within the bulk, as suggested by previous literature.

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Abstract
OP-09

Hydrogen Storage in Metal Hydrides: Experimental Approach

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Hydrogen Storage
Metal Hydrides
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Thermodinamics
Sorption Properties

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Abstract: The paper deals with the destabilization methods for improving the storage properties of metal hydrides. The experimental approach was used to point out the influence of various types of defects on the structure and stability of hydrides. As a case study, Mg-based hydrides have been investigated. As shown by our research, ion irradiation is the way to introduce a well-defined concentration of defects (Frankel pairs) at the surface and sub-surface layers of a material. Defects at the surface play the main role in sorption reactions since they enhance the dissociation of hydrogen. Further, our research shows that ball-milling introduces defects through the entire sample volume, refines the structure and thus decreases the path for hydrogen diffusion. Surface-modified material demonstrates better thermodynamic and kinetics properties than bulk modified hydride materials.

Acknowledgment

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Abstract

OP-10

Onion Bulb Extract Inhibits Airway Inflammation in a Mouse Model of Allergic Asthma

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Abstract: Asthma represents a global health challenge. The main pharmacotherapy is synthetic. Additionally, chemicals and biological-based drugs are costly and have significant side effects. In contrast, the use of natural products, such as onions (*Allium cepa* L., Amaryllidaceae), in the treatment of airway diseases has increased worldwide because of a few safety concerns and their perceived efficacy. However, their pharmacological actions remain largely uncharacterized. This research investigates whether onion bulb extract (OBE) can 1) prevent the development of the asthma phenotype (preventative treatment approach) and/or 2) reverse the established asthma phenotype (therapeutic treatment approach). Male Balb/c mice were used throughout the study. Two protocols were used: a therapeutic (21 days) and a preventative (19 days) treatment protocol. PBS and house dust mites (HDM)-challenged mice treated with vehicle or OBE (30, 60, and 100mg/kg/i.p.). Airway inflammation was determined using cytology, histology, immunofluorescence, Western blot and serum IgE. Preventative (100 mg/kg/i.p.), therapeutic (60 mg/kg/i.p.), and OBE treatments resulted in a down-regulation of HDM-induced airway cellular influx, histopathological changes, and an increase in the expression of pro-inflammatory signaling pathways (EGFR, ERK1/2, AKT, pro-inflammatory cytokines, and serum IgE).

The presented data show that OBE is an effective anti-inflammatory agent with preventative and therapeutic anti-asthma effects. These findings imply that onion or OBE may be used as an adjunct therapeutic agent for established asthma and/or to prevent the development of allergic asthma. However, further studies are needed to identify the active constituents and demonstrate proof-of-concept in humans.

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Abstract

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OP-11

Atomistic Simulations of Hydrogen Storage in Carbon-based Materials

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Hydrogen Storage
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Abstract: Hydrogen technology presents a possible strategy in the present transformation towards sustainable and responsible research, development, and production. One source of hydrogen is pyrolysis, which yields large amounts of carbon as a by-product. In the present contribution, we will use computational tools to investigate the H-storage capability of carbon-based nanostructures.

Firstly, we will present a strategy for constructing a realistic 3D atomistic model of nanoporous carbon (np-C) based on experimental measurements. Subsequently, we employ this model to investigate H sorption as a function of temperature and H2 gas pressure using molecular dynamics.

To further enhance the storage capacity of carbon, we employ the MatlantisTM platform, together with their neural network interatomic potential, to scan through the entire periodic table and quantify how a single dopant attached to graphene locally modifies the adsorption properties of hydrogen. We probe various dopant sites (on the graphene or placed as substitutional atoms within the graphene structure) and different carbon geometries (graphene or carbon nanotubes). This approach enables the identification of dopants that significantly increase hydrogen adsorption. Our work has the ambition to steer future knowledge-based experiments on the modification of carbon for hydrogen storage.

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Abstract

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PP-AC-01

Selection of Method for Determination of Enantiomeric Purity (Impurity D) for Active Pharmaceutical Ingredient Levetiracetam

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Enantiomeric Purity (Impurity D)
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Abstract: Levetiracetam is a novel antiepileptic drug used to treat partial, myoclonic, and tonic-clonic seizures. The high-performance liquid chromatography (HPLC) method for determination of Enantiomeric purity (Impurity D) in Levetiracetam is described in the European Pharmacopoeia (EP). The specified level in EP monograph for Levetiracetam Impurity D is 0.8%. To keep the level of Impurity D in finished pharmaceutical product in accordance with the guidelines, level of impurity D in active pharmaceutical ingredient should be set to 0.1%. For this reason, in-house method with higher sensitivity was developed.

In-house method is developed on Chiral Pak AD-H, 150x4.6 mm; 5µm; column, recording at 215 nm. Mobile phase (n-Hexane/dehydrated ethanol (80:20 V/V)) at a flow rate of 1.0 ml/min was used.

In house method showed a better separation of peaks of Impurity D and Levetiracetam and higher sensitivity than EP method. The developed in-house method had been applied successfully to determine Enantiomeric purity in Levetiracetam and can be used in quality control of active pharmaceutical ingredient.

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Abstract

PP-AC-02

Physicochemical and Thermal Properties of Hydrophobic Eutectic Mixtures Based on Tetrabutylphosphonium Bromide (TBPB) and Terpenoids

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Abstract: Investigations of new hydrophobic solvents prepared from a wide range of compounds, followed by testing their properties for different purposes, are increasing in scientific literature recently. Considering the requirements related to thermal and chemical stability, as well as desirable physicochemical properties of new solvents applied in liquid-liquid extraction techniques (LLE), the concept of this study was made. In this study, deep eutectic mixtures based on tetrabutylphosphonium bromide (TBPB) and terpenoids as H-bond acceptors, along with alcohols and a series of organic acids with chain lengths of 8, 12, and 18 C atoms, as H-bond donors were prepared and their stability was tested. Simultaneous thermogravimetric and differential scanning calorimetric methods (TG-DSC), were used to determine thermal properties of prepared mixtures, followed by density and viscosity measurements. Results showed that the thermal stability of the deep eutectic mixtures containing thymol and alcohols does not increase, compared to the stabilities of individual components. However, thermal stabilities for eutectic mixtures based on tetrabutylphosphonium bromide (TBPB) and both- lauric and octanoic acid, were improved and thermal decompositions occurred in two stages. Density and viscosity values were in accordance with requirements related to their application in liquid-liquid extraction procedures. Significantly lower values of viscosity and density for terpenoid based mixtures compared to TBPB makes them more suitable for LLE purposes.

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PP-AC-03

Estimation of the Heavy Metal Content in the Leaf and Prepared Tea Infusion of *Achillea millefolium* L.

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Abstract: *Achillea millefolium* L., as a medicinal plant, deserves special attention because it can be easily contaminated with metals during growth, development, and processing. The aim of this study was to achieve the quantitative determination of Cu, Mn, Fe, Co, Ni, Pb, and Zn in the leaf and leaf tea infusion of *Achillea millefolium* L. using flame atomic absorption spectrometry. Samples of the life *Achillea millefolium* L. were collected at five locations in the urban part of Central Bosnian Canton. The metal content in the leaf of *Achillea millefolium* L. ranged from: 7.42 to 10.14 mg/kg (Cu); <LOD to 0.132 mg/kg (Co); 82.14 mg/kg to 143 mg/kg (Fe); 46.16 to 100 mg/kg (Mn); <LOD to Ni; 0.684 to 3.92 mg/kg (Pb); and 4.47 to 8.79 mg/kg (Zn). The metal content in the leaf tea infusion ranged from: 0.792 to 1.95 mg/kg (Cu); <LOD (Co); 1.81 to 5.37 mg/kg (Fe); 7.90 to 12.5 mg/kg (Mn); 0.467 to 1.68 mg/kg (Ni); <LOD to 0.187 mg/kg (Pb); 1.58 to 3.18 (Zn). Analysis of *Achillea millefolium* L. leaf tea infusions revealed the presence of heavy metal in lower content than in leaf samples. Monitoring the content of heavy metals in the leaf of *Achillea millefolium* L. and their tea infusion is of high importance because heavy metals can accumulate in the human body and have a negative impact on human health.

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Abstract

PP-AC-04

Determination of Co, Fe, Ni and Zn Content in Leaf and Root of the *Taraxacum officinale*

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Abstract: Dandelion (*Taraxacum officinale* F.H. Wigg.) is a medicinal plant, but it is also commonly used in environmental quality assessment. Dandelion commonly occurs in different ecosystems, is geographically widely distributed, and is easily accessible for sampling. The main object of this study was the quantitative determination of Co, Fe, Ni, and Zn in the leaf and root of *Taraxacum officinale* F.H. Wigg. using flame atomic absorption spectrometry (FAAS). Samples of the leaves and root of *Taraxacum officinale* F.H. Wigg. were collected at seven locations in the rural part of the municipality of Visoko in Bosnia and Herzegovina during the stable weather conditions. Samples were prepared by using acid digestion. The metal content in the leaf of *Taraxacum officinale* F.H. Wigg. ranged from: 109 µg/g to 329 µg/g (Fe); 0.045 µg/g to 1.29 µg/g (Co); 2.79 µg/g to 10.01 µg/g (Ni); 15.25 µg/g to 35.47 µg/g (Zn). The metal content in the root samples ranged from: 246 µg/g to 769 µg/g (Fe); <LOD (Co); 0.33 µg/g to 4.19 µg/g (Ni); 20.35 µg/g to 41.6 µg/g (Zn). The average metal content of Co and Ni was higher in leaf samples compared to root samples, while the average content of Fe and Zn was higher in root samples. The content of the analyzed metals does not exceed the maximum allowed content prescribed by the World Health Organization, but the results indicate that it is necessary to continuously monitor the content of metals in *Taraxacum officinale* F.H. Wigg., considering that it is used for medicinal as well as food purposes.

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Optimization and Transfer of Method for Particle Size Determination on the Malvern Mastersizer 3000 using the example of Tramadol Hydrochloride

Salihović, E., Bajrović, A., Podumljak, E., Nalo, A., Avdić, N., Pašić-Kulenović, M.

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Abstract: Particle size determination (PSD) is a critical aspect of pharmaceutical development, affecting drug formulation, dissolution, bioavailability and efficacy. Most of the methods for determination of PSD are developed on the Mastersizer 2000 instrument. Because of the different instrument design there is a need for optimization of methods during method transfer in the new version of the instrument type Mastersizer 3000. Tramadol hydrochloride is used as a model compound to investigate the influence of different modifications and adaptations during the verification and optimization process. The main topic explores the differences between using the Standard Venturi and the High Energy Venturi Disperser, which is a part exclusive to the new instrument model. With the High Energy Venturi disperser, particles undergo acceleration similar to the standard one, but with the additional feature of a 90-degree curve, creating an impact zone, thereby providing high energy dispersion. The results show that although both Venturi types exhibit variations in design and dispersion energy, the choice between them does not significantly affect particle size determination result when analyzing Tramadol hydrochloride raw material. This finding confirms the robustness of the particle size determination method on the Malvern Mastersizer 3000, no matter what Venturi type is used for measurement. All results for particle size distribution are within the specified limits and conform to the acceptance criteria. RSD for repeatability and intermediate precision with both type of ventury also conform to the acceptance criteria

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Abstract

PP-AC-06

Electrochemical Behavior of Co(II) Polymer Modified Glassy Carbon Electrode for the Determination of Dopamine

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Abstract: A new electrochemical sensor for the highly sensitive and selective determination of dopamine (DA) has been developed based on the use of a glassy carbon electrode modified with a cobalt(II) coordination polymer. The Co(II) coordination polymer was prepared by a reaction of cobalt(II) nitrate hexahydrate, 2-chloronicotinic acid and 1,2-bis(4-pyridyl)ethylene (molar ratio 1:2:1) in DMF:H_2O solution at room temperature and atmospheric pressure. Dopamine (DA), a major catecholamine neurotransmitter widely distributed in the mammalian central nervous system, plays an important role in human metabolism as it is involved in many biochemical reactions. Therefore, it is of crucial importance for use in diagnostic and medical examinations. Although DA can be determined by electrochemical methods due to its electrochemical activity, the direct determination of DA on conventional bare electrodes is irreversible (due to surface fouling), requires high oxidation potentials and is prone to common interferences of biomedical samples. Modified electrodes improve the sensitivity and selectivity of electrochemical analysis by enhancing the kinetics of the reaction. In this work, both the electrochemical and morphological characterization of the Co(II) polymer-modified glassy carbon electrode were investigated. The immobilization of Co(II) polymers on the surface of the glassy carbon electrode (GCE) showed a favorable electrocatalytic effect on the oxidation of DA with a reduction of the overpotential compared to the bare GCE. Under optimal conditions, the sensor showed good anti-interference ability and stability, excellent sensitivity, low detection limit (0.003 μM) and fast response to the analyte. Furthermore, the developed sensor was successfully applied in the determination of dopamine in real pharmaceutical samples.

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Abstract

PP-AC-07

New Potentiometric Surfactant Sensor with a Pt@MWCNT-Based Ionophore

Glumac, N.[a], Momčilović, M.[b], Kramberger, I.[c], Štraus, D.[c], Sakač, N.[d],*, Kovač-Andrić, E.[e], Đurin, B.[f], Kraševac Sakač, M.[g], Đambić, K.[d], Jozanović, M.[d]

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Abstract: Pt-doped acid-activated multi walled carbon nanotubes (Pt@MWCNT) were used to produce two composites a) with cationic surfactant 1,3-dihexadecyl-1H-benzo[d]imidazol-3-ium-DHBI (Pt@MWCNT-DHBI ionophore) and b) with anionic surfactant dodecylbenzenesulfonate-DBS (Pt@MWCNT-DBS ionophore). Composites were successfully synthesized and characterized. Both surfactant sensors showed a response to anionic surfactants (dodecylsulfate (SDS) and DBS; and cationic surfactants (cetylpyridinium chloride (CPC) and hexadecyltrimethylammonium bromide (CTAB)). Pt@MWCNT-DBS sensor had sub-Nernstian response of ≈23 mV/decade of activity for CPC and CTAB and ≈33 mV/decade of activity for SDS and DBS. Pt@MWCNT-DHBI surfactant sensor showed better Nernstian response; to SDS (59.1 mV/decade) and near-Nernstian to DBS (57.5 mV/decade); with linear response regions for both anionic surfactants down to ≈2 x 10-6 M. The Pt@MWCNT-DHBI was used for critical micellar concentration (CMC) detection and showed good resilience to common anionic interferent. The sensor was successfully employed for potentiometric titration of technical grade cationic surfactant with good recoveries. The content of cationic surfactants was measured in six samples of complex commercial detergents. The results were compared with the ISE surfactant sensor and classical two-phase titration.

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Abstract

PP-AC-08

Degradation of Active Pharmaceutical Ingredients Perindopril *tert*-Butylamine and Amlodipine Besylate in Tablets During Stability Testing

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Storage Conditions

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Abstract: Stability testing is an important factor during the development of pharmaceutical products, and affects the quality, effectiveness and safety of the drug. The studies are performed at various stages of drug development with the aim of determining the expiration date, storage conditions and selection of packaging for the finished product. Perindopril *tert*-butylamine belongs to the class of angiotensin-converting enzyme (ACE) inhibitors and is used in the treatment of hypertension and heart failure. Amlodipine besylate is used in the treatment of hypertension and acts as a calcium ion blocker. The joint action leads to the expansion of blood vessels, thereby increasing the flow of blood and oxygen to the heart.

The aim of this study was to assess the stability of perindopril *tert*-butylamine and amlodipine besylate during exposure of the tablets to different temperatures and relative humidity, based on the level of active pharmaceutical ingredient degradation. The high-performance liquid chromatography (HPLC) method is used for quantification of degradation products of active ingredients (impurities).

Perindopril B, Perindopril F and Amlodipine impurity D level was monitored for 6 months under accelerated (40°C/75%RH), 12 months intermediate (30°C/65%RH), and long-term conditions (25°C/65%RH). The test results show increase in level of impurities Perindopril B and Perindopril F at all storage conditions, while Amlodipine impurity D does not have a similar trend.

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Abstract

PP-AC-09

The Influence of Temperature and Relative Humidity on Degradation of Active Substance Clotrimazole in Pharmaceutical Product for Topical Treatment

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Abstract: An important part of the drug development process is stability testing which provides information about the quality of the active pharmaceutical ingredient (API) or the drug formulation itself, under the impact of various factors such as temperature, humidity, or light. These factors can lead to a chemical degradation of API during which various degradation products are formed. Clotrimazole is a member of the class of imidazoles, that is 1H-imidazole in which the hydrogen attached to a nitrogen is replaced by a monochlorotrityl group. It belongs to the group of synthetic antifungal drugs with a wide spectrum, primarily used locally in the treatment of a large number of mycoses including candidiasis. The aim of the work was to evaluate the correlation between stability of Clotrimazole and different storage condition in pharmaceutical product, during which the level of degradation products is monitored. The high-performance liquid chromatography (HPLC) method is used to quantify growth of Imidazole and Clotrimazole impurity A, which are main products of decomposition in period of 6 months under accelerated (40°C/75%RH), 12 months intermediate (30°C/65%RH) and long-term storage conditions (25°C/65%RH). The conducted stability tests showed that an increase in level of degradation products of Clotrimazole in the pharmaceutical product is in a correlation with storage conditions. Temperature increase corresponds with the level of degradants determined in the product.

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Abstract

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The Determination of Fatty Acid Composition in Selected Olive Oil Samples

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Olive Oil,
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Pharmaceutical and Cosmetic Preparations

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Abstract: Olive oil, called "liquid gold", has been used to preserve both health and beauty since ancient times. In addition to polyphenols, strong antioxidants (vitamin E and phytosterols), olive oil is rich in fatty acids (FA), especially monounsaturated fatty acids (MUFA), and is widely used in cosmetics for the production of creams and ointments. It has a beneficial effect on the skin and soothes sunburned areas and not only deeply moisturizes, nourishes and regenerates skin cells, but also repairs and protects them from future damage. Due to its sedative, cholagogic and laxative properties, it is recommended as a mild remedy against gallstones, nephritic colic, constipation, etc. In this work, the composition of fatty acids in selected olive oil samples was determined in pharmacy, and from different manufactures. Our results of analyzed the content of fatty acids showed that the most abundant FA was oleic acid (mean 74.35%) while the content of other FAs as percentages of the mean of linoleic 5.91, palmitic 11.01, stearic 2.57, eicosanoic acids 0.32 were found. All analyzed samples of Olive oil, showed that the composition of FAs has potential and relevance in cosmetic, pharmaceutical, chemicals and other industries.

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PP-AC-11

The Analysis of Magnesium Concentration in Plasma Samples

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Abstract: Magnesium (Mg), as an essential metal, has important biochemical functions in the body and affects to normal human health. It is involved in energy metabolism, acting as a metal activator or co-factor for enzymes requiring adenosine triphosphate (ATP), in the replication of DNA and in the synthesis of RNA and proteins; it appears to be essential for all phosphate transferring systems. Modern lifestyles and bad dietary habits cause magnesium deficiency and reduced levels of magnesium. The aim of this study was to determine magnesium concentrations in plasma samples of 13 adults and 13 children from the University Clinical Centre of Sarajevo, BiH; with a chemical bioanalyzer (the Siemens Dimension® Xpand Plus Germany) using a modification of the methyl thymol blue (MTB) procedure that forms a blue complex with magnesium. The results obtained for adults ranged from 0.69 to 0.73 mmol/L, and for children from 0.73 to 0.77 mmol/L Mg. Additionally, a strong negative correlation ($p<0.01$) was found between Mg and participant age. These findings showed that magnesium concentrations lie within the reference values 0.74-1.05 mmol/L in plasma samples, and that magnesium concentration depends on the age of individuals.

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Abstract

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A Comparative Study of Different Preparation Methods for Heavy Metal Analysis in Wood Biomass (Pellets and Briquettes)

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Abstract: Pellets and briquettes are intensively being used as renewable energy sources representing an acceptable fuel considering their impact on the environment and human health. Along with their ability to renew, combustion of these biomasses does not lead to the emission of high amounts of harmful substances. Therefore, the main task in order to examine and analyze their characteristics is the selection of an appropriate method for sample preparation. In this regard, the quantification of heavy metals (Cd, Co, Cr, Cu, Fe, Mn, Ni, Pb and Zn) and metaloid (As) in these wood biomass samples after their extraction with concentrated nitric acid and aqua regia using the ultrasonic and the wet digestion method was performed by flame atomic/electrothermal atomic absorption spectrometry. The content of the three most abundant metals in the tested samples, regardless of the extraction agent or the extraction method, follows the order Fe>Mn>Zn. Regarding the solvents used, ultrasonic nitric acid extraction on average extracted about 60% Fe and 80% Mn compared to aqua regia extraction. In addition, for different extraction methods, it was found that both Fe and Mn are efficiently extracted by wet digestion in Teflon vessels with aqua regia. However, concentrated nitric acid proved to be the best extraction agent with ultrasonic digestion for Zn in pellet and briquette samples. In general, ultrasonic extraction can be applied more efficiently for the extraction of Co, Cr and Zn, satisfactory for the extraction of Fe and Mn, while not efficient for Ni, Cd, As, Cu and Pb extraction.

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Abstract

PP-AC-13

Titratable Acidity and pH of Diluting Drinks and Their Potential Effect on Dental Erosion

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Abstract: Dental erosion is the loss of hard dental tissue due to a chemical process without the participation of bacteria. Many studies have shown that measured pH, acidity, is precise indicator of the erosive potential of a drink. Three commercially available juices were tested for both pH and titratable acidity at various dilutions, showing the range of concentrations at which, such drinks can be consumed. Dilutions of citric and hydrochloric acid, with ph values similar to those of the drinks, were used as positive control acidic solutions. The results showed that all tested drinks, even diluted, were highly acidic. All drinks showed a high resistance to increasing the pH value, indicating a high internal buffering capacity. On the other hand, the titratable acidity of each drink decreased proportionally with increasing dilution, thereby significantly reducing its erosive potential. It is possible to reduce the erosive potential by adding considerable amount of water, because there is a direct relationship between dilution and titratable acidity. It remains unlikely to reach a dilution point that would be acceptable for consumption, since the dilution rations were so huge.

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Abstract

PP-AC-14

Novel ISE Enriched with Magnetite Nanoparticles for Sulfates Determination

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Abstract: Ion-selective electrodes (ISEs) are among the fastest-developing sensors in electrochemistry due to their wide range of applications. They are used in the food industry, agriculture, environmental analysis, and drug analysis, offering numerous advantages: high selectivity and sensitivity, low limit of detection (LOD), easy handling, portability, and low cost. We have therefore developed a solid-state ISE for the potentiometric determination of sulfate ions, which have potential applications in evaluation environmental parameters, such as monitoring of sulfate ions in drinking water, wastewater, or industrial water. The membranes are based on a mixture of barium sulfate, silver sulfide, binding/filling polymer and magnetite nanoparticles (MNPs). The mass ratio of barium sulfate, silver sulfide, and polytetrafluoroethylene in the membranes was: 1: 2, with an addition of 0.3–0.8% MNPs in mixture. It was found that MNPs positively affected the linear response range for sulfate anions. Specifically, the membrane containing 0.6% MNPs exhibited a linear change of potential with a slope of 27.7 mV dec^{-1}, which is very close to the theoretical Nernstian value (29.6 mV dec^{-1}), with a regression coefficient of 0.9970 in the concentration range of $4.88 \cdot 10^{-5}$ mol L^{-1} - $1.00 \cdot 10^{-2}$ mol L^{-1}, and LOD of $4.34 \cdot 10^{-5}$ mol L^{-1}. Finally, the membranes showed no response to barium ions even at high concentrations ($\geq 1.00 \cdot 10^{-3}$ mol L^{-1}). These results confirm that our newly developed potentiometric sensor has a high membrane selectivity for the determination of sulfate ions and, more importantly, that it is a fast, reliable and cost-effective tool.

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Abstract
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Deep Eutectic Solvents for the Eco-Friendly Extraction of Bioactive Compounds from the Peels of the Slovenian Onion Variety "Ptujski lük"

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HPLC-UV

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Abstract: In this study, the extraction efficiency of deep eutectic solvents (DES) using choline chloride as a hydrogen bond acceptor and various donors (propane-1,2-diol, acetic acid, lactic acid, fructose and butane-1,4-diol) for the isolation of bioactive compounds from the peels of the Slovenian onion variety "Ptujski lük" was investigated. The results were compared with those obtained with 70% ethanol, 70% methanol and water. The phytochemical profiles of all extracts obtained after ultrasound-assisted extraction were analysed both spectrophotometrically (TPC, ABTS, TPC, FRAP, DPPH antioxidation test) and chromatographically (HPLC-UV). Protocatechuic acid, quercetin, quercetin-3,4'-diglucoside and quercetin-3-β-D-glucoside were determined in all extracts. Water proved to be the most effective for the extraction of protocatechuic acid (4.3 mg/g), while 70% methanol yielded the highest levels of quercetin and quercetin-3,4'-diglucoside (4.2 mg/g and 8.6 mg/g, respectively). Among the DES solvents tested, DES based on choline chloride and acetic acid proved to be the most effective (protocatechuic acid, 1.5 mg/g; quercetin, 1.7 mg/g and quercetin-3,4'-diglucoside 4.4 mg/g). Alcoholic extracts had superior antioxidant potential, while DES with acetic or lactic acid showed comparable activity, except in the DPPH test. Water extracts showed the lowest antioxidant activity. The findings highlight onion peels' potential as rich sources of healthful phenolic compounds.

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Abstract

PP-AC-16

Removal of Metal Ions from Aqueous Solutions by Green Tea Waste Biomass

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Abstract: Rapid urbanization has resulted in large amounts of water effluents that predominantly contain high levels of pollutants, which reach the environment mainly through the discharge of wastewater into natural recipients. The wastewater treatment usually implies conventional methods for removing metal ions; however, their inability to effectively remove metal ions led to the use of (bio)sorbents. In this research, the possibility of using unmodified waste biomass of green tea for the removal of metal ions (Mn^{2+}, Ni^{2+}, Fe^{2+}, Co^{2+}, Cd^{2+}, Pb^{2+}, Zn^{2+} and Cu^{2+}) from aqueous solutions was investigated. In order to achieve maximum adsorption efficiency, the influence of the following parameters was examined: adsorption contact time, pH value of the solution and the influence of the adsorbent mass on adsorption of metal ions. The characterization of adsorbents was also carried out: the point of zero charge, cation exchange and the concentration of metals in the tea waste biomass were determined. The obtained results indicate that green tea waste biomass mainly shows good efficiency in removing metal ions at an adsorbent mass of 0.5 g. The optimal pH value was 5 for the majority of metal ions. The optimal contact time at which the maximum removal efficiency was achieved was 30 min for most metal ions. The obtained results suggest that green tea waste biomass could be used as a widely available, efficient and inexpensive natural adsorbent for the removal of metal ions from aqueous solutions.

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Abstract
PP-AC-17

TLC descriptors in Examination of Chloroacetamides' Lipophilicity

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Abstract: Since discovery of their strong herbicidal activity, chloroacetamide derivatives have been the subject of numerous researches in medicinal chemistry and pharmacology. It was found that these compounds behave as bactericidal, antioxidant and antitumor agents.

The essence of the modern approach in the design of new biologically active compounds is based on establishing the relationship between the chemical structure of the molecule and its biological activity. For these purposes, the assessment of compounds' lipophilicity is of crucial importance. In the first phase, new chloroacetamide derivatives' lipophilicity was determined *in silico*, as well as by using reversed phase thin-layer chromatography (RPTLC18F254s) in the presence of two organic modifiers (*n*-propanol and acetonitrile). The possibility of applying the chromatographic parameters (R_M^0 and m) of the tested chloroacetamides as alternative measures of their lipophilicity and pharmacokinetic behavior was studied by their correlation with partition coefficient (log$P$) and important pharmacokinetic predictors. Thereby, satisfactory mathematical models were obtained. In addition, it was confirmed that the studied bioactivity properties of the given chloroacetamides are conditioned by the type of the present hydrocarbon substituents (number, arrangement and binding of C atoms).

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POSTER PRESENTATIONS

Biochemistry and Biotechnology

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Abstract
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Binding Determination and Interaction Study of Human Serum Albumin with 6- and 7-Substituted 4-Methylcoumarins

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Abstract: The interaction of synthesized 4-methylcoumarin derivatives with human serum albumin (HSA) at three temperatures was investigated using fluorescence spectroscopy. Selected derivatives of 6-substituted coumarins were 4,6-dimethyl-2*H*-benzopyran-2-one (4K), 6-methoxy-4-methyl-2*H*-benzopyran-2-one (6K), and 4,7-dimethyl-6-hydroxy-2*H*-benzopyran-2-one (10K), while 7-substituted 4-methylcoumarins are: 4-methyl-2-oxo-2*H*-chromen-7-yl benzoate (14K), 4,5-dimethyl-2-oxo-2*H*-chromen-7-yl benzoate (15K) and 4-methyl-2-oxo-2*H*-chromene-7,8-diyl benzoate (17K). The following experimental data were calculated: Stern-Volmer constant (K_{SV}), bimolecular quenching constant (K_q), binding constant (K_b), and number of binding sites (n). The experimental results show that the fluorescence of HSA was quenched and that it is most likely static, with the strongest binding occurring with sample 17K at 296 K ($k_q = 3,46 \text{x} 10^{12}$ $M^{-1}s^{-1}$). The thermodynamic parameter (Gibbs's energy, $\Delta G°$) proves spontaneous interaction between selected 4-methylcoumarin derivatives and HAS, at room temperature. Synchronous spectroscopy and three-dimensional fluorescence spectroscopy were used to monitor conformational changes in the microenvironment near the chromophore. The results indicate slight changes in the shift of the emission maximum in the microenvironment of tyrosine and tryptophan in the HSA. FRET analysis showed that all samples are at distances $r_0 < 8$ nm, indicating the potential for energy transfer from the donor (HSA) to the acceptor (4-methylcoumarin derivatives). An *in silico* analysis was conducted to determine potential binding sites of 4-methylcoumarin derivatives to HSA, revealing that sample 10K forms a hydrogen bond *via* the oxygen heteroatom in the pyrone ring structure (1.993 Å) with Lys^{137}.

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Abstract

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Biochemical Status of Patients Suffered from Diabetic Nephropathy

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Abstract: Diabetes mellitus is one of the most common chronic non-communicable diseases and represents a major public health problem. Diabetic nephropathy is one of the many complications of diabetes and is the leading single cause of end-stage renal disease. The aim of this study is to investigate the incidence of diabetic nephropathy in patients with type 1 and type 2 diabetes in the Central Bosnia Canton and their biochemical status. The paper presents the results of research on diabetic nephropathy conducted in the Central Bosnia Canton. The processing of the obtained results was done with the aim of determining the frequency of diabetic nephropathy and the frequency of markers of renal damage depending on the present risk factors in patients with diabetes. The paper is designed as a prospective study. The research included 123 respondents. There were 51.2% men and 48.7% women in the group, with an average age of 64.32 years. 57.72% of respondents had glomerular filtration (GF) ≥ 90 mL/min/1.73m^2, while 42.27% of respondents had GF < 90 mL/min/1.73m^2. Most of the respondents had second-degree renal damage. The incidence of diabetic nephropathy in the study population is significantly high.

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Abstract

PP-BB-03

Determination of the Vitamin C Content in Various Natural Samples by Direct UV Spectrophotometric Method

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Abstract: This study aimed to determine the vitamin C content in various natural samples using the direct UV spectrophotometric method at a wavelength of 266 nm, with sodium oxalate as a stabilizer. Fifteen samples, including berries, vegetables, and bee products, were analyzed in triplicate. A calibration curve was constructed from L-ascorbic acid standards to quantify the vitamin C content in the samples. The highest vitamin C content was found in rosehip from Novi Travnik (611.16±5.10 mg/100 g), followed by samples from National park (NP) "Una" in 2021, royal jelly (RJ) from Bihać-Orašac, rosehip from NP "Una" in 2020, and RJ from the Sarajevo area. Among the vegetables, broccoli had the highest content, followed by beet and carrot. Mixed honey (goji+raspberry) and raspberry from the Cazin-Rujnica area also showed significant vitamin C content. Meadow honey had the lowest content of vitamin C. These findings highlight the richness of vitamin C in rosehip and RJ samples from Bosnia and Herzegovina.

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Chemistry of Advanced Materials

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Abstract

PP-CAM-01

Protection against Microwave Radiation Penetration by the Addition of Nanomaterials in Clay Composites

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Abstract: Fast development and widespread use of mobile telephony that uses specific wavelengths in the microwave region of the electromagnetic spectrum cause a growing interest in protecting against the penetration of radiation through building materials. While most of the studies focus on concrete, in this study, fired clay bricks with added different nanomaterials (clay composites) were investigated. Microwave radiation penetration was measured using a spectrum analyzer in the frequency range from 1.5 to 6 GHz that covers all the frequencies currently in use: LTE 1800 (2G, 1.8 GHz), LTE 2100 (3G, 2.1 – 2.3 GHz), LTE 2600 (4G, 2.6 – 2.7 GHz), and NR3500 (5G, 3.4 – 3.8 GHz), on two-component fired clay disks (clay with 5 % of antimony tin oxide - ATO, titanium dioxide – TiO2, and fly ash – FA) and three-component samples that contained clay and a combination (2.5 % + 2.5 %) of nanomaterials. All the used materials were systematically characterized: specific surface area (B.E.T.), thermogravimetry (TGA), electron microscopy (SEM – morphology and particle size), phase analysis (X-ray diffraction), and chemical and mineralogical analysis (X-ray and optical emission spectroscopy). Standard solid bricks were made from three-component mixtures to determine the usability of prepared composite materials as construction elements, and their water absorption and compressive strength were determined. The results of the research show that the addition of the tested nanomaterials to the clay significantly reduces the penetration of electromagnetic radiation in the microwave region and, at the same time, improves the tested physical and mechanical properties.

Acknowledgment

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Abstract

PP-CAM-02

Natural Clay Pyrophyllite Activation with Silver and Composite Characterization

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Abstract: In this work, a hybrid pyrophyllite/AgNPs system was designed by mechanochemical activation of pyrophyllite, $Al_2Si_4O_{10}(OH)_2$. Tuning this system's properties is especially important in terms of possible biomedical applications. The reaction was triggered by adding 2, 5, and 10wt% of silver in the form of $AgNO_3$, indicating green synthesis of AgNPs. Thereby, the grinding time was adjusted from 20 to 320 minutes. The collected samples were analyzed by FTIR, XRD, SEM with EDX, TGA, DTA and PSD. The FTIR spectra of the pyrophyllite/AgNPs system showed the disappearance of some bands characteristic of pyrophyllite itself due to breaking of some bonds during the grinding, and the appearance of some new bands. SEM-EDS analysis confirmed that pyrophyllite structure changed during the mechanochemical treatment, indicating a homogeneous distribution of silver along the analyzed surface. PSD analysis showed that the average particle size distribution is approximately the same for all samples, despite the different wt% of silver. While XRD patterns of samples with 2 and 5 wt% of $AgNO_3$ did not show reflections originating from silver, the peak at 38.16˚ of the pyrophyllite sample milled for 20 minutes with 10 wt% of silver could be assigned to silver in the metal form. DTA curves of pyrophyllite/$AgNO_3$ samples milled for 20, 80 or 320 min had similar shapes for different silver content added. TGA curves of pyrophyllite/$AgNO_3$ samples milled for 20 min with 2, 5, and 10 wt% of silver showed a total weight loss of about 10% while for samples milled for 320 min reduced weight loss was observed due to the agglomeration of particles.

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Abstract

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Eco-Friendly Quaternization of 2-Hydroxyethyl Cellulose: Structural Characterization and Multifunctional Applications

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2-hydroxyethyl Cellulose
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Abstract: Quaternizing polysaccharides with trimethyl ammonium compounds expands their applications, including use as conductive materials, in water purification, and biomedicine. Recent research has been more focused on environmentally friendly derivatization methods and green reactants. This study examines the derivatization and structural characterization of choline and betaine substituted 2-hydroxyethyl cellulose. Covalently bound cationic charges were quantified via polyelectrolyte titration. The binding of choline, a naturally occurring material, and its derivative betaine, corresponds to the use of green reactants for more environmentally friendly approaches. Biological properties, such as antimicrobial properties and cytotoxicity, were tested against *S. Aureus*, *P. Aeruginosa*, and mouse fibroblasts (NCTC clone 929- CCL-1) and were compared with succinylated polyallylamine hydrochloride. Electrospinning with polyvinyl alcohol produced nanofibers, with diameters measured via SEM. Potential use of quaternized HEC as a flocculant was assessed using UV-VIS for flocculating kaolin substrate. This research advances the understanding of quaternized cellulose derivatives and presents eco-friendly applications for these materials.

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Abstract

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Inhibition of Copper Corrosion in Acidic Solution by Selected Thiazole Derivatives

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Thiazole Derivative

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Abstract: Among the biggest material losses in the world are those caused by corrosion of construction materials, raw materials, products, or semi-finished products. Therefore, the successful protection of materials against corrosion is one of the most important issues today. When it comes to protecting materials, the industry pays the most attention to metals. Reducing the degree of metal degradation is in many cases successfully achieved by using corrosion inhibitors. Copper, as one of the most important non-ferrous metals, is widely used in various parts of the industry. Therefore, the aim of this research was to investigate the inhibition properties of the selected thiazole derivative for the protection of copper against corrosion in acidic sulphate solution. Inhibition efficiency of 5-(4'-hydroxybenzylidene)-2,4-dioxotetrahydro-1,3-thiazole on copper corrosion in acidic (pH=3) 0.1mol/dm^3 sodium sulphate solution was investigated using potentiostatic polarization measurements and electrochemical impedance spectroscopy (EIS). It was found that the investigated thiazole derivative has inhibitory properties on copper corrosion in acidic media. The inhibitory effect of the tested compound is manifested by adsorption on the copper surface, which results in a decrease in the cathodic corrosion current, an increase of the polarization resistance of the system in relation to the corrosion solution. Inhibition efficiency of the tested compound largely depends on its applied concentration.

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POSTER PRESENTATIONS

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Abstract

PP-CNP-01

Chemical Composition of *Helichrysum italicum* Essential Oil from Bosnia and Herzegovina

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ABSTRACT: Volatile constituents of the hydrodistilled essential oil of *Helichrysum italicum* collected in Herzegovina (Bosnia and Herzegovina) were analyzed by GC-MS. Similarities in qualitative, but with differences in quantitative composition among the analyzed samples were indicated. Of the ten samples analyzed, 32 - 46 components were identified, representing 89.9% - 93.5% of the total essential oil composition. The results showed significant content of monoterpenes and sesquiterpenes, while terpene components such as aromatics and non-terpenes like diketones and esters were also identified. The content of italidiones, found only in *H. italicum*, in the analyzed essential oils (samples 1 - 9) was 1.5% do 4.1%. Among the identified constituents of samples from 1 to 9 those present in the highest percentage were: *α*-pinene (13.9% - 22.2%), *β*-selinene (10.9% - 16.9%), *γ*-curcumene (3.5% - 16.9%), neryl acetate (6.0% - 15.3%), *α*-selinene (4.4% - 7.5%), β-caryophyllene (5.1% - 7.3%), italicene (3.1% - 4.7%), *α*-copaene (2.1% - 3.9%) and limonene (2.3% - 3.4%). Sample 3 contains a significant amount of *β*-selinene with 16.9±0.8%, as well as neryl acetate with 15.3±0.6%, which is also the highest content of these two components compared to all other samples. The main components of sample 10, which composition differs significantly from other samples, are: *α*-thujone (12.2%), eucalyptol (11.6%), *α*-caryophyllene (9.9%), camphene (9.2%), camphor (9.1%), *α*-pinene (7.7%), *β*-pinene (7.6%), borneol (7.4%) and bornyl acetate (3.9%).

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Abstract

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Chemical Composition and Biological Activity of Volatile Extracts from Plants Ground Ivy and Mediterranean Buckthorn

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GC-MS
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Abstract: The aim of this work was to determine chemical composition and biological effect of the volatile extracts from plants ground ivy (*Glechoma hederacea* L.) and mediterranean buckthorn (*Rhamnus alaternus* L.). Of all of the chemical compounds that constitute ground ivy volatile extract, germacrene D (37.05%) was the most abundant, while *α*-pinene (22.03%) and linalool (17.53%) were two most abundant constituents in the volatile extract of mediterranean buckthorn. Antioxidant potential tests of these volatile extracts were conducted using the DPPH and FRAP assays. Results have shown that extracts with concentration of 1 g/L, tested using DPPH and FRAP assays, display very low antioxidant activity. The inhibition potential of those volatile extracts with the same concentration (1 g/L), was conducted by Ellman's method for enzymes AChE and BChE, and the Brueggan-Hollingsworth method for *α*-glycosidase. Sample of a volatile extract from ground ivy exhibits very good ability to inhibit AChE, while the extract from mediterranean buckthorn shows weaker ability to inhibit AChE enzyme. Extract from ground ivy inhibits BChE poorly, while extract from mediterranean buckthorn has no ability to inhibit BChE. Volatile extract from ground ivy inhibits *α*-glycosidase well, but the extract from mediterranean buckthorn does not inhibit this enzyme.

Acknowledgment

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Abstract

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Anti-inflammatory Properties of *Calendula officinalis* L. Extracts

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Abstract: Based on the abundance of many phytochemicals, extracts derived from *Calendula officinalis* L. demonstrate certain biological activities. This study seeks to assess the anti-inflammatory effects of extracts from *C. officinalis*. These extracts were obtained from leaves, flowers, stems, and roots collected in Lukavica during 2020 and 2021, and in Hotonj in 2021. Soxhlet and ultrasonic methods were employed with 96% ethanol (EtOH) as the solvent for extracting these compounds. Furthermore, cold extraction was conducted using an improvised vertical stirrer with distilled water (dH_2O) as the solvent, while hot and cold extraction was carried out on a magnetic stirrer. The protein denaturation assay was applied to estimate the anti-inflammatory properties of analyzed *C. officinalis* extracts. Based on the results, among the *C. officinalis* samples harvested in 2020, the flower extract prepared by cold extraction on a vertical stirrer, showed the most significant anti-inflammatory properties (65.18 ± 1.11 %), at a concentration of 15 mg/mL. On the other hand, among the samples harvested in 2021, the highest anti-inflammatory potential (80.37 ± 0.22 %), at a concentration of 1 mg/mL, was noticed by the root extract prepared by cold extraction on a magnetic stirrer. Furthermore, no correlation was found between the concentration of analyzed extracts and their anti-inflammatory properties. In conclusion, the protein denaturation assay demonstrated the anti-inflammatory properties of *Calendula officinalis* L. extracts.

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Abstract

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Phytochemical Characterization and Biological Activity of *Geranium robertianum* L. and *Geranium molle* L.

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Abstract: The aim of this study are two *Geranium* species, namely *Geranium robertianum* and *Geranium molle* collected in the surroundings of Sarajevo. Extracts were prepared by successive Soxhlet extraction, using three solvents in order of increasing polarity, chloroform → ethyl acetate →ethanol. The sample with the highest content of total phenolic compounds was the ethyl acetate extract of *G. molle* (2.73 mg GAE/g), while the highest content of total flavonoids was recorded in the ethanol extract of the same species (25.94 mg QUE/g). The highest content of total phenolic acids was determined in the ethyl acetate extract of *G. robertianum* (96.16 mg CAE/g). Qualitative and quantitative analysis of phenolic compounds was performed using high-performance liquid chromatography with a diode array detector (HPLC-DAD). Five compounds were identified and quantified in the samples, namely gallic acid, protocatechuic acid, rutin, quercetin, and kaempferol.

The biological activity was determined through the analysis of antioxidant activity using two methods, ABTS and DPPH. The ethanol extracts of the examined species showed the best antioxidant activity according to both methods, while the chloroform extracts showed the weakest activity. Besides antioxidant activity, enzyme inhibition activity was determined for two enzymes, acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE). The enzyme inhibition activity for AChE ranged from 47.11% for the chloroform extract to 79.08% for the ethanol extract of the *G. robertianum*. The obtained results for BuChE inhibition activity were slightly lower, ranging from 16.59% for the ethyl acetate extract to 41.04% for the ethanol extract of *G. molle*.

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Chemical Composition, Antioxidant and Enzyme Inhibitory Activity of *Achillea collina* (Wirtg.) Heimerl

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Abstract: This work presents the first investigation of chemical composition and antioxidant activity in different extracts of the plant species *Achillea collina* (Wirtg.) Heimerl collected from the area of Konjic, Bosnia and Herzegovina. The above-ground part of *A. collina* was subjected to Soxhlet and ultrasound extraction with 70% ethanol as solvent. Spectrophotometric methods were used for the phytochemical evaluation and testing of antioxidant activity. Soxhlet extract had a higher content of total phenolic compounds (TPC) 146.15 mg GAE/g and total phenolic acids (TPA) 112.21 mg CAE/g, while the content of total flavonoids (TFC) was similar for Soxhlet 33.29 mg QE/g and 34.05 mg QE/g for ultrasound extract. The results obtained for antioxidant activity according to the DPPH and ABTS methods were expressed as IC_{50} values, where Soxhlet extract demonstrated higher antioxidant activity than ultrasound extract, 0.25 mg/mL and 0.27 mg/mL, respectively. For the FRAP method, results were expressed as ascorbic acid equivalents, where also the Soxhlet extract demonstrated higher antioxidant activity 130.99 mg AAE/g extract compared to the ultrasound extract 112.85 mg AAE/g, respectively. The determination of selected phenolic acids and flavonoids was performed by the HPLC-DAD method. Analysis confirmed the persence of chlorogenic acid, 3,4-dicaffeoylquinic acid, 3,5-dicaffeoylquinic acid, 4,5-dicaffeoylquinic acid, vitexin, and luteolin-7-glucoside. Extracts of *A. colina* are rich sources of phenolic compounds and show good antioxidant activity.

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Abstract

Analysis of Phenolic Compounds and Biological Activity of *Achillea abrotanoides* Vis.

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Abstract: The aim of this work was the phytochemical characterization and determination of the biological activity of Achillea abrotanoides, from two natural habitats from Prenj mountain, Velika kapa and Tisovica, Bosnia and Herzegovina. Isolation of secondary metabolites was done by Soxhlet extraction using 70% ethanol as solvent. The sample from Velika kapa had a higher content of total phenolic compounds (56.06 mg GAE/g of extract), as well as a higher content of total phenolic acids (61.91 mg CAE/g of extract) than the sample from Tisovica. On the contrary, the sample from Tisovica had more than twice the content of total flavonoids (53.01 mg QE/g of extract) than the sample from Velika kapa. The extract of this sample also showed a better antioxidant activity by FRAP method (62.81 mg AAE/g of extract) and a better ability to inhibit acetylcholinesterase (IC50 0.52 mg/mL) than the sample from Velika kapa. The latter showed better antioxidant activity determined by the ABTS and DPPH method where IC50 was 0.34 mg/ml and 0.59 mg/ml respectively. Thirteen phenolic compounds, 7 phenolic acids and 6 flavonoids were selected as standards for the qualitative and quantitative chemical analysis of the investigated samples. The analysis was done by HPLC-DAD method. Luteolin (0.93 mg/g DM) and chlorogenic acid (2.14 mg/g DM) were found in the extract of A. abrotanoides from Velika kapa, while only chlorogenic acid (5.98 mg/g DM) was identified in the sample from Tisovica

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Abstract
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Total Phenolic and Flavonoid Content and Antioxidant Activity of Some Raspberry Varieties

Topčagić, A.[a], **Muftić-Brdar, D.** [a], **Klepo, L.**[a], **Mujezin, A.**[a,c], **Toromanović, J.**[b], **Tahirović, I.**[a*]

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Abstract: This paper presents the study of total phenolics (TPs), total flavonoids (TFs), and antioxidant activity (AA) of fruits and juice of raspberry varieties from the area of the municipality of Cazin. Five raspberry varieties grown according to the integral concept were analyzed: Fertodi, Meeker, Polka, Tulameen, and Willamette. The TPs (before and after precipitation with formaldehyde) were quantified using the Folin-Ciocalteu method. The TFs were calculated from the difference between the TPs and the non-flavonoid fraction determined after precipitation. Gallic acid was used as a standard. In addition, the AA of the raspberry samples was tested by the ABTS radical scavenging method, using Trolox as a standard. The TPs of fresh raspberry fruit ranged from 1608.77 mg GAE/100 g for the Tulameen variety to 1443.82 mg/100 g for the Polka variety, while the TPs of raspberry juice ranged from 1006.45 mg GAE/100 ml for Meeker to 154.66 mg GAE/100 ml for the Polka variety. The Tulameen variety had the highest TFs in raspberry fruit (1488.40 mg GAE/100 g) and the Willamette variety in raspberry juice (789.99 mg GAE/100 ml), while the Polka variety had the lowest content in both samples tested (1345.58 mg GAE/100 g in fruit and 100.43 mg GAE/100 ml in juice). Raspberry fruits are significantly richer in TPs and TFs content than raspberry juice. All samples exhibited AA, with values for raspberry fruit samples ranging from 0.146 g TE/100 g for the Polka variety to 1.211 g TE/100 g for the Fertodi variety, while values for raspberry juice samples ranged from 0.031 g TE/100 ml for the Polka variety to 0.163 g TE/100 ml for the Meeker variety.

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Determination of Vitamin C Content in Amaranthaceae Plants by UV/Vis Spectrophotometry

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Abstract: The Amaranthaceae family includes annual and perennial plants. The leaves of these plants contain considerable amount of vitamin C. The antioxidant characteristics of vitamin C make it helpful in the treatment of a variety of disorders, including atherosclerosis, diabetes, infertility, and neurological diseases.

Given the importance of vitamin C in the body, this study aims to determine vitamin C levels in the dry and fresh leaves of Amaranthaceae plants, which are commonly used in human nutrition. The plants chosen are spinach (*Spinacia oleracea* L.), Swiss chard (*Beta vulgaris* L ssp. vulgaris), and Goosefoot (*Chenopodium album* L.).

UV-Vis spectrophotometry was used to determine the concentration of vitamin C in samples. The procedure with 2,4-dinitrophenylhydrazine (DNPH) is one of precise, and dependable methods for determining vitamin C content in plants. Vitamin C reacts with the acidic DNPH in samples. The addition of bromine water in the presence of acetic acid oxidizes vitamin C to dehydroascorbic acid. L-dehydroascorbic acid then mixes with DNPH to generate osazone, which reacts with 85% sulfuric acid to make the solution red. After cooling, absorbance was measured at 521.5 nm.

A quantitative analysis of vitamin C in the dry leaves of the analyzed plants showed concentrations ranging from 0.013 to 0.069 mg/g, and fresh leaves from 0.072 to 0.674 mg/g. Based on these results, we may conclude that dry samples of analyzed plants have a considerably smaller quantity of vitamin C than fresh ones. The difference could be a result of a variety of factors, including light, temperature, enzymes, and the drying process itself.

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Abstract

PP-CNP-09

Determination of Total Phenols and Flavonoids in Fruit and Leaves of White Mulberry (*Morus alba* L)

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Total Flavonoids

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Abstract: White mulberry (*Morus alba* L.) is a deciduous tree from the Morus genus in the Moraceae family. Almost every component of the white mulberry tree is utilized in traditional medicine, with the leaves and fruit being particularly essential. White mulberry leaves and fruits have long been used in traditional Chinese medicine to treat a variety of diseases, including asthma, cough, edema, sleeplessness, and diabetes. Flavonoids and phenols both have antioxidant activity, which can help to prevent the start of some diseases and free radical damage to cells, as well as delay aging and inhibit the creation of molecules implicated in inflammation.

Due to the above, the objective of this study is to determine the total phenols and flavonoids contained in white mulberry fruit and leaf. Total phenols have been determined using the Folin-Ciocalteu method. The total flavonoid content has been determined using the spectrophotometric method, which is based on the reaction of aluminum chloride with flavones and flavonols resulting in complex molecules. For the preparation of the extracts, the ultrasonic extraction was performed.

The spectrophotometric determination of total phenols and flavonoids in ethanolic extracts of white mulberry fruit and leaves showed higher concentrations in the fruit (0.86 and 3.28 mg/g) than in the leaf (0.24 and 1.80 mg/g). The factors that impact the total phenol and flavonoid content of white mulberry fruit and leaves are not well understood. However, the proportion of total phenols and flavonoids is likely impacted by the ecotype and method of extract preparation, as several studies have shown.

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Abstract

PP-CNP-10

Characterisation of Volatile Compounds in Kumquat

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Abstract: Citrus fruits have wide acceptance due to their attractive flavour and nutritional value. All citrus fruits originate from five recognized parent species, namely pomelo (*Citrus grandis*), citron (*Citrus medica*), pure mandarin (*Citrus reticulata*), micrantha (*Citrus micrantha*) and kumquat (*Fortunella japonica* Swingle). Although kumquat is commercially marketed as a citrus fruit, it is scientifically classified as a different genus from the common citrus fruits and has a different chemical composition from the other fruits of the *Citrus* genus. Volatile compounds of rare citrus fruits such as kumquat are still insufficiently researched. Since flavour is one of the most appreciated fruit characteristics, volatile aroma compounds probably play a key role in consumer perception and acceptance of products. In this research, the composition and content of volatile compounds from the peel and pulp of the kumquat were analyzed. The volatile compounds were isolated by solid-phase microextraction (HS-SPME) using two fibers of different compositions (divinylbenzene/carboxen/polydimethylsiloxane (DVB/CAR/PDMS) fiber and polydimethylsiloxane/divinylbenzene (PDMS/DVB) fiber). Adsorption of the volatile compounds on the fibers was carried out for 40 and 80 minutes. All samples were analysed by coupled gas chromatography-mass spectrometry system on an HP-5MS column, and the results were compared. A total of 22 volatiles were identified in the kumquat samples. The major compounds in all samples were limonene (79.8-93.1%), germacrene D (1.8-7.6%), *β*-myrcene (1.9-4.3%) and geranyl acetate (1.1-2.7%). The results have shown that a longer adsorption time increased the number of identified compounds.

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Abstract

PP-CNP-11

Headspace SPME–GC/MS Analysis of *Hyssopus officinalis* L. Volatile Constituents

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PDMS/DVB Fibre
Methyl Eugenol

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Abstract: Hyssop (*Hyssopus officinalis* L., Lamiaceae) is a perennial shrub with violet-blue flowers in vertical clusters and a spicy taste with a pungent flavour. Besides being used as a culinary herb for flavouring and food preservation, this plant is also a traditional remedy for respiratory and digestive disturbances. Hyssop essential oil is used in the pharmaceutical, fragrance, and cosmetics industries, as well as in aromatherapy. In the sense of presenting a broader olfactory profile research is conducted to determine the chemical composition of plant volatiles by headspace-solid phase microextraction (HS-SPME) coupled with gas chromatography (GC/MS) of Hyssop harvested in the Herzegovina area. Depending on the type of fibre utilized, the analysis found 16 compounds (97.92% with Divinylbenzene/Carboxen/Polydimethylsiloxane-DVB/CAR/PDMS fibre) and 26 compounds (97.38% with Polydimethylsiloxane/Divinylbenzene-PDMS/DVB fibre). The disparity in the number of compounds detected can be attributed to the varying polarity of the fibre coatings in relation to the polarity of the constituents. The main component identified was methyl eugenol, with a content of 70.65% (DVB/CAR/PDMS) and 54.29% (PDMS/DVB). It is a naturally occurring chemical compound classified as phenylpropene, found in various essential oils, and important for insect behaviour and pollination. Other predominant compounds were 1,8-cineole, limonene, germacrene D, (Z)-β-ocymene, and bicyclogermacrene. As expected, most of the other dominant compounds identified were found to be monoterpenes, oxygenated monoterpenes, and sesquiterpenes. The HS-SPME method can achieve comparable results to those obtained by essential oil analysis. Advantages of method are a very small number of samples, a shorter extraction time, and a much simpler procedure but it is not available in many laboratories.

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Abstract

PP-CNP-12

GC/MS Volatile Constituents of *Taxus baccata* L. Fruit and Seed Essential Oil

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Abstract: The genus *Taxus* (yews) is the largest and most important genus of the family Taxaceae. It comprises about 24 species, with 55 varieties distributed mainly in Asia, Europe, North Africa, and North America. Essential oils (EOs) of fresh fruit and seed of *Taxus baccata* L. from Sarajevo gardens were obtained by hydrodistillation in a Clevenger-type apparatus, yielding 0.02% (w/w). The GC and MS analyses enabled the identification of 95 constituents, which accounted for 89.83% of the total fruit EO, and 80 constituents from seed EO, which accounted for 92.86%. Acids, alcohols, and aldehydes were found to be the main compounds of EOs extracted from *Taxus* plant parts. The fruit oil was mainly composed of *n*-hexadecanoic acid (22.22%), tetradecanoic acid (6.33%), linolenic acid, ethyl ester (4.75%), and 1-hexadecanol (4.04%), while *n*-hexadecanoic acid (38.15%), hexanal (10.55%), benzaldehyde (4.04%), and *cis*-9-hexadecenoic acid (2.70%) were the main compounds of the seed oil. *Taxus* species are in high demand for the extraction of taxol or related taxanes, a drug for the treatment of various cancers. In addition to taxane diterpenoids and the anticancer drug taxol, *Taxus* species contain essential oils with actual or potential biological activity.

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Abstract

PP-CNP-13

Phytochemical Profile of *Taxus baccata* L. Needles Essential Oils from Sarajevo Gardens

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Abstract: *Taxus baccata* L., originally known as common or European yew, is an evergreen tree from the family Taxaceae, native to western, central, and southern Europe. All parts of the plant, except the red flesh berry, act as antispasmodics, cardiotonics, expectorants, and purgatives. Yew contains numerous toxic compounds, including several alkaloids and nitriles (esters of cyanogenic glycosides), but the most important toxins are taxine alkaloids, which are cardiotoxic chemical compounds. In the present study, the extraction of fresh and dried yew needle essential oils (EO) was obtained by hydrodistillation in a Clevenger-type apparatus and phytochemical profiled by gas chromatography coupled with mass spectrometry (GC/MS). A total of 108 components were identified in fresh needles EO and 82 in dried needles EO. The major components in fresh yew needles EO were (*Z*)-3-hexen-1-ol (21.85%) and (*E*)-2-hexenal (18.87%), and in the dried needles EO 3-octanone (14.70%) and 1-octen-3-one (11.33%). The other predominant components in both samples were as follows: hexanal, 1-octanole, (*E*)-2-hexen-1-ol, and myrtenole. (*E*)-9-octadecenoic acid was detected only in dried needle EO samples. Containing taxol, which shows significant potential in the treatment of cancer, especially ovarian cancer, *Taxus baccata* L. can be used for many medicinal purposes. Due to the toxicity of the plant, it should not be used at home without the supervision of an authorized person.

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Abstract

PP-CNP-14

In Silico DFT and Docking Studies on β-sitosterol Compared to *In vitro* Studies on the Antiproliferative Properties of Sloe Plant Extracts Against Prostate Cancer Cells (DU 145 and PC3)

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Abstract: Medicinal plants have been used to alleviate human pain since ancient times. Due to their therapeutic efficacy, the pharmaceutical industry has included crude extracts of these plants in the production of medicines. Extracts of sloe (*Prunus spinosa* L.) are a rich source of natural bioactive compounds, including phytosterols, which are known for their use in the treatment of various prostate diseases. Investigation of the *in vitro* antiproliferative activity of ethanolic extracts of sloe flowers, leaves and fruits, sourced from three habitats in Bosnia and Herzegovina, against human prostate cancer cell lines PC-3 and DU145 using the MTT assay has been performed and their results were published. In addition to previous research, this work aims to theoretically investigate the β-sitosterol molecule due to its biological and medical significance. Theoretical approaches such as molecular mechanics, semiempirical methods, Hartree-Fock and density functional theory (DFT) calculations were used to explore the structural, vibrational and electronic properties of β-sitosterol. The frontier molecular orbitals are mainly localized at the C-C double bond, with a relatively small energy difference that contributes to the kinetic stability of the molecule. The dipole moment of β-sitosterol is 2.01 Debye's, indicating that it is a polar molecule.

To understand how β-sitosterol binds to the androgen receptor, which exists in two isoforms (AR-A and AR-B), we also performed molecular docking using AutoDock Vina integrated with YASARA Structure and Schrödinger's Glide. The results showed that β-sitosterol fits well to the binding sites of both androgen receptor models, suggesting a possible mechanism for its antiproliferative effects.

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Abstract

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Antimicrobial Evaluation of European Pharmacopoeia Quality Essential Oil Combinations for Mouthwash Application

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Abstract: In this study, the potential antimicrobial effects of 4 different (*Foeniculum vulgare, Lavandula angustifolia, Carum carvi, Pinus pumilionis*) European Pharmacopoeia quality essential oils were evaluated. The plant preparations are known and used ethnobotanically against throat infections. *In vitro* antimicrobial evaluation of the commercial essential against *Morexella catharrallis, Streptococcus mitis, Staphylococcus aureus* and *Streptococcus mutans*, were performed using a microdilution assay. Active samples were then prepared for mouthwash formulations and the effects were challenged and compared also using the agar-well diffusion method. Mouthwash formulations were designed from studied essential oils, including binary combinations and quadruple combinations with all oils. Of the seven different combinations studied in total, the most effective ones were *F. vulgare-L. angustifolia* (240 mm zone diameter against *S. mitis*) and *L. angustifolia-C. carvi* (300 mm zone diameter against *S. mutans*) essential oil combinations. While none of the combinations tried was effective against *M. catarrhalis* microorganism, it was observed that all combinations were generally more effective against *S. mutans* microorganism. As a result, it is thought that mouthwash formulations developed with these oils can be used especially in preventing dental caries.

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Abstract

PP-CNP-16

Antioxidant Properties of Alien Plant Species: Assessing Phenolic and Flavonoid Content, Antioxidant, Oxidant Capacities, and Antimicrobial Activity

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Abstract: Alien plant species pose significant threats to natural ecosystems due to their adaptability and invasive potential. In this study we investigated the antioxidant activity of 13 alien and invasive plant species, regarding their total phenolic content, flavonoid content, total antioxidant capacity, total oxidant capacity, and antimicrobial activity. Plant tissues were macerated, evaporated to dryness, and the extracts were dissolved in water. Total phenolic content ranged from 6.55 mg GAE/g extract to 30.82 mg GAE/g extract. Flavonoid content spanned from 3.04 mg quercetin/g extract to 40.81 mg quercetin/g extract. The total antioxidant capacity ranged between 662 CEAC µM and 1540 CEAC µM. Total oxidative capacity can be correlated to the abiotic stress. *Rhus typhina* L. and *Impatiens balfourii* Hooker f., exhibited positive total oxidant capacity values of 122.56 ± 7.85 µM H_2O_2 Equiv./L and 141.38 ± 4.33 µM H_2O_2 Equiv./L, respectively. These two species also showed the highest total antioxidant capacity that were 1190,06 ± 137,36 CEAC µM for *Rhus typhina* L and 1540,34 ± 270,84 for CEAC *Impatiens balfourii* Hooker f.. We determined antimicrobial activity against *Escherichia coli*, *Staphylococcus aureus*, *Proteus mirabilis*, *Pseudomonas aeruginosa,* and *Candida albicans*. *Rhus typhina* L was active against *E. coli* and *P. mirabilis*.

This data indicates plant increased antioxidant defense systems against abiotic stresses. Clearly, correlation between total oxidant capacity and total antioxidant capacity values in plants is valuable factor indicating the mechanism of the plant defense.

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Abstract

PP-CNP-17

Effect of Temperature on the Content of Bioactive Compounds in Commercial Teas

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Abstract: The most widely consumed beverage in the world is tea, which is made from the *Camellia sinensis* tea plant. Teas have anti-inflammatory and antioxidant properties and are rich in bioactive substances including flavonoids and phenols. For this experiment, fifteen various commercial tea samples—both in bulk and in bags—were used. To determine the impact of temperature on the amount of total phenolic content (TPC) and flavonoid content (TFC), as well as how temperature changes affect the content of TPC and TFC, each sample was prepared for three minutes at each of four distinct temperatures (20, 50, 80, and 100 °C). Using gallic acid (GA) as a standard, the TPC was determined spectrophotometrically using the Folin-Ciocalteu method. Using quercetin (QE) as the reference, an aluminum chloride colorimetric test was used to determine the TFC. Looking at all the results, it is evident that the highest content of TPC and TFC was when the samples were prepared at 100 °C and the lowest at 20 °C. Of all tested samples, green and black tea have the highest values of total phenols (from 14.58 ± 0.002 µg GA/g_{sample} to 60.42 ± 0.005 µg GA/g_{sample} for all tested temperatures, i.e., 6.55 ± 0.0002 µg GA/g_{sample} to 58.84 ± 0.01 µg GA/g_{sample}), and the lowest was the chamomile sample (from 2.71 ± 0.002 µg GA/g_{sample} to 11.96 ± 0.002 µg GA/g_{sample}). The content of total flavonoids was the highest in the St. John's wort sample (from 5.36 ± 0.001 mg QE/g_{sample} to 27.96 ± 0.005 mg QE/g_{sample}), and the lowest in the nettle, green, and black tea samples (from 2.99 ± 0.002 mg QE/g_{sample} up to 6.43 ± 0.007 mg QE/g_{sample}; 2.93 ± 0.003 mg QE/g_{sample} up to 7.03 ± 0.005 mg QE/g_{sample}; 0.08 ± 0.001 mg QE/g_{sample} do 9.11 ± 0.006 mg QE/g_{sample}). From the obtained results, it is evident that temperature affects not only the content of total phenols but also of flavonoids.

POSTER PRESENTATIONS

Education in Chemistry

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Abstract

PP-EDC-01

Spatial Visual Abilities as a Predictor of Successfully Understanding the Content of Organic Chemistry

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Abstract: Though often neglected in education, skills in spatial visualisation have an important role in student achievements when learning chemistry. Spatial reasoning is a demanding but essential skill which includes research in the process of recollecting acquired knowledge. It contributes to the development of critical thinking and problem-solving aptitude. Not only it encourages the development of essential student skills, but also helps them to develop skills in terms of learning outcomes. Insufficiently developed visual-spatial abilities in students can be an obstacle to academic achievement, but given their ability to adapt, active learning strategies are essential in encouraging their development. The organic chemistry curriculum at the secondary school level (in Croatia, last four years of high school) aims to develop spatial visualisation skills, as well as form and apply active teaching and learning strategies suitable for secondary school students. This approach helps students achieve better results on exams and motivates them to learn more complex content. The aim of this research is to determine whether modelling as an active learning strategy for organic chemistry content contributes to development of spatial reasoning skills in students who have shown above average or average results in the Spatial Test.

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POSTER PRESENTATIONS

Environmental Chemistry

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Abstract

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Assessment of Physicochemical Properties and Microbial Quality of Water in Poultry Farms in Bosnia and Herzegovina

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Microbial Quality
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Abstract: Water plays a critical role in poultry production. Contaminated water used as drinking and processing water on poultry farms can result in infections among animals and contamination of animal products and is unsuitable for water administered medications. This study assessed the physicochemical and microbiological quality of water used on poultry farms producing broilers in the northeastern region of Bosnia and Herzegovina. The majority of broiler farms had private wells (n =58) or public water supplies (n = 34). Samples from 92 farms were collected and examined for color, odor, taste, turbidity, pH value, $KMnO_4$ consumption, chlorides, ammonia, nitrates, nitrites, conductivity and enumeration of *E. coli*, fecal coliforms and *Enterococcus* spp. All parameters were analyzed using an appropriate ISO method accredited according to the requirements of BAS EN ISO/IEC 17025:2008. Mean values with standard deviation for turbidity, pH, $KMnO_4$ consumption, chlorides, ammonia, nitrates, nitrites and, conductivity were as follows: 0,16±0,04; 7,51±0,25; 1,37±0,64; 11,91±10,49; 0,09±0,31; 12,78±13,64; 0,06±0,09 and 612,61±216,40, respectively. Ammonia and nitrates contents exceeded the recommended standard in one sample. Total coliform, *E. coli* and *Enterococcus* spp. were found in 41,30 %, 22,83% and 34,78% of water samples, respectively. The water used on the analyzed poultry farms has satisfactory physicochemical properties but a high microbial load and could represent a potential source of pathogenic organisms. This indicates that water from poultry farms needs more treatment to improve its quality especially its microbial contamination. Regular monitoring of water used in animal farms in order to prevent the use of contaminated water must be conducted.

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Abstract

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Application of a Pyrophyllite Modified Carbon Paste Electrode for the Detection of Carbendazim Fungicide in Water

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Abstract: This work aims to design an electrochemical sensor for pesticide detection in food and water based on modified pyrophyllite. Pyrophyllite is a phyllosilicate mineral of the chemical formula $Al_2Si_4O_{10}(OH)_2$. Modification of the carbon paste electrode was made by the addition of mechanochemically modified pyrophyllite. This type of modification is an environmentally friendly green chemistry method because it avoids using solvents. It was found that the best physicochemical characteristics for constructing the electrochemical sensor were shown by the sample that was milled for 15 minutes. Due to the delamination and bending of the layers, the size of the particles and crystallites decreases, and the electrocatalytic activity of the modified electrode is improved. Electrochemical measurements were performed by cyclic voltammetry in 0.5 mol/L H_2SO_4 and 1 mmol/L $K_4Fe(CN)_6$ in 0.1 mol/L KCl. The results showed that the electrode made of 50 % carbon paste and 50 % mechanochemically ground pyrophyllite for 15 minutes had the best properties. Quantitative detection of carbendazim was done by differential pulse stripping voltammetry at different pH in the Britton Robinson buffer. The developed method shows the linearity at pH 4 in the range of (1–10) mg/kg, with r = 0.999 and a detection limit of 0.3 mg/kg. In contrast to earlier works, in which carbendazim was determined electrochemically with different types of electrodes, the detection limits obtained with the carbon paste electrode modified with pyrophyllite, which was ground for 15 minutes in this work, are significantly lower.

Acknowledgment

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Abstract
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Physico-Chemical, Histological, Microbiological Analyses and Organic Pollutants Determination of Water and Fish Samples From Miljacka River

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Abstract: River ecosystems differ fundamentally from most other ecosystems in their (i) openness, which is characterized by close functional links to adjacent ecosystems, and (ii) dynamic physical and ecological structures that change spatially and temporally. Continuous monitoring of water quality in Sarajevo Canton is central to effective water management, pollution migration, and conservation efforts in the area. This study uses a comprehensive analytical approach to assess the water quality of the Miljacka river, located in Otoka. The water samples were analysed to assess their physico-chemical properties, the presence of microorganisms, and the content of heavy metals and pollutants. In addition, organic pollutants such as pesticides or phthalates were analysed in fish samples (muscle and gill tissue). All findings were considered as combined environmental stressors and further validated by histopathological examination of fish tissues. The water sample showed elevated levels of lead (1.52 µg/L), ammonia (0.78 mg/L), orthophosphates (0.11 mL/L), and BOD_5 (7.98 mgO_2/L). In addition, according to microbiological analysis, the water sample had a high content of fecal impurities and a high number of total coliform bacteria. Various environmental pollutants such as plasticizers, emulsifiers, solvents, surfactants, and additives used in the pharmaceutical and cosmetic industries were identified in the collected water and fish samples by GC-MS analysis. These types of compounds were found more frequently in gill and water samples than in muscle tissue. Increased levels of tissue damage were found in the gills and muscles of fish caught in the area.

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Abstract

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Assessment of Mosses as Bioindicators of Indoor Air Pollution: A Study on Metal Accumulation in Working Areas

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Abstract: The research aim was the assessment of mosses as bioindicators of metal air pollution (indoor pollution) in working areas. The moss bag method of active biomonitoring was applied by exposing mosses for 20 days in two working areas, a permitted smoking area (approximately 3 cigarettes were smoked daily) and a non-smoking area. After 20 days of exposure, flame atomic absorption spectrometry (FAAS) was used to determine total metal content (µg/g) for Cr, Co, Cd, Pb and Fe. In order to assess the metal uptake of the studied moss species, relative accumulation factor (RAF) was calculated as the moss content of each metal after exposure (C exposed) was subtracted and then divided by the metal content before exposure (C initial). The highest RAF value was for Cr and Pb in the permitted smoking area (3.38 and 2.04) and non-smoking area (1.18 and 1.02). The lowest RAF value was for Fe in the permitted smoking area (0.06) and non- smoking area (0.04). The results show that there is a higher concentration of determined metals in permitted smoking areas compared to non-smoking areas. Consequently, it was confirmed that the mosses exposed in working areas accumulate heavy metals such as Cr, Co, Cd, Pb and Fe.

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Abstract

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Determination of Heavy Metals in the Soil After Disposal of Wood Pellet Ash

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Abstract: As the production of energy from wood pellet combustion has increased, the processing and disposal of the resulting ash has become an environmental and economic issue. Ash produced from wood biomass can be used in agriculture as a soil fertilizer due to the constituted nutrients and vital inorganic components. Unfortunately, ash can be a source of heavy metals, which usually accumulate in the soil. Uncontrolled disposal of ash can cause air pollution with small particles carried by the wind, groundwater pollution due to the leaching of heavy metals from the ash, and the entry of heavy metals into the food chain. Ten soil samples were treated with wood pellet ash, in the heating season. Samples of soils were prepared by wet digestion using nitric acid (HNO_3), and heavy metals are determined by atomic absorption spectroscopy-flame and graphite furnace. The obtained results show that the heavy metal concentrations in the soil after disposal of wood pellet ash range from 29625.00 mg kg^{-1} for Fe to 0.60 mg kg^{-1} for Cd.

The mean concentrations of analyzed heavy metals decrease as follows Fe > Mn > Ni > Zn > Cu > Cr > Pb > Co > Cd.

Uncontrolled disposal of ash can cause air pollution with small particles carried by the wind, pollution of groundwater due to leaching of heavy metals from ash, and entry of heavy metals into the food chain. When using ash in agriculture, it is necessary to monitor heavy metals (Cd, Cr, Cu, AS, Ni, Pb and Zn) and potentially toxic essential elements (Zn and Cu) that can have a significant negative impact on the soil.

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Abstract

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Foeniculum Vulgare: An Overall Study from Seeds to Simultaneous Cd/Cr/Cu/Pb Biosorption Application

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Abstract: The presence of heavy metals in the environment initiates numerous studies in order to determine their content, distribution, mobility, removal, and reduction of metal ion concentrations due to their harmful effects and toxicity. Therefore, the efficiency of simultaneous removal of Cd, Cr, Cu, and Pb ions using fennel seed (native and NaOH - modified) - based biosorbents from aqueous solutions as an efficient and cheap biomaterial for solid phase extraction was examined. Furthermore, the feasibility of the developed procedure for purifying real water samples was investigated. It was found that optimal conditions for simultaneous removal of four analyte metal ions by native fennel seed biosorbent were: pH 5, sorbent mass 300 mg, and 20 minutes of contact time, while NaOH-modified fennel seed biosorbent pH 4, sorbent mass 200 mg and 20 minutes of contact time were optimal. Under these conditions and for the same initial concentration of each of the analyzed metals (50 mg L^{-1}), total theoretical equilibrium capacities of 22.2 mg g^{-1} and 38.5 mg g^{-1} for native and modified fennel seed biosorbents, respectively, were achieved. Furthermore, both biosorbents showed the best/worst binding affinity toward Pb/Cd ions. According to infrared spectra, the chemical modification of native fennel seed biosorbent caused significant intensity loss of bands in the carbonyl region, while sorption caused deprotonation of hydroxyl groups along with the formation of a weaker metal-oxygen bond, confirming the importance of oxygen-active sites for the sorption of metal ions. Successful application to galvanic wastewater indicated biosorption by fennel seeds as a potential alternative to classical wastewater treatments.

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Abstract

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Heavy Metal Content in Wood Briquettes

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Abstract: The preparation of alternative fuels from wood biomass in the form of wood briquettes belongs nowadays to one of the most frequent ways of ecological fuel preparation used in households and in biogas stations. Wood briquettes are a form of renewable energy that offers numerous benefits, including environmental conservation, the use of local resources, economic feasibility, and versatility. The study focuses on determining the heavy metal content of wood briquets available in the Bosnia and Herzegovina market.

Sample preparation was carried out by wet digestion with nitric acid (HNO_3) in Teflon vessels, and heavy metals (Cd, Co, Cr, Cu, Fe, Mn, Ni, Pb, and Zn) and metalloid (As) are determined by atomic absorption spectroscopy-flame and graphite furnace.

The results indicated that the most abundant heavy metals in the analyzed samples were Fe, Mn, and Zn, all of which can be toxic if absorbed in significant amounts. The Ni content was lower than allowed according to standards used in European Union countries. Only in sample B6 was it within the limit values. Ni, Cd, Cu, Pb, and Cr is present in all tested samples. Arsenic (As), a carcinogenic non-essential metalloid, is the least represented in wood briquette samples, with levels below the detection limit in three samples.

Based on the obtained results, it can be concluded that monitoring of heavy metals in wood briquets is necessary in order to achieve a clean and healthy environment that will not affect human health.

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Abstract

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Grapefruit Peel as a Promising Sorbent for Biosorption Removal of Eriochorme Black T Dye from Aqueous Solution

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Abstract: Water contamination from various industrial plants due to the uncontrolled release of toxins (i.e., dyes) results in intensive biosorption studies aiming to investigate the possibility of using different biomaterials for their remediation.

In this regard, a batch study using pulverized grapefruit peel (native, and $ZrOClx8H_2O$ modified) for the removal of Eriochrome Black T (EBT) was optimized in the mean of key biosorption parameters followed by ultraviolet-visible spectrophotometry (UV-ViS) determination. Different physico-chemical characterization methods of grapefruit peels before/after EBT removal were conducted.

The determined zero charge values were 4.15 and 2.75 along with 4.11 and 2.56 pH values of the biosorbent suspension in water for native and modified peel, respectively. According to Boehm's titrations, both native and modified biosorbents are rich in acidic functional groups, 2.95 mmol/g and 3.90 mmol/g, respectively. Fourier transform infrared spectroscopy (FTIR) showed that most of the bands after EBT sorption shift to lower wave numbers, which further indicates the role of hydrogen bonds as the main reason for the sorption of this dye.

For the initial EBT concentration of 60 mg/L at room temperature, removal by native peel was optimum at pH 3-6, biosorbent mass 100 mg under 60 minutes of contact time, while by modified peel, the best conditions were pH 5-7, biosorbent mass 100 mg, and contact time 30 minutes. Under these conditions the maximum adsorption capacity was 24.3 mg/g for native peel, and 52.3 mg/g for modified peel.

Based on the results, pulverized grapefruit peel can be an efficient biosorbent for removing EBT dye from contaminated waters.

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Abstract

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Lignocelulosic Waste Lemon Peel Enrolled as a Biosorbent for the Emerging Contaminant (Aspirin) Removal

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Abstract: An extremely high consumpted drug, aspirin, can often be found in surface/sewage/waste waters since it is partially metabolized within both animals and human's organism. Recently, many traditional methods have been applied to mitigate the pharmaceutical's health harmful effects through its removal from water, but certain green methods such as using of biosorbents have important role to sustainable chemistry. Therefore, the main objective of this research was to develop a new, efficient and cheap biosorption process for the removal of aspirin from aqueous solutions using lignocellulosic material (lemon peel). In the experimental study, the effect of pH, biosorbent dose, contact time and initial aspirin concentration were considered followed by aspirin quantification by ultraviolet-visible spectrophotometry.

The results obtained from the experimental analyses showed that the removal of aspirin on the surface lemon peel biosorbent (1g) under pH 4 is relatively fast (60 min), eco-friendly with high yield (Removal efficiency 91.50%) treatment. Obtained adsorption capacity was 3.10 mg/g for 40 mg/L aspirin content in water. This study demonstrates the feasibility of lemon peel biosorbent in removing aspirin from aqueous solution, therefore the potential of such adsorbent in treatment of different effluents (municipal, hospital and pharmaceutical) should be investigated in further studies.

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Abstract

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Enhancing Pyrophyllite Adsorption Capabilities Via Sonic Treatment

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Abstract: Adsorption, a highly efficient water purification method and tool for pollution control, utilizes materials like clay. Compared to other commercial adsorbents, clay offers notable advantages including affordability, large specific surface area, accessibility, high ion exchange capacity, excellent adsorption properties, and non-toxicity. Pyrophyllite, among abundant natural clays, stands out due to its layered structure without interlayer cations or water molecules, offering favorable physical and chemical attributes.

This study specifically examines the characterization of natural pyrophyllite ore treated with ultrasonic waves for 30 minutes and 6h. Analysis of samples using X-ray diffraction (XRD) technique indicates the removal of hard phases such as quartz and calcite from both treated samples in comparison to the raw ore. Energy dispersive X-ray spectroscopy (EDS) analysis, conducted as part of SEM-EDS analysis, revealed a significant reduction in the weight % of silicon. Specifically, the Si content decreased from 35.1 weight % in the raw ore to 28.7 after half an hour of treatment. Subsequently, after 6 hours, the most effective purification was achieved, with the Si content reaching only 18.6 weight %.

Furthermore, UV-VIS analysis testing the sorption of a methylene blue solution in water reveals that ultrasonically treated pyrophyllite for 30 minutes achieves 97% efficiency after 24 hours, surpassing the 89% efficiency of the raw ore. Notably, after 6 hours of ultrasonic treatment, efficiency reaches nearly 98% after just 1 hour, confirming high efficacy of ultrasonic treatment on adsorption ability of pyrophyllite.

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Abstract

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Forced Degradation Study of Sofosbuvir

Miloloža, M. *, Tomić, F., Martinjak, V., Bule Možar, K., Furač, L., Markić, M., Kučić Grgić, D., Cvetnić, M., Bolanča, T., Ukić, Š.

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Abstract: In recent decades, the so-called "new pollutants" have become increasingly important in scientific research and environmental protection. One of these is sofosbuvir, an antiviral drug that has been increasingly used during the COVID-19 pandemic to treat people infected with the SARS-CoV-2 virus. Unfortunately, this led to an increased release of sofosbuvir into the environment.

In this work, a forced degradation study of sofosbuvir was conducted to get an idea of its fate in the environment, especially in the aquatic medium. The behavior and stability of a 0.1 mM solution of sofosbuvir was tested by forced degradation experiments: a) alkaline hydrolysis, b) acid hydrolysis, c) oxidation, d) thermal degradation, and e) photolytic degradation. The samples were analyzed using HPLC, for which the analytical method had to be developed and validated beforehand. The developed method showed good linearity with a coefficient of determination of more than 0.99, high accuracy with analytical recoveries between 70 and 130% and acceptable precision with RSD values of less than 10%. In the forced degradation study, sofosbuvir was found to be stable under most conditions tested, suggesting that sofosbuvir has a low tendency to degrade easily and accordingly has the potential to be highly persistent in the aquatic environment. This emphasizes the danger of the presence of sofosbuvir in the environment and the need for detailed investigation of its ecotoxicological properties and methods for its efficient removal from the environment.

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Abstract

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Glyphosate Adsorption onto Pyrophyllite: Effects of Aluminum and Zinc Ion Addition

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Abstract: The aim of this research is to examine the adsorption behavior of glyphosate on pyrophyllite spectrophotometrically using the ninhydrin reaction. The investigated conditions included changes in pH values over time intervals of 60, 120, and 180 minutes, along with the addition of Al(III) and Zn(II) ions. The research results are presented in terms of adsorption capacity (q_e), removal efficiency (R), distribution coefficient (K_d), and recovery. The study was conducted in a slightly acidic to basic environment, with pH ranging from 6, 8, 9, 10, to 11, wherein the best results were obtained in a basic medium at pH 8. Comparing the removal efficiency results (R%) of glyphosate with and without the presence of Al ions, it is evident that at pH 8, the removal efficiency increases in the presence of Al and ranges from 46.52% to 76.69% across all contact times. The removal efficiency without the presence of Al ranges from 8.35% to 23.40%. Regarding the results with Zn, the removal efficiency (R%) of glyphosate with and without the presence of Zn ions shows that at pH 8, the removal efficiency increases in the presence of Zn and ranges from 77.65% to 85.49% across all contact times. The removal efficiency without the presence of Zn ranges from 8.35% to 23.40%. Based on the recovery data, it can be observed that the amount of metal adsorption depends on time and follows an increasing trend as the contact time prolongs, especially with aluminum. Throughout the entire study, it has been proven that a basic environment is more suitable for the adsorption of glyphosate on pyrophyllite, especially at pH 8 and a contact time of 120 minutes in the presence of Al and Zn ions. Without the presence of these ions, adsorption is best at pH 12-13.

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Abstract

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The Influence of the Addition of Copper and Iron Ions on the Adsorption of Glyphosate on Pyrophyllite

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Abstract: Glyphosate (GLY) is a non-selective herbicide whose main function is to interfere with the synthesis of essential secondary metabolites in plants and microorganisms. The effect of herbicides is less harmful weeds but also less nutrients in our food. GLY molecules stably bind to metals in the soil, impoverishing it for future planting. Today, adsorption is being researched as a very economical and efficient method for eliminating herbicides from the environment, with the basic principle of binding herbicide molecules to the surface of the adsorbent. In this research, pyrophyllite (PRL) was used as an adsorbent due to its good ability to remove harmful components. The quantification of GLY before and after adsorption was determined spectrophotometrically using the ninhydrin reaction, as was the quantification of Cu and Fe ions using the FAAS method. The efficiency of GLY removal in the presence of Cu ions was best demonstrated in the basic medium (pH 11; R = 43.67%). Data for the Langmuir and Freundlich adsorption isotherms show that the Freundlich isotherm better describes the adsorption process. The data also indicate an unfavored chemical type of adsorption. The efficiency of GLY removal from an aqueous solution in the presence of Fe ions is at pH = 6 (27.80%). This pH is also the normal pH in the presence of GLY and PRL. It is also seen that at pH 11, there is constant maintenance of GLY removal at all concentrations and contact times (R = 11.07%, 15.27%, 7.44% (60'); R = 10.29%, 15.36%, 7.28% (120'); R = 12.01%, 14.80%, 6.66% (180')). When Fe ions are present, the data show that the Langmuir isotherm better describes the adsorption process. It is also evident from the obtained results that there is a non-faorized and physical type of adsorption. Kinetic data show that the adsorption reaction of GLY on PRL takes place with pseudo-second-order kinetics in the presence of Cu and Fe ions.

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Abstract

PP-ENC-14

Pyrophyllite as a Sustainable Material for Purification of Mine-Waste Water

Trtić-Petrović, T.[a], Lazarević, D.[a], Jovanović, J.[a], Šaraba, V.[a], Kurtanović, E.[b], Marković, I. [b], Harbinja, M.[b]

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Abstract: Wastewater from mines poses a significant problem as it often contains high concentrations of metals, which are discharged into river systems, thereby contributing to environmental pollution. Pyrophyllite is a natural hydrous aluminum silicate clay mineral ($Al_2Si_4(OH)_{10}(OH)_2$) with a high melting point, stable chemical properties, and low cost. The elementary sheet of pyrophyllite is composed of an aluminum-oxygen/hydroxyl octahedral layer between two tetrahedral layers of silicon-oxygen. The layered silicate structure of pyrophyllite crystals has natural adsorption activity. Mechanochemical activation (MCA) is a simple method for modification of solid materials that causes structural disorder, amorphization and increased chemical reactivity. MCA, usually performed by grinding, is an environmentally friendly process because of low energy consumption, processing temperatures and cost. This study investigates the adsorption kinetics of the divalent metal ions (Cd, Ni, Cu, Zn, and Pb) from aqueous solutions using pyrophyllite as an adsorbent. It was found that the removal depends on the mechanochemical treatment of pyrophyllite, contact time with the aqueous solution, and the mutual competition of ions. The conditions were optimized for maximum removal of metal ions from synthesized aqueous solutions. Subsequently, pyrophyllite was applied under optimal conditions for removing Zn (II) from the wastewater of the closed Red Hill mine on mountain Avala. Based on the obtained results, it can be concluded that pyrophyllite completely removes zinc from mine water in a very short time (10 minutes) and thus has great potential for application.

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Abstract

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Microplastic Pollution in Skadar Lake, National Park of Montenegro

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Abstract: Pollution of aquatic ecosystems with microplastics (particles of 0.1-5.0 mm in size) is of great concern to the scientific community, due to the unfathomable consequences for the entire biodiversity, ecosystems and humans. In this study, a preliminary investigation of microplastic pollution was performed in the coastal sediments of the Skadar Lake, National Park of Montenegro. Skadar Lake is the largest lake on the Balkan peninsula. About 65% of the surface of Skadar Lake belongs to Montenegro, and 35% to Albania. Skadar Lake is an area of regional importance and was declared a National park of Montenegro in 1983. The quality and pollution of lake are equally affected by anthropogenic activities in Montenegro and Albania. Microplastics were identified in all examined samples of coastal sediment from the Skadar Lake, during the autumn of 2022. In the coastal sediments of the Skadar lake the most commonly identified microplastic shape type was fibers, size 1–3 mm and blue color. Fourier transform infrared spectrometry (FTIR) was used to identify types of polymers in the coastal sediments of the Skadar Lake, of which polypropylene and polyethylene were the main identified polymers. The results of the study indicate that microplastics of different polymer composition are present in the coastal sediment of the Skadar Lake, which can have a significant impact on aquatic habitats, the food chain and human health.

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Abstract

PP-ENC-16

Desorption of Metals from Pyrophyllite and use as a Sustainable Construction Material

Lazarević, D.[a], Jovanović, J.[a], Šaraba, V.[a] , Trtić-Petrović, T.[a], Kurtanović, E.[b], Marković, I.[b], Harbinja, M.[b]

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Pyrophyllite
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Abstract: Developing efficient water purification technologies is critical due to the limits of present approaches and the enormous environmental and human health dangers posed by polluted water. Pyrophyllite is a natural mineral composed of aluminum and silicate hydroxides ($Al_2Si_4O_{10}(OH)_2$) with a high cation exchange capacity and affinity for metals from water. This study aimed to investigate the adsorption and desorption of metals from pyrophyllite in aqueous solutions as a potential solution for this problem of contamination. The concentration of metal ions in water was quantified by anodic stripping voltammetry. The row natural pyrophyllite used in experiments was obtained from the deposits "Parsovići" - Konjic (AD HARBI d.o.o., Sarajevo, Bosnia and Herzegovina). Pyrophyllite (granulation 0.045) adsorbed > 98% Pb(II) from the aqueous solution after only 10 min of contact and Cd(II) reached the maximum of 95% after 24 h. The findings of our studies have shown that the desorption of metals was higher in the solution that was shaken compared to the stationary one. Our results proved that ions of Pb(II) can be desorbed under shaking conditions after 48h about 26%, and Cd(II) at the same conditions desorbed at 44%. The desorbed pyrophyllite can be consolidated into building materials using processes such as cementitious solidification or polymer encapsulation. By adding pyrophyllite to building materials, the pollutants held inside the Pyrophyllite are successfully contained, limiting the release into the environment. This technique turns polluted pyrophyllite into ecologically beneficial construction materials, ideal for diverse infrastructure projects.

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POSTER PRESENTATIONS

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Abstract

PP-IC-01

Crystallographic Evidence of Oxidative Dehydrogenation in Copper(II) Complexes of Schiff Bases Derived from Salicylaldehyde and 8-Aminoquinoline: Synthesis, Characterization, and Antimicrobial Activity

Zahirović, A.[a,*], Fetahović, S.[a], Višnjevac, A.[b], Žilić, D.[b], Bešta-Gajević, R.[c], Dahija, S.[c], Roca, S.[b]

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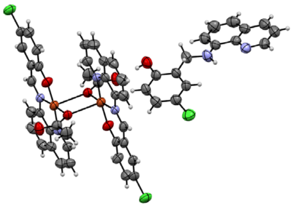

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Abstract: The reaction between copper(II) acetate and reduced Schiff base ligands derived from salicylaldehyde and its 5-chloro- and 5-bromo-substituted derivatives and 8-aminoquinoline was investigated. The reaction led to the oxidative dehydrogenation of secondary amines and the coordination of corresponding Schiff base ligands to copper(II), resulting in the formation of three novel copper(II) complexes. Additionally, a co-crystal of copper(II) complex featuring the 5-chloro moiety with the corresponding secondary amine ligand was isolated, indicating non-catalytic stoichiometric oxidative dehydrogenation. The complexes were characterized by elemental analysis, infrared, electron, and EPR spectroscopies, conductometry, and single-crystal X-ray diffraction. Detailed characterization of the secondary amines and corresponding Schiff bases was achieved using 1D and 2D NMR spectroscopy. The isolated compounds are neutral binuclear complexes featuring paramagnetic copper(II) centers embedded in a square-pyramidal environment and coordinated with di-μ-acetato-κ*O*:κ*O* bridging ligand and tridentate monobasic ONN donor Schiff base. Geometry optimization and quantum chemical reactivity parameters were calculated using DFT, and Hirshfeld surface analysis was performed. The complexes and ligands exhibited promising antimicrobial activity against several strains of Gram-positive and Gram-negative bacteria and the yeast *Candida albicans*.

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Abstract

PP-IC-02

The Two-Dimensional Heterometallic Sodium-Palladium(II) Coordination Networks with Differently Substituted Nicotinate Ligands

Politeo, N.[a], **Kodrin, I.**[b], **Rodríguez, M.**[c], **Soldin, Ž.**[b], **Rončević, T.**[d], **Čikeš Čulić, V.**[e], **Sokol, V.**[a], **Doctorovich, F.**[c], **Kukovec, B.-M.**[a,*]

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6-Fluoronicotinate
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Abstract: Heterometallic coordination polymers contain different metal ions in a single framework, leading to enhanced properties, functionalities and new applications. Previously, we have prepared the 2D heterometallic sodium-palladium(II) coordination polymers with 2-halonicotinates (2-chloro- or 2-bromopyridine-3-carboxylate) in aqueous solutions in the presence of $NaHCO_3$. We have now prepared the 2D heterometallic sodium–palladium(II) coordination polymers with 2-methylnicotinate (2-Menic) and 6-fluoronicotinate (6-Fnic), $\{[Na_2(H_2O)_2(\mu\text{-}H_2O)_4PdCl_2(\mu\text{-2-Menic-}N{:}O')_2]\cdot 2H_2O\}_n$ (**1**) and $\{[Na_2(H_2O)_2(\mu\text{-}H_2O)_4PdCl_2(\mu\text{-2-Fnic-}N{:}O')_2]\cdot 2H_2O\}_n$ (**2**), respectively, by using a similar experimental procedure. The crystal structures of **1** and **2** were determined by single crystal X-ray structural analysis. The 2-methylnicotinate and 6-fluoronicotinate ions are engaged as *N:O′*-bridging ligands between the adjacent palladium(II) and sodium ions. The resulting $[PdCl_2(2\text{-Menic})_2]^{2-}$ (in **1**) or $[PdCl_2(6\text{-Fnic})_2]^{2-}$ (in **2**) moieties and sodium ions are the main building units. The water-bridged sodium ions are connected into a zigzag chain and these symmetry-related chains are bridged by $[PdCl_2(2\text{-Menic})_2]^{2-}$ moieties in **1** or by $[PdCl_2(6\text{-Fnic})_2]^{2-}$ moieties in **2**, resulting in the formation of the infinite 2D coordination networks of **1** and **2** (**Figure 1**). The compounds **1** and **2** were also characterized by IR spectroscopy, PXRD and TGA/DSC methods. The experimental findings were correlated and explained by DFT calculations. The compounds exhibited no antibacterial and no antitumor activity *in vitro*. *Escherichia coli* and *Staphylococcus aureus* bacteria and bladder (T24) and lung (A549) cancer cell lines were used in these studies.

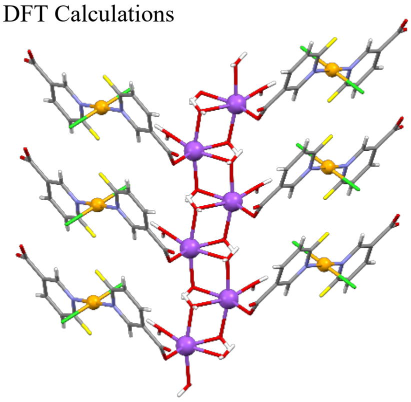

Figure 1. The sodium-palladium(II) coordination network of **2**

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Abstract

PP-IC-03

Functional Iron-Sulfur Clusters: Model Studies Using Synthetic Analogues

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Proton-Coupled Electron Transfer

Abstract: Iron-sulfur clusters are amongst the most prevalent biological cofactors found in living organisms across all kingdoms of life. As such, they have been a focal point of research in bioinorganic chemistry. An increasing number of them is found to feature alternative (non-cysteine) ligation. To understand and emulate the intricate functions of these metal containing sites, a variety of synthetic analogues have been synthesized over the past years. Herein we report the synthesis and characterization of proton-responsive clusters with alternative N-donor ligation, which were further evaluated for their reactivity towards biologically relevant reactive species.

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Abstract

PP-IC-04

Heterometallic Bridged Pt(II)-Zn(II) Complexes: Influence of the Substituent In 4´-Position in Inert Terpy Ligand on Mechanism of Interactions of the Complexes with Biomolecules

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Heteronuclear Complexes
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Terpy-Cl Ligand

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Abstract: Platinum complexes have significant applications in medicine. However, patients often experience a large number of side effects when taking these drugs. While they exhibit rapid efficacy, they also demonstrate toxicity, and resistance commonly develops. One approach to mitigate these unwanted effects is through the synthesis of heteronuclear complexes. In addition to platinum(II), these heteronuclear complexes incorporate another metal that naturally occurs in the human body. The novel heteronuclear complexes [{*cis*-PtCl(NH$_3$)(*μ*-4,4´-bipyridyl)ZnCl(terpy-Cl)}] (ClO$_4$)$_2$, [{*cis*-PtCl(NH$_3$)(*μ*-pyrazine)ZnCl(terpy-Cl)}(ClO$_4$)$_2$, [{*trans*-PtCl(NH$_3$)(*μ*-4,4´-bipyridyl)ZnCl(terpy-Cl)}](ClO$_4$)$_2$ and [{*trans*-PtCl(NH$_3$)(*μ*-pyrazine)ZnCl(terpy-Cl)}](ClO$_4$)$_2$, (where terpy-Cl = 4´-cloro-2,2′:6′,2″-terpyridine) were synthesized and characterized.

The stability and interaction of heteronuclear complexes with biologically relevant molecules 5´-GMP and GSH were investigated spectroscopically. It was shown that chloride in 4´ position of 2,2´:6´, 2´´-terpyridine has great influence on the stability of complexes. The decrease of electrophilicity of metal centers leads to the higher p*K*a values and to moderate stability of the complexes at physiological conditions. In the case of all complexes the decomposition was noticed. These complexes without strong independent cytotoxicity can be a starting point in further research in combined treatments with the aim to reduce side effects.

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Abstract

PP-IC-05

A New Polymeric Adduct of Copper(II) Formate with Pyridine

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Abstract: A new polymeric adduct of copper(II) formate and pyridine has been synthesized and characterized using single-crystal X-ray diffraction, ESR and IR spectroscopy. The adduct crystallizes in the orthorhombic space group P*nma* with lattice parameters a = 9.7350(2) Å, b = 14.3863(3) Å, c = 10.2885(2) Å, and Z = 8. The crystal structure reveals two coordination modes of the formate ion: *syn*-monodentate and *syn-anti* bridging. The copper(II) ions exhibit a distorted square pyramidal coordination geometry, with the equatorial positions occupied by two alternating oxygen atoms from formate ions and two nitrogen atoms from pyridine rings. The axial position is occupied by an oxygen atom from the bridging formate ion, which is at a longer distance [2.313 Å] compared to the Cu(II)-oxygen distances [1.952 Å, 1.972 Å] in the equatorial plane. The compound exhibits antiparallel zig-zag chains without crosslinking hydrogen bonds from co-crystallized water molecules. Instead, the water molecules form hydrogen bonds between the terminal oxygen of the unidentate formate and the bridging formate oxygen in the equatorial plane. The IR spectra match crystallographic data, displaying notable shifts in C–H wagging and ring bending vibrations indicative of coordinated pyridine, and broadening in the symmetric and asymmetric C-O stretching regions due to various formate ion coordination modes. Additionally, X-band ESR reveals rhombic spectra (gx ≠ gy ≠ gz) for paramagnetic d^9 Cu(II) ions, without any hyperfine interaction detected.

Acknowledgment

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Abstract

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Glassy Black/Brown Crystals from Various Cu(I) Complexes with Azopyridine Ligand

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Coordination Polymers
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Azopyridine
Mixed-Ligand

Abstract: Novel mixed-ligand Cu(I) coordination polymers have been investigated by using Cu(I) precursors reacting with pyrazolate, diphosphine and azopyridine ligands. Glassy black/brown single crystals were formed. The single crystal X-ray diffraction analysis shows extended chains of conjugated units due to the “back-to-back” bridging ligands. The presentation shows the crystal structure and the spectral properties of the black complexes capable of absorbing solar radiation within the entire visible region and most of the near-infrared (NIR) portion (~200-900nm). In addition, the presentation will exhibit the effect of varying the ligand substituents on the crystal structures of the resulting products.

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Abstract
PP-IC-07

Molecular and Crystal Structure of the Tetrakis(4-Methyl-1H-Pyrazole)-bis(acetato)Nickel(II)

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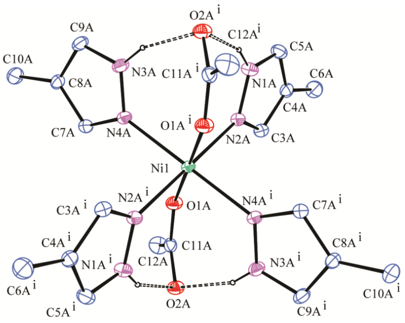
Abstract: Ligands with multiple coordination sites are often used in the synthesis of the extended metallo-organic structures. Both pyrazolyl and acetato ligands can have a role of a "bridge" between the metallo-organic fragments. As a part of the study of the coordination capabilities of pyrazole-based ligands we are reporting the molecular and crystal structure of the tetrakis(4-methyl-1H-pyrazole)-bis(acetato)Nickel(II). The asymmetric unit contains two halves of the title molecule with nickel (II) ions sitting on inversion centers. Four 4-methyl-pyrazole and two acetato ligands are coordinated to Ni (II) in a distorted octahedral geometry. Deviations from ideal octahedral geometry are associated with acetato ligands involved in intramolecular hydrogen bonds.



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Abstract

PP-IC-08

Interaction of Vanadium(IV) Thiosemicarbazonato Complexes with BSA and CT DNA

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Abstract: The interaction of a vanadium(IV) complex [VO(phen)L], where L is a ligand derived from 5'-fluoroacetophenone and 4-methylthiosemicarbazide, with BSA and CT DNA was investigated using spectroscopic methods. Spectrofluorimetric analysis of the interaction of the complex with BSA revealed significant fluorescence quenching, indicating a notable conformational change in the protein upon binding with the complex. The data suggest a static quenching mechanism, where the complex forms a stable adduct with BSA in the ground state. The value of the binding constant calculated indicates moderate binding strength and excludes irreversible binding at the target site. FRET analysis confirms nonradiative energy transfer between the donor and the acceptor. The interaction of the ligand and complex with CT DNA was studied using electronic spectroscopy and spectrophotometric titration methods. The binding constants of the same order of magnitude suggest a moderate affinity of both the ligand and the complex for DNA. Notably, no significant shift in the absorption bands, which would indicate intercalation, was observed. The results suggest groove binding as the likely mode of interaction. These preliminary findings encourage further investigation of the complex as a biologically active substance.

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Abstract

PP-IC-09

Catecholase-like Activity of Heteroleptic Copper(II) Complexes with Schiff Base and Flavonol/Chalcone Coligands

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Abstract: The investigation into the catecholase-like activity of copper complexes aims to develop functional models that mimic natural catechol oxidases, with the goal of creating robust catalysts for quinone production, as the operational versatility of native catecholases is limited for broader application due to their sensitive dependence on specific pH and temperature conditions. The catalytic activity of four neutral heteroleptic copper(II) complexes was studied using spectrophotometry. Each complex features copper(II) coordinated by a Schiff base ligand derived from 2-aminophenol and benzaldehyde or terephthalaldehyde, with 3-hydroxyflavonol or 2'-hydroxychalcone as coligands. The biomimetic catalytic performance of these complexes was assessed in oxidation reactions of 3,5-di-tert-butylcatechol (DTBC) using hydrogen peroxide as a co-oxidant in methanol. The kinetic of DTBC oxidation catalyzed by copper(II) complexes was analyzed spectrophotometrically under pseudo-first order conditions. Catalytic parameters including maximum reaction rate, Michaelis-Menten constant, catalytic reaction rate constant, catalytic efficiency, turnover number, and turnover frequencies were calculated. Results demonstrate that all complexes exhibited catalytic activity, with copper(II) complexes incorporating flavonol ligands showing superior catalytic efficiency, as evidenced by higher catalytic reaction constants.

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Abstract

PP-IC-10

Unveiling Iodo Analogs: Novel Tricarbonylrhenium(I) Complexes with Diimine Ligands

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Abstract: Tricarbonylrhenium(I) complexes with diimine ligands have recently seen increased structural diversity and varied applications. Among the halogen derivatives featuring the tricarbonylrhenium(I) motif, iodo analogs are the least studied. Here, we present the synthesis and characterization of two novel tricarbonylrhenium(I) diimine complexes. The diimine ligands, bipyridines, are obtained in good yield from known 2'-hydroxychalcones via the Kröhnke pyridine synthesis. The complexes are synthesized almost quantitatively and with high purity by briefly refluxing equimolar amounts of $ReI(CO)_5$ and the bipyridine in dry toluene under argon. Characterization of the ligands and complexes was performed using ESI-ToF mass spectrometry, IR spectroscopy, and elemental analyses. The mass spectra of the complexes showed molecular ion peaks of $[M - H]^-$ at m/z 748.9716 and 778.9821, confirming the molecular weights of $[C_{26}H_{17}IN_2O_5Re]^-$ (748.9717) and $[C_{27}H_{19}IN_2O_6Re]^-$ (778.9823), respectively. The IR spectra display three distinct bands in the carbonyl stretching region, with symmetric stretching bands around 2020 cm^{-1} and asymmetric bands around 1925 cm^{-1} and 1880 cm^{-1}, consistent with a fac-isomer arrangement of the three CO ligands on the rhenium center. The phenolic group bands in the ligands and their complexes remain largely unchanged in position relative to each other, indicating that the ligand coordinates to the rhenium center not as a phenolate, but rather as an N, N-donor.

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Abstract

PP-IC-11

Rhenium Complexes with Benzodioxole-Containing Bipyridine Ligand: Synthesis and Analysis

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Abstract: Benzodioxole-containing compounds exhibit significant bioactivity and favorable structure-activity relationships due to the electron-rich benzodioxole ring, enhancing molecular interactions and efficacy in various biological applications. Despite these advantages, the utilization of benzodioxole-containing compounds as ligands in metal complexes is rarely observed. In this study, we present the synthesis and characterization of a novel bipyridine ligand containing benzodioxole. The ligand was synthesized by condensing equimolar quantities of 3,4-(methylenedioxy)-2'-hydroxychalcone and pyridacylpyridinium iodide via the Kröhnke reaction. Subsequently, two tricarbonylrhenium(I) complexes were derived from this ligand using $ReBr(CO)_5$ or $ReI(CO)_5$, resulting in both compounds being obtained in analytically pure form with a yield exceeding 95% in a one-pot synthesis. Characterization involved ESI-ToF mass spectrometry, IR spectroscopy, and elemental analyses. IR spectra revealed distinctive patterns in the carbonyl stretching region, with symmetrical stretching bands at ~2020 cm^{-1} and asymmetrical bands at ~1915 cm^{-1} and ~1890 cm^{-1}, suggesting a fac-isomer configuration of the three CO ligands surrounding the rhenium center. Additionally, both the ligand and the complexes exhibited a characteristic stretching band of the benzodioxole methylene group at ~2890 cm^{-1}. The positions of the phenolic group bands in the ligand and its derivatives showed minimal variation, suggesting coordination with the rhenium center as an N, N-donor rather than a phenolate. The mass spectra of the complexes exhibited molecular ion peaks of $[M - H]^-$ at m/z 714.9651 and 762.9510, confirming molecular weights of $[C_{26}H_{15}BrN_2O_6Re]^-$ (714.9643) and $[C_{26}H_{15}IN_2O_6Re]^-$ (762.9505), respectively, while the ligand displayed a peak at 367.1080, confirming the molecular ion as $[C_{23}H_{15}N_2O_3]^-$ (367.1088).

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Abstract

PP-IC-12

Synthesis and Characterization of Zinc(II) Complexes with Selected Amino Acids

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Abstract: Considering zinc's role as a biogenic element, primarily operating within coordination compounds alongside biomolecules, particularly amino acid residues within peptides or proteins acting as heteroatom donors, it's crucial to assess zinc's coordination behavior with individual proteinogenic amino acids.

In this paper, the reaction of zinc (II) hydroxide with L-alanine and L-histidine, separately, and the reaction of zinc (II) chloride and L-tryptophan in aqueous solution were examined. The reaction products of the subjects were determined by FT-IR and UV-VIS spectroscopy to differentiate the products of reaction from, in the literature, previously described amino acids as reactants.

UV-VIS absorption spectra of three separate amino acids and possible formed complexes of those amino acids with zinc (II) were recorded and compared. Notable discrepancies in FT-IR spectra of potential complexes must be noted, differing from literature descriptions of individual amino acids.

"Rocking" or "wagging" vibrations of the amino group in the spectrum of Zn-alanine complex occur at 1150 cm^{-1} and 1020 cm^{-1}, respectively. It is also necessary to mention the band of possible coordination of N-atoms with Zn, which occurs at 472 cm^{-1}. The amino group of the aliphatic chain in the spectrum of the Zn-histidine complex gives a band of symmetrical "scissoring" deformation at about 1625 cm^{-1}. The spectrum of the Cu-tryptophan complex shows a band at 3420 cm^{-1}, which corresponds to the vibration of the N – H bond of indole, and this fact is related to possible coordination through the indole ring.

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Abstract

PP-IC-13

Synthesis and Structure–Antihyperglycemic Activity Relationship in Vanadium(IV) Complexes of Acetophenone Isoniazid Hydrazones

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Abstract: Four novel heteroleptic neutral paramagnetic mononuclear vanadium(IV) complexes, denoted as [VOL(phen)], where L represents acetophenone isoniazid hydrazone and its 5-halogenated derivatives, were synthesized and characterized using chemical analysis, spectroscopy, and diffraction methods. The molecular and crystal structures of the vanadium complex with 5-bromoacetophenone isoniazid hydrazone were determined by single-crystal X-ray diffraction, revealing an octahedrally coordinated vanadium(IV) center with tridentate ONO donor hydrazone in its deprotonated enol-imine form, 1,10-phenanthroline, and one terminal oxygen. The interaction of these complexes with bovine serum albumin (BSA) was investigated by spectrofluorimetric titration, yielding binding constants in the order of 10^4 M^{-1}. Thermodynamic data suggest that moderately strong binding to BSA is driven by hydrophobic interactions and van der Waals forces, without involving irreversible processes. The antihyperglycemic effects of aroylhydrazonato vanadium(IV) complexes were investigated in streptozotocin-induced diabetic rats. All four complexes demonstrated significant *in vivo* antidiabetic activity, reducing hyperglycemia after one week of treatment. Notably, the complex with 5-bromoacetophenone isoniazid hydrazone was most effective in lowering blood glucose levels to normoglycemic status without causing hypoglycemia.

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Abstract

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Antibiotic Sensitivity of *Acinetobacter baumannii* to H_2S

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Abstract: Antimicrobial resistance is increasing and represents a major threat to public health. Endogenous hydrogen sulfide (H_2S) production has been shown to cause antibiotic resistance in all bacteria studied so far. Assuming that all bacteria produce endogenous H_2S, it represents a universal defense mechanism against antibiotics in bacteria. In this study we tested the effect of exogenous H_2S on antibiotic tolerance in a bacterium that does not produce it. We also showed that exogenous H_2S sensitized *A. baumannii* to several antibiotic classes, rather than inducing antibiotic tolerance In this research we treated two strains of *A. baumannii* with different concentrations of Na_2S. We found that higher concentrations of 1M and 0,1M Na_2S were lethal for both strains. Lower concentrations of Na_2S (80µM and 160µM), stimulate the sensitivity of already sensitive antibiotics, while in resistant ones, it slightly increases the growth inhibition zone around the antibiotic discs. Na_2S is a toxic substance, and at a concentration that has been shown to be lethal for colonies of *A. baumannii*, it is not suitable for use in human medicine. A higher concentration could be used in cleaning agents and treating surfaces inside hospitals, where this bacterium lingers. A lower, micromolar concentration is possible in human medicine, and further studies are needed to determine which concentration would be effective and sensitize *A. baumannii* to antibiotics.

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Abstract

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DNA and HSA Binding Of Copper(II)-Complexes With Imine-Based Ferrocene Derivatives

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Abstract: Copper, a crucial transition metal ion in biological systems, showcases distinctive redox activities and exhibits strong binding affinity toward nucleobases. In this study, three novel copper(II) complexes were synthesized and characterized, employing imine-based ferrocene derivatives as ligands. Characterization was achieved through MS and UV spectrophotometry, followed by an examination of the complexes' reactivity towards biomolecules. Specifically, the interaction of these complexes with CT-DNA and human serum albumin (HSA) were investigated. The findings demonstrate good CT-DNA and HSA interaction ability of the studied complexes.

These results underscore the potential of incorporating imine-based ferrocene derivatives as ligands to enhance the stability and reactivity of copper(II) complexes. This research contributes to expanding the understanding of metal-ligand interactions in biological systems and offers insights into the design of novel metal-based therapeutics.

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Abstract

PP-MC-03

Analysis of Kidney Stones

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Abstract: Urolithiasis is a disease that causes the formation of kidney stones in various organisms, mainly in mammals such as humans, cats, dogs, etc. In recent decades, urolithiasis has been diagnosed with increasing frequency and affects about 10-15% of the population in Western countries. Fast-paced lifestyles have dramatically changed dietary habits, including high protein and salt consumption. High consumption of fructose-rich carbonated beverages is one of the main causes of the increased incidence of calcium oxalate kidney stones, which are now the most commonly diagnosed type of stone. Although kidney stones consist mainly of calcium oxalate, many usually contain less or more phosphate. Stones composed of calcium oxalate may include whewellite (calcium oxalate monohydrate) and weddellite (calcium oxalate dihydrate), and a small percentage of stones are also composed of magnesium ammonium phosphate, uric acid or cystine.

Stone analysis is an important part of evaluating and further treating patients with stones. X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR) are currently used to analyze stones. They identify each component and provide a qualitative and semi-quantitative assessment of stone composition. In this study, an analysis of several kidney stones collected from patients after surgical treatment was performed. Using three analytical methods (FTIR, XRD, TGA-DSC), the results showed that oxalate stones (whewellite and weddellite) were the most common, but phosphate stones were also present.

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Abstract

PP-MC-04

Comparison of the Diagnostic Significance of Lipid Parameters and Lipid Ratios in Subjects with T2 DM

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Abstract: Early detection and treatment of dyslipidemia in individuals with T2DM is significant to prevent or slow the progression of lipid abnormalities and reduce the risk of cardiovascular diseases. Attention is directed towards lipid ratios (logTG/HDL (AIP), TC/HDL (CRI-I), LDL/HDL (CRI-II)) as predictors of both T2DM and cardiovascular complications. The aim of the study is to explore the diagnostic significance of lipid parameters (TC, TG, LDL, and non-HDL) and lipid ratios as predictive biochemical models in T2DM.The study presents ROC (Receiver Operating Characteristic Curve) analysis to determine the threshold values and discriminatory ability of lipid parameter biomarkers compared to lipid ratios. A case-control study was conducted in a group of n = 44 subjects with T2DM and n = 30 control subjects.

ROC analysis of lipid ratios showed greater discriminatory power (AUC > 0.8; $P < 0.001$) compared to individual lipid parameters (AUC > 0.7; $P < 0.001$). The ratio of TC/HDL had the highest discriminatory power and sensitivity at a threshold value of >1.7 (AUC=0.849; sensitivity 88.64%; specificity 66.67%), while the ratio of LDL/HDL had the highest specificity (90%) and sensitivity (65.91%) for a threshold value of >2.87. The results indicate that lipid ratios have greater diagnostic significance compared to lipid parameters and can be used as predictive models for T2DM, and therefore, it would be beneficial to include them in diagnostic practice, especially in individuals with a genetic predisposition for T2DM and in a prediabetic state.

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Abstract
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Heterobinuclearity *vs.* Homobinuclearity in Ruthenium(II) and Gold(I) Organometallics with Diphosphine Ligands: Synthesis, Characterization, BSA Binding, and *In Vivo* Toxicity

Zahirović, A.[a,*], Roca, S.[b], Fočak, M.[c], Fetahović, S.[a], Višnjevac, A.[b], Topčagić, A.[a], Suljević, D.[c], Mitrašinović-Brulić, M.[c], Ostojić, J.[a], Muzika, V.[d]

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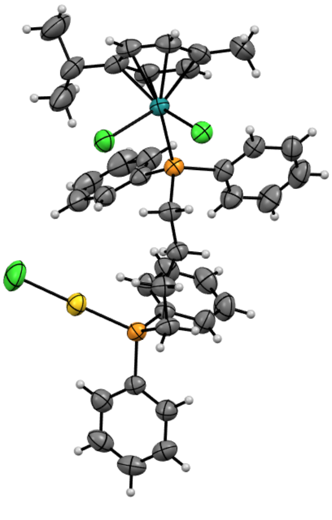
Pathohistology



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Abstract: Solution synthesis yielded two new heterobinuclear ruthenium(II)-gold(I) organometallics featuring bridging bis(diphenylphosphino)alkane ligands, with either butane (**AuRu1**) or pentane (**AuRu2**) as bridges. Additionally, a homobinuclear ruthenium(II) complex (**Ru2**) with a bis(diphenylphospino)pentane ligand was prepared. Furthermore, two homobinuclear gold(I) complexes with the same ligands (**Au1** and **Au2**), as well as a homobinuclear ruthenium(II) complex (**Ru1**) with a bis(diphenylphospino)butane ligand, were synthesized using the described procedures. Complexes were characterized by elemental analysis, infrared and electronic spectroscopy, as well as 1D and 2D NMR spectroscopy. The crystal structure of **AuRu1** was determined using single-crystal X-ray diffraction. In heterobimetallic ruthenium-gold and homobimetallic ruthenium complexes the metals are bridged by diphosphine ligands in μ-ligand-κ*P*:κ*P*' fashion, while homobimetallic gold complexes show di-μ-ligand-κ*P*:κ*P*' bridging. Ruthenium complexes feature coordination with ^{6}η-cymene and two chlorido ligands, while gold(I) exhibit additional coordination with chlorido ligands. Quantum chemical calculations using DFT and Hirshfeld surface analysis of **AuRu1** were performed. Hydrolytic behavior under physiological conditions was explored *via* electron spectroscopy. The investigation of complex interactions with BSA employed spectrofluorimetric titration, synchronous fluorimetry, and FRET analysis, revealing binding constants dependent on the metal center and length of the bridging linker. Molecular docking was utilized to determine binding sites on BSA. The *in vivo* effects of administering the **AuRu1** complex on the biochemical and hematological parameters of healthy Wistar rats, as well as the histopathological findings of the liver, indicate a safe toxicity profile of the heterobimetallic compound, allowing for further testing as a potential thioredoxin reductase inhibitor on Wistar rats with induced colon cancer.

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Abstract

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Docking Study of Antitumor Activity for Some Compounds with Thiazole Ring

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Abstract: Cancer is one of the main causes of death worldwide. Multidrug resistance (MDR) is responsible for over 90% of deaths in cancer patients receiving traditional chemotherapeutics or novel targeted drugs. Rapidly increasing numbers of biomedical studies are focused on designing chemotherapeutics that are able to evade or reverse MDR. Our previous research on xanthenes and coumarins showed that these compounds are good candidates for the development of new antiproliferative agents. In this study, we investigate how the introduction of a thiazole heterocycle affects the inhibition of protein kinase B (PDB: 1GZO). Using the YASARA Structure software for molecular docking, we examined the values of binding energies and dissociation constants for 8 different compounds of acridine, xanthene and coumarin scaffold with a thiazole heterocycle. The binding energy values ranged from -7.22 to -10.73 kcal/mol, and the dissociation constant values ranged from 0.014 to 5.130 mM. Coumarin derivatives with thiazole ring showed to be the best potential inhibitors for protein kinase B. We also tested the inhibitory activity of these derivatives on the human CYP2C9 enzyme (PDB: 4NZ2), where binding energies ranged from -7.54 to -8.88 kcal/mol, and dissociation constants from 0.310 to 2.972 mM. Compounds of the coumarin core with a thiazole heterocycle have shown to be promising candidates capable of inhibiting protein kinase B at very low concentrations and therefore represent a good basis for further *in vitro* studies.

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Abstract

PP-MC-07

In Silico Screening of Antibacterial Activity for Some Compounds with Thiazole Ring

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Abstract: The evolution of new bacterial strains, along with excessive use and reckless consumption of antibiotics have led to the unfolding of antibiotic resistance to an excessive level. Multidrug resistance is a potential threat worldwide, and is escalating at an extremely high rate. Therefore, the discovery and development of new antimicrobial agents is a constant need. Our previous research on coumarins and xanthenes showed that these compounds are good candidates for the development of new antimicrobials. In this study, we investigate how the introduction of a thiazole heterocycle affects the inhibition of bacterial DNA gyrase (PDB: 4DUH). Using the YASARA Structure software for molecular docking, we examined the values of binding energies and dissociation constants for 8 different compounds of acridine, xanthene and coumarin scaffold with a thiazole heterocycle. The binding energy values ranged from -5.41 to -9.53 kcal/mol, and the dissociation constant values ranged from 0.103 to 8.247 mM. Coumarin derivatives with thiazole ring showed to be the best potential inhibitors for bacterial DNA gyrase. We also tested the inhibitory activity of these derivatives on the human CYP3A4 enzyme (PDB: 6UNE), where binding energies ranged from -8.08 to -10.91 kcal/mol, and dissociation constants from 0.01 to 1.195 mM. Compounds of the coumarin core with a thiazole heterocycle emerged as the most promising candidates capable of inhibiting bacterial DNA gyrase at low concentrations and therefore represent a good basis for further *in vitro* studies.

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Abstract

PP-MC-08

Penicixanthene D – a Potent Inhibitor of SARS-CoV-2 Papain-like Protease

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Penicixanthene D
Druglikeness Properties

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Abstract: COVID-19 has transitioned from a pandemic to an endemic phase, but the virus responsible, SARS-CoV-2, continues to spread and pose public health challenges globally. New variants with multiple mutations in their spike proteins are now capable of evading neutralization by antibodies in both vaccinated and recovered individuals. As a result, there is an urgent need to develop broad-spectrum antivirals to address current and future outbreaks. Marine natural products are valuable biomedical resources for creating marine pharmaceuticals, bioactive compounds, and therapeutic agents. Evaluating the antiviral properties of well-known marine natural products can assist in identifying innovative therapies to treat or prevent COVID-19 by screening these compounds against SARS-CoV-2. Using the SeeSAR software for molecular docking, we screened 118 compounds that naturally occur in marine organisms, against the papain-like protease SARS-CoV-2 (PDB: 7TZJ). Compound Penicixanthene D emerged as the most potent inhibitor, with the lower boundary for estimated affinity as low as 0.089 μM and the upper boundary for estimated affinity 9 μM. Optibrium – ADME properties were also calculated for this lead compound, and resulting parameters for 2C9 pKi, 2D6, BBB, HIA, P-gp, PPB90, hERG pIC_{50}, logD, logP, logS, TPSA, Mw, number of rotatable bonds, H-bond acceptors and donors were all within the limits of recommended *druglikeness* properties, predicting good bioavailability after oral administration. All these results position the Penicixanthene D as promising antiviral for further preclinical research.

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Abstract

PP-MC-09

Radiopharmaceuticals in Prostate Cancer Diagnosis

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Ga^{68}-PSMA
Tc^{99m}-PSMA

Abstract: Prostate specific membrane antigen (PSMA) is a protein that can be found in various tissues and organs, such as the prostate, kidneys, small intestine, and salivary glands, but most importantly in prostate cancer, its concentration increases exponentially, allowing for excellent binding of radioisotopes for both therapeutic and diagnostic purposes.

PSMA binding started with Ga^{68}, but Tc^{99m} is the most used radioisotope globally, so the possibility of binding PSMA to it was also explored. Tc^{99m} PSMA-T_4 complex was successfully synthesized in time (less than 10 min), with an exceptional RCP and reasonable radiochemical yield (over 95%). The preparation of Ga^{68}-PSMA-11 requires a specialized module for binding Ga^{68} to PSMA, efficiency is over 95%, but the preparation time exceeds 40 minutes, because the preparation and quality control time is longer than of Tc^{99m} radiopharmaceuticals.

Ga^{68}-PSMA-11 is more used because it has proven to be better at detecting tumor lesions when PSA is less than 2 ng/mL and lesions in the prostatic bed, while being equally effective with Tc^{99m} PSMA-T_4 in detecting bone metastases and lymph nodes. However, Tc^{99m}-PSMA-T_4 is cheaper (about 7 times less expensive).

In essence, both radiopharmaceuticals provide good results in detecting prostate cancer and its metastases. Essentially, it does not matter which variant of the radiopharmaceutical is available; what is important is enabling radio guided surgeries with a gamma probe, which significantly increases the percentage of cancer and lesion removal. And of course, ultimately binding PSMA to Lu^{177}, which gives excellent results in the therapy and treatment of prostate cancer.

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Abstract

PP-MC-10

Antimicrobial Assessment of Ethanol Fruit Extracts from *Prunus spinosa* L.

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Abstract: *Prunus spinosa* L., a plant of the Rosaceae family, also known as sloe or blackthorn, grows as a shrub on the slopes of wild, uncultivated terrain. Fresh fruits were gathered in late fall from three distinct habitats: Trnovo, Vareš, and Borije in Bosnia and Herzegovina. The antimicrobial activity of *n*-hexane, ethanol, diethyl ether, and dichloromethane fruit extracts obtained from the Soxhlet device was the subject of research. For that purpose, in vitro analysis was performed by the agar-well diffusion method against standard bacterial strains: Gram-negative (*Salmonella enterica* ATCC 31194, *Escherichia coli* ATCC 25922, *Pseudomonas aeruginosa* ATCC 9027), Gram-positive (*Staphylococcus aureus* ATCC 25923, *Bacillus subtilis* ATCC 6633, *Enterococcus faecalis* ATCC 29212), and fungus (*Candida albicans* ATCC 1023). Antibiotic streptomycin and antimycotic nystatin were used as positive controls, and four solvents were used as negative controls. It can be noted that all plant extracts exhibited varying degrees of antimicrobial activity against the bacterial strains tested. The best antibacterial efficacy was shown by ethanol fruit extracts from Borije, Trnovo, and Vareš, with inhibition zones of 21.00, 23.50, and 25.00 mm against the gram-positive bacterial strain *S. aureus*, respectively. The sample from Trnovo and Vareš is more potent against this bacterial strain compared to the control sample. Diethyl ether extract from Vareš against *E. faecalis* shows a sensitive inhibition zone (22.00 mm), and it is more potent than streptomycin. The data obtained indicate that there is high antibacterial activity in the blackthorn fruit extracts under investigation.

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Abstract

PP-MC-11

Chemical Composition and Cytotoxic Activity of *Hyssopus officinalis* L. Essential Oil from Bosnia and Herzegovina

Alispahić, A.[a], Džudžević-Čančar, H.[a,*], Dedić-Mahmutović, A.[a], Jerković, I.[b], Matić, I.[c], Petrović, N.[c,d], Stanojković, T.[c], Boškailo, E.[e]

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Abstract: *Hyssopus officinalis* L. (Lamiaceae), also known as Hyssop, is a genus of herbaceous or semiwoody plants that includes about 10 to 15 species and is distributed mainly in the East Mediterranean, central Asia, and Mongolia. Hyssop essential oils (EOs) have been evaluated for various biological activities and pharmaceutical applications, as they are known to possess insecticidal and attractant properties and are honey-bearing plants. The objective of the present study was to determine the chemical composition of *H. officinalis* L. EO obtained from samples collected in the region of Herzegovina and to assess its antiproliferative activity. Extraction was performed by hydrodistillation in a Clevenger-type apparatus. The produced oil was a pale-yellow liquid with a characteristic pleasant odor and yielded 0.724%. Gas chromatography coupled with mass spectrometry was used for determination of phytochemical composition. Hyssop EO was investigated against human cervical adenocarcinoma HeLa cells and non-transformed human lung fibroblasts MRC-5 by an MTT cell viability assay. A total of 22 compounds were detected, with the most abundant monoterpenes 1,8-cineole (25.75%), methyl eugenol (25.66%), and limonene (23.44%) comprising 74.85%, followed by β-pinene (9.16%) and (Z)-β-ocymene (5.92%). *H. officinalis* EO exhibited a fairly strong cytotoxic effect against HeLa and MRC-5 cell lines, with IC_{50} values of 2.29 µL/mL and 1.68 µL/mL, respectively, indicating that MRC-5 cells are more sensitive to this EO than HeLa cells. The tested EO showed concentration-dependent cytotoxic effects on HeLa and MRC-5 cells. Additional investigations are necessary to explore the cytotoxic effects of this EO against various cancer cell lines and the mechanisms underlying its anticancer effects.

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Abstract

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Permeability Characteristics of Metformin Across Biological Barriers

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Abstract: Metformin, a basic therapy for type 2 diabetes mellitus, exhibits notable permeability characteristics across various biological barriers. Understanding the factors influencing metformin's transport mechanisms is crucial for optimizing its therapeutic efficacy and designing effective drug delivery systems. In this review, we explore the permeability characteristics of metformin across various biological membranes from a chemical perspective. By synthesizing existing research, it describes the factors influencing its transport mechanisms and underscores the implications for drug development and therapeutic optimization in type 2 diabetes management. A literature review was conducted to synthesize evidence from studies investigating the permeability of metformin across various biological barriers. Studies revealed that metformin exhibits differential permeability patterns across biological barriers. In vitro investigations demonstrated that metformin permeability is influenced by factors such as pH, concentration, and interaction with transporters. Metformin's permeability across the blood-brain barrier was found to involve organic cation transporters and was altered under pathological conditions such as hypoxia. Furthermore, intestinal transport studies In vivo indicated concentration-dependent permeability behavior, with metformin primarily absorbed in the duodenum via both passive and active carrier-mediated mechanisms. Positioned within class III of the biopharmaceutical classification system, metformin's chemical properties pose challenges for formulation and delivery. The literature review highlights the intricate interplay between metformin's permeability characteristics across biological barriers and its therapeutic implications.

POSTER PRESENTATIONS

Organic Chemistry

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Abstract

PP-OC-01

Synthesis, Characterization of Metal Complexes of Mg(II) and Cu(II) Ions with *N*-(4-hydroxyphenyl) Acetamide

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N-(4-Hydroxyphenyl) Acetamide
Mg(II)-Ion
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Complexes
FTIR
MS

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Abstract:

N-(4-hydroxyphenyl) acetamide or paracetamol is an acylated aromatic amide used as analgesic and antipyretic to relieve pain and reduce body temperature. In medicinal chemistry, there is a growing interest in the development of drugs based on metal complexes, which are of great importance in therapeutic and diagnostic possibilities. In this research, complexes of Mg(II) and Cu(II)-ions with *N*-(4-hydroxyphenyl) acetamide were synthesized and confirmed with FTIR, UV and MS spectroscopy. The results of the analysis of the synthesized complexes spectra indicate interactions between *N*-(4-hydroxyphenyl) acetamide and metal Mg(II)-ions and Cu (II)-ions via O-donor atom (-C=O) and N-donor atom (- NH) groups.

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Abstract

PP-OC-02

Synthesis and Biological Evaluation of Mannosylated Desmuramyl Peptide with Lipophilic Cholesterol Subunits

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Mannose
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Immunostimulating Activity

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Abstract: Adjuvants are substances incorporated into vaccines that increase the immunogenic responses of antigens. Muramyl dipeptide (MDP, *N*-acetylmuramyl-L-alanyl-D-isoglutamine) and its analogue without the hydrophilic *N*-acetylmuramyl unit, desmuramyl peptide (DMP, L-Ala-D-*iso*Gln) are the well-known adjuvants. Structure-activity studies of DMP derivatives suggest that introduction of lipophilic substituents into the DMP pharmacophore as well as its subsequent mannosylation can increase their adjuvant activity. We recently reported the preparation of mannosylated derivatives of DMPs containing lipophilic subunits such as adamantan-1-yl, adamantan-1-ylethyl and C_{12} alkyl chain, each connected to DMP *via* triazole ring, at the C-terminus (α- or γ-position of D-*iso*Gln) of DMP. Their adjuvant activities were tested *in vivo*. The obtained results showed that the α-position of D-*iso*Gln is the best position for the attachment of lipophilic substituents.

In this work we described the synthesis of mannosylated DMPs with cholesteryl (**I**) and cholesteryl-triazole (**II**) subunit linked to α-position of D-*iso*Gln through an amide bond (Figure 1). Protected dipeptide L-Ala-D-Glu was synthesized first. It was modified by an amidation reaction on α-position of D-*iso*Gln with previously prepared cholesterol amine and cholesterol-triazole amine. The mannose subunit, protected with acetyl groups, was linked to the N-terminal amino group of alanine *via* glycolyl linker. After the removal of protecting groups in the final step of the synthesis, target molecules **I** and **II** were obtained. They will be tested for their adjuvant activity.

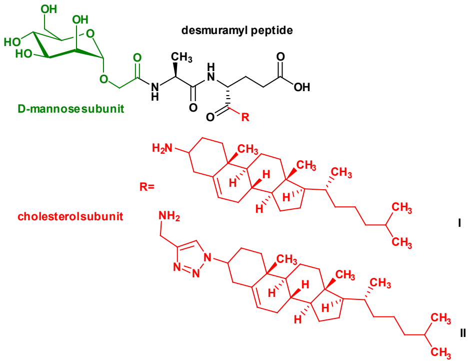

Figure 1. Mannosylated desmuramyl peptide with lipophilic cholesterol subunits

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Abstract

PP-OC-03

Synthesis, Structural Characterization and *In Vitro* Biological Evaluation of Novel B-Ring Trifluoromethylthio-Substituted Flavonoids

Bosno, M.[a,*], Deumić, S.[b], Crnčević, N.[b], Tuka, P.[a], Topčagić, A.[a], Avdić, M.[b], Dizdar, M.[a]

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Abstract: Flavonoids, a group of natural substances with a variable phenolic structure, are one of the most studied bioactive compounds. Within this research, a series of flavonoids bearing trifluoromethylthio group on the B ring were designed, synthesized and evaluated for their biological activity. While the chalcone was prepared by Claisen-Schmidt condensation of 4'-fluoro-2'-hydroxyacetophenones with 4-((trifluoromethyl)thio) benzaldehyde, the aurone, flavone and 3-hydroxyflavone were prepared by oxidative cyclization of the corresponding chalcone. The purity and structures of all synthesized compounds were confirmed by elemental analysis, ATR-FTIR and NMR spectroscopy. All synthesized compounds were tested for their ability to neutralize the stable free radical DPPH, inhibition of acetylcholinesterase and tyrosinase, as well as antimicrobial activity. While the chalcone showed the highest ability to reduce the DPPH free radical (IC_{50} 59.46 µM), the 3-hydroxyflavone showed the highest inhibitory activity against both tested enzymes, acetylcholinesterase (IC_{50} 5.37 µM) and tyrosinase (IC_{50} 24.12 µM). Additionally, all synthesized compounds showed moderate antibacterial activity against Gram-positive (methicillin-resistant *Staphylococcus aureus*, *Staphylococcus aureus* and *Listeria monocytogenes*) and Gram-negative (*Escherichia coli*, *Pseudomonas aeruginosa* and *Klebsiella pneumoniae*) bacteria, and antifungal activity against *Candida albicans*.

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Abstract

PP-OC-04

Antioxidative Profiling of Novel Schiff Bases: A Comprehensive EPR and DPPH Analysis

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Abstract: Schiff bases, obtained in the reaction of carbonyl compounds with thiocarbohydrazide, have been extensively studied for their potential biological and pharmacological activities, including antioxidant, antimicrobial, anti-inflammatory and anticancer properties. Their versatile nature and ability to modulate biological processes make them promising candidates for further exploration in drug discovery and other biomedical applications. To evaluate the antioxidative potential of our Schiff bases, we employed electron paramagnetic resonance (EPR) spectroscopy, widely regarded as the gold standard in antioxidant research. Distinguished by its exceptional sensitivity and selectivity, EPR offers significant advantages over other spectroscopic techniques. Notably, its results remain independent of the optical properties of the sample. By employing EPR, we were able to precisely measure the scavenging capacity of Schiff bases against free radicals, offering a deeper understanding of their antioxidative properties. Assessment of the samples' antioxidative activity was conducted using the 2,2-diphenyl-1-picrylhydrazyl (DPPH) assay, a renowned standard in the field. This assay is widely recognized for its simplicity, reproducibility, and ability to provide semi-quantitative estimates of antioxidant capacity. All EPR spectra were recorded using a Bruker ELEXSYS-II X/L spectrometer with R4123SHQE X-band resonator, 2 minutes upon the addition of DPPH into the solution of Schiff bases in DMSO. EPR spectra were analyzed using Xepr software (Bruker BioSpin). Our findings reveal that all compounds exhibit antiradical activity against DPPH radicals, with bases derived from *o*-hydrohyacetophenone and thiophen-2-acetylcarbaldehyde demonstrating particularly potent effects. These results underscore the promising application of Schiff bases as potential antioxidants, warranting further exploration in biomedical and pharmaceutical research contexts.

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Abstract

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Optimization Of Schiff Bases Synthesis Reaction between Carbonyl Compounds and Thiocarbohydrazide (dHS) using Ultrasound

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Abstract: Schiff bases, obtained in the reaction of carbonyl compounds (aldehydes and ketones) with thiocarbohydrazide (dHS), have been extensively studied for their potential biological and pharmacological activities, including antioxidant, antimicrobial, anti-inflammatory and anticancer properties.The usual way of synthesizing imines (Schiff bases) between aldehydes and ketones with thiocarbohydrazid involves heating mixtures for 3 hours in a mixture of solvent: water and ethanol (volume ratio $H_2O/EtOH = 7:3$) with the addition of a catalytic amount of concentrated (36%) hydrochloric acid. The optimal pH value for these syntheses is 4,5. Heating in the presence of acid catalysts over a long period of time may be unsuitable for acid-sensitive, labile, reactive or thermally unstable aldehydes or ketones, which are prone to polymerization under these conditions. Therefore, we tested the condensation reaction at room temperature with a series of aldehydes and ketones, while maintaining the described ratios (equimolar ratio of aldehydes and dHS), with the addition of a few drops of 36% HCl. In this sense, we examined the synthesis reaction of a series of aldehydes and ketones with dHS using an ultrasonic sonde (UP200Ht ultrasonic processor, for manual or stand use, 200 W, frequency 26 kHz autom. tuning). The course and completion of the reaction were monitored using infrared spectroscopy (FTIR) or, in some cases, TLC-analysis (petroleumether/acetone = 8:2, uv/vis visualization). By applying ultrasound, the reaction time was significantly shortened (to 30 min) and the yields of obtained Schiff bases were 80-95%, which in some cases far exceeds the yields obtained by synthesis.

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Abstract

PP-OC-06

Synthesis and Characterization of a Copper(II) Complex With N'-[(1E)-1-(2-Hydroxyphenyl)ethylidene]hydrazinecarbothioamide Ligand

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Abstract: Initially, a suspension of copper(II)-nitrate was mixed with a warm suspension of ligand in DMF, yielding a dark brown solution. Despite prolonged standing, no precipitate was observed. Therefore, this synthesis was repeated under different conditions. The synthesis of a copper(II) complex with the ligand N'-[(1E)-1-(2-hydroxyphenyl)ethylidene]hydrazinecarbothioamide was successfully accomplished under reflux conditions, using ethanol as the solvent with 1:2 metal-to-ligand ratio. Upon cooling and evaporation, a homogeneous green powder was obtained.

Infrared spectra of obtained green powder shows a shift in the apsorption of primary NH_2 and OH functional groups indicating that the functional group was coordinated to the central Cu^{2+} atom (**Figure 1**). Additionally, a shift of the band from 1222 to 1296 cm^{-1} was observed.

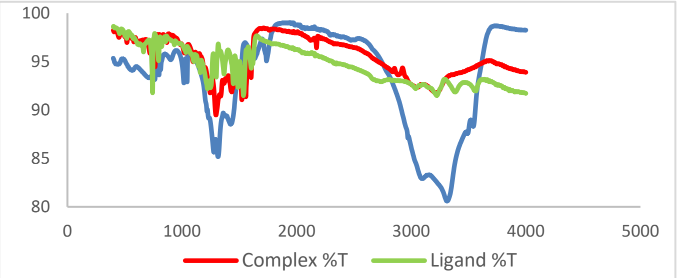

Figure 1. FTIR spectra of complex compound, ligand and copper(II)-nitrate

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Abstract

PP-OC-07

Antioxidant Activity of Schiff Bases Derived from Acetophenones and Benzaldehyde

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Abstract: Given that Schiff bases are known for their biological activities, we performed antioxidant determinations using the DPPH method for two disubstituted Schiff bases derived from benzaldehyde and *o*-hydroxyacetophenone, respectively, as well as two disubstituted Schiff bases with 3,4-dihydroxyacetophenone and 3- hydroxyacetophenone. We also compared the antioxidant value of mono-substituted and di-substituted Schiff bases with *o*-hydroxyacetophenone. A solution of vitamin C was used as a standard for determination. Schiff's base with *o*-hydroxyacetophenone as well as that with 3,4-dihydroxyacetophenone showed very good antioxidant properties, because the IC_{50} value is significantly lower than the value of vitamin C, which is known as a good antioxidant. A Schiff's base with a hydroxyl group in the meta position has a slightly lower value, although there is information that the BDE value is lower compared to the compound with a hydroxyl group in the ortho position, which tells us that the position of the hydroxyl group itself, i.e. the structure, used solvents, but also thermodynamic parameters such as bond dissociation energy, ionization potential, proton affinity and the like, significantly affect the antioxidant properties of a compound.

POSTER PRESENTATIONS

Physical and Theoretical Chemistry

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Abstract

PP-PTC-01

Modification of Briggs-Rauscher Reaction

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Oscillating Reaction
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Abstract: The Briggs-Rauscher reaction, a classic oscillating chemical reaction, has been widely studied due to its intriguing oscillatory behavior. In this research, modifications to the Briggs-Rauscher reaction, which was comprised of hydrogen peroxide, potassium iodate, malonic acid, sulfuric acid, manganese(II) sulphate and starch, were investigated to explore its potential applications and understand its underlying mechanisms. Reactant concentrations (hydrogen peroxide, malonic acid, starch, and manganese(II) sulphate) were systematically varied to modulate the oscillation frequency, oscillation period, and amplitude. The effects of these modifications on the reaction kinetics and oscillation patterns were analyzed using potentiometric technique at 25°C.

When changing parameters such as concentration, one might expect alterations in the overall kinetics of the reaction. Higher concentrations of reactants typically lead to faster reaction rates due to increased collision frequency among reacting species, potentially resulting in shorter oscillation periods. Our findings showed typical behavior, where all reactants in higher concentration increased oscillation period except for the starch.

A change in the concentration of reacting species led to a change in the total number of oscillations. An increase in the total number of oscillations was observed when using a lower concentration of manganese(II) sulphate, a higher concentration of malonic acid and in the reaction without starch. The frequency of oscillations in the first minute was not significantly changed, except in the case when the concentration of malonic acid was increased.

These modifications provide valuable insights into the reaction dynamics and can be utilized to tailor the reaction for specific applications or to elucidate underlying mechanisms.

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Abstract

PP-PTC-02

Electrochemical Behaviour of Aluminium in Artificial Seawater in Presence of *Artemisia annua* L.

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Abstract: Plant extracts are increasingly explored for their corrosion inhibition properties on metals and alloys due to their strong antioxidant characteristics. This study investigated the use of *Artemisia annua* L. aqueous extract (AAE) as a corrosion inhibitor for aluminum in artificial seawater (ASW) using cyclic voltammetry (CV), potentiodynamic polarization (PP) and electrochemical impedance spectroscopy (EIS) measurements. The active compounds in AAE were analyzed using Fourier-transform infrared spectroscopy. Both PP and CV showed a decrease in anodic current densities with increasing inhibitor concentration. Additionally, the corrosion current (E_{corr}) shifted to more positive values indicating AAE acts as an anodic inhibitor of Al corrosion. EIS data obtained for Al in ASW showed the capacitive behavior of the electrode in the middle-frequency range. Simultaneously an inductive loop was observed in the low-frequency region, which was associated with the dissolution of the surface film on the Al electrode. However, with the addition of AAE (0.25-1.00 g L^{-1}) inductive loop disappeared and Al behavior was described with a simplified Randles cell, where (*QR*) represented a double-layer capacitor and a charge transfer resistance. The inhibition efficiency deduced from electrochemical data increased with the increasing concentration of AAE. The adsorptive behavior of AAE on the Al surface followed a Freundlich adsorption isotherm with a free energy of adsorption ΔG_{ads} of −17.18 ± 0.66 kJ mol^{-1}. Calculated value suggested that the caffeic acid and its derivatives present in AAE were physically adsorbed onto the Al surface, forming a thin layer that acted as a barrier from aggressive seawater.

Acknowledgment

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Abstract

PP-PTC-03

Experimental Characterization, *In Silico* Study and Antimicrobial Activity of Newly Synthesized Ionic Liquids with Carboxylate Anions

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Abstract: The COVID-19 pandemic highlighted an urgent need to synthesize and study new antimicrobial and antiviral substances. Among them, ionic liquids (ILs) with antibacterial properties are of a crucial importance due to their tunable properties. Most ILs have strong antibacterial effects, but ILs containing the imidazolium cation are more effective than the positive control. In this study, ionic liquids containing 1-butyl-3-methylimidazolium cation, (Bmim), combined with various carboxylate anions (phenylacetate (Phe), benzoate (Ben), and 4-methoxyphenylacetate (CH_3OPhe)) were synthesized and fully characterized. In order to obtain [Bmim][Phe], [Bmim][Ben] and [Bmim][CH_3OPhe], potentiometric titrations were performed. In this phase, the methanol solution of phenylacetic acid, benzoic acid, and 4-methoxyphenylacetic acid was titrated with an aqueous solution of [Bmim][OH]. The interactions between the cation and anion were discussed based on density, viscosity, and electrical conductivity measurements. These properties were analyzed and calculated also by *in silico* approach and hierarchical cluster analysis with Ward's minimum variance as the clustering method and Euclidean distances as the distance method. The antimicrobial activity of the prepared ionic liquids was tested, confirming that all studied Ils show improved antimicrobial activity compared to the starting components.

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Abstract
PP-PTC-04

Adsorption Mechanism of Polyphenols Extracted from *Artemisia annua* L. on the Al 5083 Alloy Surface during Microbial Activity

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Abstract: Approximately 80% of marine corrosion is due to microbial activity, costing billions of dollars annually. The main challenge in combating microbiologically influenced corrosion (MIC) is finding effective, nontoxic, and biodegradable inhibitors. Thus, this study examined the anticorrosive and antimicrobial properties of *Artemisia annua* L. (AAE) extract as a greener substitute for biocides. The impact of AAE on the MIC of Al 5083 alloy in artificial seawater was determined using electrochemical, surface, and spectroscopic techniques. The characterization of the AAE by HPLC and FTIR revealed the presence of well-known antimicrobial and anticorrosive compounds in the extract. Corrosion kinetic parameters obtained from electrochemical measurements showed poor corrosion resistance of Al 5083 alloy against aggressive biotic seawater. XPS and FTIR analysis of the treated surfaces revealed that the main corrosion products during MIC were porous Al oxyhydroxides. In contrast, the corrosion resistance of Al 5083 alloy increased with the addition of *A. annua* to the biotic seawater. The latter was associated with the coordination of chlorogenic acid with Al 5083 surfaces through bidentate bridging via carboxylate, as well as the formation of a more compact $\alpha\text{–}Al_2O_3$. As confirmed by ICP-OES, the formed layer slowed the diffusion rate of Al^{3+} to and from the electrode surfaces. The inhibition efficiency of *A. annua* against MIC deduced from electrochemical data was 80%. These results represent a basis for advancing green protection strategies of Al alloys from MIC by utilizing *A. annua* extract in antibacterial coatings.

Acknowledgment

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Abstract

PP-PTC-05

Anomalous Properties of the Central Force Water Model

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Abstract: In 1975 Stillinger, Lemberg and Rahman proposed an isotropic coarse-grained central force (CF) model of water which was later revised (CF1) by Haymet *et al.*. In this model, water is regarded as a weak electrolyte, where oxygen and two hydrogens spontaneously form ion-triplets, i.e. a H_2O molecule. The most appealing feature of the central force models of water lies in the fact that a system of water molecules is treated as a mixture of partially charged particles representing oxygen and hydrogen atoms in the 1:2 number ratio. Compared to commonly used atomistic water models (e.g. SPC and TIP models), no angular dependent terms are included in the CF model. This is an advantage for simulations as well as for theoretical manipulations.

We employed Monte Carlo computer simulations to investigate the properties of bulk CF1 water, focusing on hydrogen bonding, tetrahedral (q), and translational (τ) order parameters to shed light on the water-like anomalous behaviour of CF1 water. The model accurately reproduces the intramolecular structure of the H_2O molecule. Using an energetic definition of the hydrogen bond yields more consistent results for the average number of hydrogen bonds compared to a one-parameter distance criterion, with an average value of 3.8 obtained at 300 K. The structural anomalies lead to the density anomaly, and the model's density aligns well with experimental $\rho(T)$ trends. We explored the chemical potential-density projection of the model's equation of state, observing vapor-liquid coexistence at sufficiently low temperatures.

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Abstract

PP-PTC-06

Application of Briggs-Rauscher Reaction for Measurement of Antioxidant Capacity of Atorvastatin

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Abstract: Atorvastatin, primarily known for its cholesterol-lowering properties, has been the subject of research regarding its potential antioxidant effects. While its main mechanism of action involves inhibiting the enzyme HMG-CoA reductase to reduce cholesterol synthesis, some studies suggest that atorvastatin may possess additional antioxidant properties.

In this research, the antioxidant capacities of atorvastatin and its active substance were evaluated using the Briggs-Rauscher method. This method is based on the inhibitory effects by antioxidants on the oscillations of the Briggs-Rauscher reaction system. The inhibition times producted on the Briggs-Rauscher reaction system, which was comprised of hydrogen peroxide, potassium iodate, malonic acid, sulfuric acid, manganese (II) sulfate and starch, were recorded potentiometrically.

Results indicate that both atorvastatin and its active substance exhibit notable antioxidant activity, as evidenced by their ability to inhibit the oscillating reaction effectively. The active substance as assumed showed higher antioxidant capacity than the drug itself.

The conclusion suggest that atorvastatin and its active substance possess antioxidant properties, which may contribute to their therapeutic effects beyond lipid-lowering mechanisms. Further exploration of their antioxidant capabilities could provide valuable insights into their potential applications in managing oxidative stress-related disorders.

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Abstract

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Volumetric Properties of Solutions of the Ionic Liquid 1-Ethyl-3-Methylimidazolium Chloride in *N,N*-Dimethylacetamide and Dimethyl Sulfoxide

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Volumetric Properties
1-Ethyl-3-Methylimidazolium Chloride
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Abstract: This work represents the continuation of the systematic (ionic liquid – solvent) system research in our laboratory. Namely, the volumetric properties of binary mixtures, containing the ionic liquid 1-ethyl-3-methylimidazolium chloride, [C_2mim][Cl] and *N,N*-dimethylacetamide (DMA) or dimethyl sulfoxide (DMSO) were investigated in the temperature range of (278.15 to 313.15) K in DMA or (293.15 to 318.15) K in DMSO and in the molality range of [C_2mim][Cl] (~0.0050 to ~0.1000) mol kg^{-1}. The measured density data, were used to calculate the thermal expansion coefficient, the apparent molar volume, partial molar volumes for the solvent and the solute, the apparent molar volume at infinite dilution, Masson's interaction coefficient, Heppler's coefficient, and the limited apparent molar expansibility. The validity of the Masson's equation was verified and applied to describe the dependence of apparent molar volume on molarity. The apparent molar volume at infinite dilution and Masson's interaction coefficient were determined from this dependence at each temperature. Finally, the structure-maker or structure-breaker properties of the investigated ionic liquid in both solvents are discussed. In our case, the values of the Hepper's coefficients are negative, indicating that [C_2mim][Cl] in DMA or DMSO solvents could be described as structure-breaking.

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Abstract

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Spectrophotometric Determination of the Influence of Metformin on Enzyme Activity

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Abstract: Metformin is clinically used in the treatment of diabetes patients 1, 2. The major action of Metformin is to increase glucose transport across the cell membrane in skeletal muscles. The effect of metformin consists in increasing anaerobic glycolysis. Therefore, there is a reduction in intestinal absorption of glucose, a reduction in glucose resynthesis in the liver, as well as an increase in tissue glucose consumption as a result of the enhancement of the effect of insulin. The spectrophotometric method was used in this study. Absorbance was recorded at a wavelength of 570 nm. The influence of metformin on catalase enzyme activity in phosphate buffer was monitored. The obtained results show that the reaction follows the Michaelis-Menten model. Using the Lineweaver-Burk equation, the values of the kinetic parameters of maximum velocity (V_{max}) and Michaelis-Menten constant (K_m) were calculated. A competitive type of inhibition has been proven, where the value of the maximum velocity is constant, and the value of K_m is variable. By binding metformin to the active site of the enzyme, metabolic processes in the body are inhibited, resulting in the development of the disease.

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Abstract

PP-PTC-09

Electrochemical Characterization of Nickel-Based Cathodes for Hydrogen Evolution Reaction in Alkaline Water Electrolysis

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Abstract: Alkaline water electrolysis is one of the simpler methods for obtaining hydrogen. Since seawater is among the most abundant natural resources globally, its electrolysis offers a promising avenue for generating clean hydrogen energy. Thanks to the alkaline electrolyte, non-precious metals, such as nickel or its alloys with other metals, have been considered as alternatives to noble metal catalytic electrodes. This work investigates the electrocatalytic activity and corrosion of nickel-based cathodes for the hydrogen evolution reaction in alkaline media using electrochemical and spectroscopic methods. Various nickel/molybdenum alloys on stainless-steel mesh were obtained by chronoamperometric electrodeposition at different deposition potentials and times. Electrochemical research was conducted using techniques such as cyclic voltammetry (CV), linear voltammetry (LV), Tafel plots (TP), and potentiostatic electrochemical impedance spectroscopy (PEIS). Tests were performed in 1 M KOH solution, 1 M KOH solution containing 0.5 M chlorides, as well as in 1 M KOH solution containing chlorides (0.5 M) and bromides (5 mM). NiMo alloys exhibited better electrocatalytic activity than Ni and blank stainless-steel mesh. As expected, the corrosion potentials obtained from Tafel plots were higher in the electrolyte containing KOH and chlorides compared to those containing only KOH, chlorides, and bromides. However, in some cases, the corrosion potentials in pure KOH solutions were lower, while in others, they were higher than those containing the aforementioned ions.

POSTER PRESENTATIONS

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Gammaspectrometric Analysis of ^{226}Ra, ^{40}K, ^{232}Th and ^{137}Cs through Soil Profiles (0-30 cm) in Fojnica Area, B&H

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Abstract: Monitoring of radionuclides migration through the soil represents a special challenge. Hence, the aim of this study was to assess vertical distribution of radionuclides (^{232}Th, and ^{226}Ra, ^{40}K and ^{137}Cs) through soil depths (0–10, 10–20, 20–30 cm) at three sampling sites in the Fojnica area (site 1; the location of the thermal recreation center "Reumal" Fojnica, site 2; spring of the thermal water and site 3; a park in the vicinity of the thermal pool), to evaluate possible effect of radioactive thermal water presence on the content of the determined radionuclide in the surrounding soil. The obtained values of activity concentrations for ^{137}C showed that sites 1 and 2 had untreated soils, while at location 3 soil was treated. In addition, the measured activity concentrations of ^{137}C were low (from 1.52 to 53.75 Bq/kg) and in correlation with the values obtained at different locations in B&H and in the region. Among three tested natural radionuclides, ^{40}K was the most abundant, with the activity concentrations ranging from 251.97 to 852.19 Bq/kg, with a slight tendency to increase its content with soil depth. Activity concentrations of ^{232}Th ranged from 19.74 to 84.70 Bq/kg, and of ^{226}Ra from 47.65 to 850.15 Bq/kg for all tested soil samples. The obtained values for the activity concentrations of ^{226}Ra had a higher value compared to other tested radionuclides, which could be attributed to the naturally present uranium in the soil as well as the migration of uranium from the thermal water into the soil.

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Abstract

PP-RC-02

Determination of ^{238}U, ^{234}U and ^{226}Ra Concentrations in Bottled Waters Commercially Available in Bosnia and Herzegovina

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Alpha Particle Spectrometry

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Abstract: Bottled water consumption is increasing in Bosnia and Herzegovina, and the intake of water is a relevant pathway for human exposure to environmental radioactivity. Alpha particle spectrometry is a powerful method for the determination of alpha-emitting radionuclides such as ^{238}U, ^{234}U and ^{226}Ra. Radiochemical separation is essential for the preparation of samples before they are submitted for alpha particle counting in the alpha particle spectrometry system. The aim of the investigation was the determination of ^{238}U, ^{234}U and ^{226}Ra concentrations in bottled waters. A total of 12 bottled water samples were collected for investigation. The concentrations of ^{238}U, ^{234}U and ^{226}Ra were determined by alpha particle spectrometry following radiochemical separation and purification. Radionuclides ^{238}U and ^{234}U were separated by ion exchange and prepared for measurement by electroplating, while ^{226}Ra was preconcentrated with $Pb(Ra)(Ba)SO_4$ and prepared for measurement by micro-precipitation. The results for ^{238}U, ^{234}U and ^{226}Ra ranged from 0.80 mBq/L to 23.90 mBq/L, 0.35 mBq/L to 100.00 mBq/L, and 0.84 mBq/L to 12.50 mBq/L, respectively. The activity ratios of ^{234}U/^{238}U are in the ranges 0.29 to 4.21 indicating that analyzed waters are more enriched in ^{234}U in relation to ^{238}U, which is typical for natural waters. The activity ratios of ^{238}U/^{226}Ra are in the ranges 0.24 to 4.82. The lower concentration of ^{226}Ra compared to the ^{238}U parent radionuclide is because of the lower transfer rate of ^{226}Ra in water during rock weathering processes and the removal of ^{226}Ra from water by precipitation. Total activity concentrations of ^{238}U, ^{234}U, and ^{226}Ra are significantly lower than guideline values prescribed by the WHO.

POSTER PRESENTATIONS

Topics Related to Chemistry

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RP- HPLC Method for Determination of Perindopril Related Compounds

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Abstract: Perindopril is a long-acting angiotensin-converting enzyme (ACE) inhibitor used for the treatment of high blood pressure, heart failure, and coronary artery disease in the form of perindopril arginine, perindopril erbumine, or perindopril tert-butylamine. A literature search of the available papers on the determination of related compounds of perindopril led to the conclusion that all methods are fundamentally based on the same concept of gradient elution with an acidic buffer/aqueous phase, a low starting proportion of acetonitrile, and a gradual increase through the gradient program in order to elute more non-polar components.

The in-house method was developed on an Inertsil ODS-3, 250 mm x 4.6 mm; 5 µm column, recording at 210 nm. The gradient is achieved by mixing mobile phase A (phosphate buffer pH 2.2 / Acetonitrile = 90:10) and mobile phase B (Phosphate buffer pH 2.2 / Acetonitrile = 40:60) at a flow rate of 1.0 ml/min.

Forced degradation of perindopril tert-butylamine was performed by treatment in an acidic, alkaline, oxidizing environment, as well as examination of the influence of heat and light. The main degradation products are perindopril impurity B and perindopril impurity F. The developed method is selective, sensitive, accurate, robust, and can be used for testing related substances in the finished product.

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Abstract

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Development of RP-HPLC Method for Determination of Carbocisteine Related Compounds

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Abstract: Carbocisteine is a mucolytic used as an adjunctive therapy in the treatment of diseases of the respiratory system characterized by the production of excessive viscous mucus, including chronic obstructive airways disease. European Pharmacopoeia (EP) prescribes the monitoring of related compounds of Carbocisteine (ninhydrin positive substances) by thin-layer chromatography (TLC) method. TLC method is not sufficiently sensitive, accurate and reliable, which is why the in-house method was developed.

The in-house high-performance liquid chromatography (HPLC) method for determination of related compounds of carbocisteine was developed on a SAX column. A Zorbax SAX column (250x4.6 mm, 5 µm) was used, recording was performed at 220 nm and the gradient is achieved by mixing the mobile phase A (0.05 M phosphate buffer pH 5.5/ acetonitrile = 37 /63) and mobile phase B (0.05 M phosphate buffer pH 6.0/acetonitrile = 80/20) with a flow rate of 1.0 ml/min.

The developed method had adequate resolution between the peaks of impurities and the active substance. The method is selective for determining the following carbocisteine impurities: carbocisteine lactam, carbocisteine sulfoxide, L-cystine, L-tyrosine as well as other individual related substances. The sensitivity of the method is 0.05% and can be used for further development of the method for the determination of related carbocisteine substances in drug samples.

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Abstract

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Orodispersible Films with Ascorbic Acid: Formulation and Characterization

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Abstract: Orodispersible films are a very suitable dosage form for pediatric and geriatric populations. They don’t need additional water for application, quickly hydrate with saliva, adhere to the mucosa, and disintegrate within 60 seconds. As there are no orodispersible films with ascorbic acid available on the market, a total of nine formulations (F1-F9) were prepared using the solvent casting method. Three different hydrophilic polymers (hydroxypropyl methylcellulose, gelatin, and sodium carboxymethyl cellulose) were used for the preparation, with a variation in the concentration of the polymer and glycerol as a plasticizer in the formulation. The concentration of ascorbic acid as an active substance also varied in different formulations. After extracting the films, the formulations with hydroxypropyl methylcellulose (F1-F3) were selected for further testing due to their optimal characteristics. After evaluation of ascorbic acid content uniformity, F2 was chosen for further characterization, while formulations F1 and F3 were excluded due to uneven content and crystallization of the active substance, respectively. Formulation F2 had a satisfactory disintegration time, with an average of 25,64 seconds, and was flexible. It proved to be very hygroscopic, considering the concentration of glycerol, and transparent. The compatibility of all substances in the formulation was examined using FTIR spectroscopy. Ascorbic acid, glycerol and hydroxypropyl methylcellulose were found to be compatible as signals from individual substances were observed on the spectrum of formulation F2. FTIR spectra also confirmed the formation of a film between polymer and plasticizer.

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Optimization of Biogas Production with Emphasis on Waste Recovery

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Abstract: Energy generation from alternative sources is of major importance in Bosnia and Herzegovina. Since there are numerous dairy and poultry farms in this country, biogas productions from organic waste has significant potential. The following experiment was conducted on a lab-scale reactor system, aiming to optimize a full-scale biogas plant in Bosnia and Herzegovina. Multiple mixtures of cow manure, chicken manure and corn silage in varying ratios were prepared. Emphasizing the importance of waste and material recovery, equal amounts of digestate were fed to all mixtures, reducing both the amount of waste generated and the operating cost of the biogas plant. Through this research, the mixture used for biogas production at the full-scale plant was optimized. The optimized mixture resulted in a maximum specific methane yield of 0,15 Nm3/kgVSi and 60.02% CH_4, compared to similar experiments reporting specific methane yield from 0,07 to 0,14 Nm3/kgVSi at 47 and 55% CH_4. Furthermore, the digestate proved to be a valuable component, as it served as inoculum in the lab-scale plant but is also returned to the process in the full-scale plant to contribute to the overall organic matter content and harness the waste recovery potential of anaerobic digestion processes.

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