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10th Conference of Young Chemists of Serbia

Book of Abstracts

26th October 2024

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All scientific contributions are divided into the following categories:

Chemistry and Society (CS)
Chemistry meets Biology (CB)
Developments in Chemical Synthesis (DCS)
Environmental Awareness (EA)
Physical and Computational Chemistry (PCC)
Phytochemistry and Food Chemistry (PFC)
Solution Chemistry and Chemical Equilibrium (SCCE)
Supramolecular Chemistry and Functional Materials (SCFM)

POSTER NUMBER is the last part of the contrubition code, e.g. XY PP 15.

VENUE:

- Lectures, oral and flash presentations will take place at the **large chemistry amphitheater (VHA)** on the ground floor, Faculty of Chemistry, University of Belgrade (address: Studentski Trg 12–16, Belgrade).
- The Poster sessions will take place in the hallway **in front of the library** on the 1st floor.
- The lunch will take place in Faculty council meeting room (SZS) on the 1st floor.

Plenary Lecture

PP OP 01

Transition-metal catalysis in organic synthesis

Andrea M. Nikolić

University of Belgrade – Faculty of Chemistry, Belgrade, Serbia

With the high demand for reactions to be efficient, selective and practical, catalysis became a vital part of the chemical synthesis. Transition-metal based catalysts enabled the transformations previously unattainable, which in turn made the significant progress in the fields of chemical, pharmaceutical, agricultural and other industries and they are now considered essential in synthesis [1,2]. This field is ever-expanding and herein, the application of palladium-catalyzed reaction was used for the N-arylation of 1-substituted-1*H*-tetrazol-5-amines for the first time. This reaction is characterized with the broad substrate scope and excellent functional group tolerance. As an extension of this study, the method for the synthesis of *N*,1-diaryl-1*H*-tetrazol-5-amines under mild reaction conditions was developed. Palladium catalysts can also be employed in complex reaction mixtures, which was shown in a one-pot, two step synthesis of isochromene-fused pyrazoles. One of the obstacles in transition-metal catalyzed reactions is finding the best catalyst that will ensure high yield of the desired products while being applied in low quantities under reasonable conditions. The rational design of the catalytic system can be accelerated and made more environmentally friendly with *in silico* methods, especially with the prominent machine learning models. Here, a targeted generation of ligands with desired properties for palladium was achieved and its utility was demonstrated experimentally in Mizoroki-Heck reaction. Another machine learning model was developed for retrosynthetic planning, a strategy that enabled a more efficient synthesis of a precursor of the anti-cancer molecule.

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Invited Lectures

PPP OP 01

Biocatalysis in the spotlight: exploring the complexities of enzymatic processes with a reaction engineering approach

Nevena Milčić, Martina Sudar, Zvjezdana Findrik Blažević
University of Zagreb – Faculty of Chemical Engineering and Technology, Zagreb, Croatia

Once seen as a promising green technology, biocatalysis has developed into a transformative tool for sustainable chemical production in recent decades. However, the complexity of enzymatic systems can pose a major challenge for broader applications. Scaling up these processes requires a multidisciplinary approach that integrates insights from molecular biology, biotechnology, organic and process chemistry, and reaction engineering.

Enzymatic reactions are very sensitive to environmental factors such as pH and temperature. Limitations in substrate specificity and selectivity can lead to unintended side reactions or inefficient main reactions, especially with non-natural substrates. Complex kinetic behavior, including multiple inhibitions and reactions involving more than one substrate, further complicate process design. The selection of suitable media for enzymes and substrates also requires a balance between substrate availability and enzyme compatibility. Maintaining the operational stability of the enzyme over multiple cycles or longer reaction times is also critical for practical applications. Mass transfer limitations, especially with whole cell or immobilized enzymes, can also be a problem. Furthermore, although often advertised as a green technology, biocatalysis is not inherently sustainable, so its environmental impact must be assessed and minimized on a case-by-case basis. All these complexities increase significantly when multiple enzymes are involved in cascade reactions.

In this lecture, such challenges are explored and explained using a reaction engineering approach. Case studies based on experiments are used to illustrate how reaction engineering helps to discover and minimize reaction bottlenecks, leading to the optimization of biocatalytic processes for more efficient and sustainable applications [1,2].

References

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Acknowledgments

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PPP OP 02

Harnessing the power of plants: the science behind natural antioxidants in cosmetic formulations

Nevena R. Mihailović, Vladimir B. Mihailović, Nikola Srećković
University of Kragujevac – Faculty of Science, Department of Chemistry, Kragujevac, Serbia

In recent years, the demand for natural ingredients in cosmetics has surged, driven by consumer preference for safer, eco-friendly products. These evolving requirements have spurred innovative approaches within the cosmetic industry, resulting in the formulation of numerous products utilizing natural ingredients, predominantly derived from botanical sources [1]. Among these, natural antioxidants have garnered significant attention not only for their ability to protect cosmetic products, especially creams, against oxidative degradation, but also to protect the skin from cellular damage, as well as тo enhance skin repair and rejuvenation, making them a critical component in modern skincare formulations [2]. This study explores the efficacy of natural antioxidants extracted from plants in cosmetic formulations, focusing on their potential to replace synthetic alternatives. The primary objective of this study is to give an insight into the beneficial use of plant-base ingredients in the formulation of cosmetic creams, as well as experimentally confirm the antioxidant properties of some cosmetic cream formulations, containing plant-derived ingredients, in correlation with the content of plant phenolic compounds, known as the most effective natural antioxidants. The total phenolic content was quantified in all cream samples with values ranging up to 0.2 mg gallic acid equivalents (GAE)/g of sample. However, certain formulations, lacking flavonoids, demonstrated negligible antioxidant activity. The formulations with the highest percentage of plant-derived ingredients demonstrated the most elevated phenolic content and the strongest antioxidant capacity. These results suggest that cosmetic formulations containing plant-derived ingredients do not inherently provide beneficial effects, such as antioxidant activity, solely due to the presence of bioactive plant components. To achieve any measurable biological activity, it is essential that the formulation includes an adequate concentration of the selected plant-based ingredients.

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Oral Presentations

CB OP 01

HPTLC-FTIR-MS identification of anti-MRSA and antioxidative compounds from *Dysidea avara*

Marko D. Jović[1], Petar M. Ristivojević[2], Vukosava M. Živković-Radovanović[2], Jelena Đ. Trifković[2]

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The marine sponge *Dysidea avara* is recognized as a rich source of bioactive compounds [1]. This study aimed to evaluate its effect on anti-methicillin resistant *Staphylococcus aureus* (anti-MRSA) activity and antioxidant activity. The methanolic extract was analyzed using high-performance thin-layer chromatography (HPTLC) on silica gel with a mobile phase of toluene: ethyl acetate: acetic acid (60:37.5:2.5, *v/v/v*). Separated zones were visualized under UV light at 254 nm and 366 nm before derivatization, and under white light after derivatization with *p*-anisaldehyde/sulfuric acid reagent. Anti-MRSA and antioxidant activities were assessed using HPTLC-effect direct analysis (HPTLC-EDA). Antibacterial zones were detected for compounds at $hR_F \approx 50$, 65, 75, and 95, which were isolated by preparative TLC. Attenuated total reflectance-Fourier transform infrared (ATR-FTIR) spectroscopy revealed the presence of saponins, sterols, and sesquiterpenes in the isolated fractions. Antioxidant activity was determined using the DPPH assay, identifying a single active zone at $hR_F \approx 75$, which coincided with the most potent anti-MRSA region. Further analysis of this bioactive compound using ultra-high-performance liquid chromatography coupled with linear ion trap-OrbiTrap (UHPLC-OrbiTrap) mass spectrometry confirmed the presence of avarol, a phenol-type sesquiterpene derivative. Chromatograms were analyzed using ImageJ software, and bioactivity was quantified as milligram streptomycin equivalents per gram of extract (mg StrptE/g) for anti-MRSA activity, and milligram gallic acid equivalents per gram (mg GAE/g) for antioxidant activity. The results indicated significantly higher anti-MRSA potential compared to antioxidant potential, with avarol identified as the major contributor to the bioactivity of *D. avara* extract.

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Acknowledgments

This work has been supported by the Ministry of Science, Technological Development and Innovation of Republic of Serbia, Contract numbers: 451-03-66/2024-03/200168 and 451-03-66/2024-03/200288.

CB OP 02

Optimization of chromatographic conditions for separation of bee venom constituents by high–performance thin–layer chromatography

Danilo Trajković[1], Mihajlo V. Jakanovski[2], Olivera Bo Brenjo[1], Sandra Šegan[3], Dušanka M. Milojković-Opsenica[1]
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Bee venom (BV), or apitoxin, is biotoxin naturally produced by the venom glands of honeybees. A major role of BV is defence of the bee colony, while it possesses a wide range of pharmacological and biological activities [1]. Several techniques and methods have been used for separation and quantification of BV constituents. Selection is usually done by proportionality of BV components, as melittin has the highest proportion among three most important components, and is followed by phospholipase A_2 (PLA2) and apamin [2]. So far no method has been standardized for full characterization of BV. The majority of analytical procedures revolve around qualification and separation of melittin, PLA2 and apamin using the HPLC method. The main drawback of this method is that it consumes large amounts of mobile phase and it is a relatively slow process. In this work, we have tried to develop and optimize a more efficient, faster and greener HPTLC method, for the complete separation of three main components of BV [1, 2].

The separation of BV components was effectively accomplished with each component's peak areas aligning closely with the R_F value ranges of standard solutions for the individual components. The mobile phases were composed of a solution of 0.1% trifluoroacetic acid (TFA) in acetonitrile (ACN) and a solution of 0.1% TFA in water (H_2O) in different ratios. The same solvent ratio was applied for the separation of melittin and PLA2, while a different solvent ratio was necessary for the separation of apamin.

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CB OP 03

Physicochemical characteristics, antimicrobial activity and effect on Chard (*Beta vulgaris L.var.cicla*) of newly synthesised nicotine-based ionic liquids

Andrija Vukov[1], Milica Živković[2], Tijana Jovanović Paunović[1], Milana Rakić[2], Ivana Maksimović[3], Milan Vraneš[1]
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Nicotine is a natural compound found in a large array of plant species. It is widely believed that the role of this secondary metabolite is that of a pesticide, due to its ability to bind to acetylcholine receptors in the nervous systems of animals, exhibiting harmful effects. Due to nicotine's structure the tertiary nitrogen atom is susceptible to alkylation. The increase of an alkyl side-chain has shown to lead to, among other effects, the increase in antimicrobial activity and toxicity of a substance. Further, ionic liquids (ILs), ionic compounds with melting points below 100°C, are also known to have high biological activity. Due to potential synergistic effects of the base substance, an added alkyl side-chain and the form of an IL, we synthesised four nicotine-based ionic liquids with varying alkyl chain lengths: N-octylnicotinium bromide, N-decylnicotinium bromide, N-dodecylnicotinium bromide and N-tetradecylnicotinium bromide.

Density, viscosity and sound velocity measurements of their water solutions were performed in a concentration range from 0.02 to 0.12. $mol \cdot kg^{-1}$ and in a temperature range from 293.15 to 313.15K. The measured values are further discussed in terms of solute-solute and solute-solvent interactions. The antimicrobial activity of these ILs and nicotine was also tested against several strains of gram-positive and gram-negative bacteria, yeasts and molds and compared. It was found that all nicotine-based ILs have significantly higher antimicrobial activity than nicotine, for all examined species. The effects of N-dodecilnicotinium bromide was investigated on *Beta vulgaris* and compared with nicotine, finding no harmful effects on the examined plants.

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EA OP 01

Insight on the deterioration phenomena of cultural heritage objects

Marija K. Kovač[1], Bojan B. Miljević[1], Helena M. Hiršenberger[2], Snežana B. Vučetić[1]
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Climate changes throughout different seasons are one of the most crucial factors for materials degradation. Different degradation mechanisms can lead to the devastation of cultural heritage objects if they are not adequately protected and maintained. For the preservation of these objects, the suggested approach is an examination of degradation patterns, their removal and the protection/restoration processes. The most affected materials by harmful environmental impact are building materials like natural stone, bricks and mortars, which are often affected by air pollution, freeze-thaw weathering, soluble salt presence *etc*. These climatic conditions can cause similar degradation patterns in the different types of materials in buildings [1]. In this research, natural stone, brick and mortar samples from the Serbian Orthodox Church dedicated to Saint Mary in Sremski Karlovci were examined in-situ, to determine degradation patterns and their consequences on materials degradation using a multi-analytical approach that includes: digital microscopy, VIS-colorimetry, FTIR analysis, XRF analysis, soluble salt content analysis and thermography analysis.

Results of used instrumental analyses included information for complete characterization of materials condition and chemical composition, presence of degradation patterns (cracks, black crusts, peeling and crumbling, etc.), presence of soluble salts, etc. Obtained results have shown that degradation patterns can be examined and identified with different instrumental methods to achieve a better understanding of material degradation caused by climatic conditions. Moreover, the obtained conclusions are a starting point for appropriate conservation decisions about the further conservation, cleaning and protection processes which will be performed on church.

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Acknowledgments: This study was supported by the programs 451-03-66/2024-03/200134 and 451-03-65/2024-03/200134 funded by the Ministry of Science, Technological Development and Innovations of the Republic of Serbia.

EA OP 02

The application of green ZnO nanoparticles based on tartaric acid for the sustainable removal of the antipsychotic sulpiride

Đorđe T. Todorović, Dušica K. Jovanović, Daniela V. Šojić Merkulov
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Antipsychotic drug, sulpiride (SLP), is widely used today in the treatment of schizophrenia, anxiety, mild depression, *etc*. Even small amounts of this drug in water bodies can cause major changes in the ecosystem, since SLP can disrupt aquatic plants and microorganisms. Namely, SLP may affect plant growth, metabolism, and nutrient uptake. Additionally, studies have shown that SLP can be lethal to aquatic fauna by its huge effect on central nervous system of aquatic animals.[1] Heterogeneous photocatalysis, as a green and eco-friendly method, poses suitable for the degradation of pollutants such as SLP. It is based on the formation of reactive radicals that can oxidize organic pollutants to harmless products.[2] The aim of this study was to investigate the effects of several different factors (catalyst loading and doping, initial pH value) on the photocatalytic degradation of SLP in the presence of the newly synthesized green ZnO nanocomposite based on tartaric acid (ZnO/TA) under simulated sunlight. After 60 min of irradiation, 90.7% of SLP was removed in the presence of 0.5 mg/cm^3 of ZnO/TA, whereas non-adjusted pH value was chosen as the optimal one. Lastly, photocatalytic activity of ZnO/TA was enhanced when it was doped with SnO_2.

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PCC OP 01

An efficient electrochemical sensor based on Y_2O_3 nanoparticles doped with graphitic carbon nitride for sensitive detection of triclosan in real samples

Aleksandar Mijajlović[1], Vesna Stanković[2], Filip Vlahović[2], Slađana Đurđić[1], Dalibor Stanković[1]

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Triclosan (TSC), a chlorinated aromatic compound, is an antimicrobial agent widely incorporated into various consumer products (soaps, toothpaste,...) due to its efficacy in inhibiting bacterial and fungal growth. Despite these uses, skin irritation, allergic reactions, and effects on immune system function have been linked to exposure to triclosan [1].

In the current study, a new electrochemical sensor for TSC detection was developed using a carbon paste electrode (CPE) enhanced with Y_2O_3 nanoparticles doped with graphitic carbon nitride (GCN).

Yttrium (Y), a rare-earth metal, has emerged as a key component in the development of novel electrode nanocomposites with enhanced electrocatalytic performance. Graphitic carbon nitride (g-C_3N_4, GCN) is a polymeric material composed of carbon and nitrogen arranged in a layered, graphitic structure. Due to its unique properties, GCN has garnered attention for use in electrochemical sensors [2].

The synthesis of Y_2O_3 was carried out using the Pechini method for the first time, and the morphology and nanostructure of the material were confirmed by the use of X-ray powder diffraction (XRPD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). The electrochemical sensor that was suggested had a remarkable response to TSC, displaying a broad linear range of 0.5 to 100 μM, a detection limit of 0.137 μM, and a sensitivity of 2.112 $\mu A\ \mu M^{-1}\ cm^{-2}$. Furthermore, the Y_2O_3 /GCN - CPE sensor showed good recovery results when used to detect TSC in water and toothpaste samples.

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PCC OP 02

Application of carbon aerogels for supercapacitors

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Supercapacitors, also known as electrochemical capacitors, emerged as promising candidates in fulfilling the growing need for more effective and faster storage and release of energy. Development of high-performance electrodes and electrolytes is crucial in achieving that goal. Carbon aerogels stand out among various electrode materials due to their large specific surface area, light weight and outstanding electrical conductivity. The goal of this research was probing potential use of carbon aerogels with iron and cobalt as electrode materials for supercapacitors in alkaline, neutral and acidic medium. Fe-CA, $Co_{70}Fe_{30}$-CA-1 and $Co_{70}Fe_{30}$-CA-2 were synthesized with labels 1 and 2 referring to one-step and two-step synthesis procedure. Research was conducted by using cyclic voltammetry method [1,2]. All three materials delivered the highest currents and the highest specific capacitance in 1 M H_2SO_4, while the smallest capacitance values were determined in 1 M Na_2SO_4. Voltammograms further reveal pseudo-capacitance contribution to the total capacitance values as evident by redox processes giving rise to small redox peaks in 0.45 – 0.55 V region. Comparison of performance of two $Co_{70}Fe_{30}$-CA, revealed that $Co_{70}Fe_{30}$-CA-1 delivers higher currents and higher capacitance in every medium, indicating that the one-step synthesis gives better results. However, the addition of cobalt, besides iron, in carbon aerogels lowers its performance as electrode material for supercapacitors.

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PCC OP 03

Comparative study of synthetic, natural, and blended graphite anodes in lithium-ion batteries

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Graphite remains a key anode material in lithium-ion batteries (LIBs) due to its balanced representation of low-cost, high-energy density, and power density. This study focuses on the electrochemical performance of three types of graphite—synthetic, natural, and a 70:30 blend of synthetic to natural graphite—used as anode materials for advanced LIBs. Within this experiment, ten cells of each graphite type were tested, and performance was evaluated after more than 350 hours of cycling. Key parameters, including charge-discharge cycles, actual capacity, and Coulombic efficiency, are analyzed, with particular emphasis on SEI layer formation. The results reveal how each type of graphite influences battery performance, providing insights for optimizing the choice of anode material in next-generation LIBs.

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All experiments were conducted in the R&D laboratory of ElevenEs. The authors would like to express their gratitude to ElevenEs for providing comprehensive support in conducting the experiments, as well as for supplying high-quality natural and synthetic graphite samples, and assisting in the interpretation of the data.

PCC OP 04

Magnetic properties of *per*iodo-bicyclic hydrocarbons

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The concept of double aromaticity was introduced by Schleyer [1]. Compounds that possess two circularly delocalized electron systems can be considered as double aromatic. A well-known example is the hexaiodobenzene dication, $[C_6I_6]^{2+}$.[2] In this molecule, both π and σ electrons generate diatropic currents: the π electrons induce diatropic currents within the benzene ring, while the σ electrons induce diatropic currents in the outer ring formed by the iodine atoms. In this study, the double aromatic character of *per*iodo-bicyclic hydrocarbons was examined based on their magnetic properties and electronic aromaticity indices. Current densities, computed using the diamagnetic-zero variant of the continuous transformation of the origin of the current density (CTOCD-DZ) method, proved to be a powerful tool for both qualitative and quantitative assessments of double aromaticity. The magnetic aspects of double aromaticity were further compared with electronic aromaticity indices.

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PFC OP 01

Correlation between phenolic compounds and mineral content in wood species generated from cooperage

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Maturation of some alcoholic beverages, including fruit brandy (in Serbia known as 'rakija'), in contact with wood, is an important practice for obtaining high-quality products with improved sensorial characteristics, such as appearance and aroma. The type of wood used in that process influences significantly the quality of alcoholic beverages. Oak is the most commonly used wood species, because of its unique mechanical, physical and chemical properties. Due to the high price and limited quantity of high-quality oak wood, other wood species, such as cherry, black locust and mulberry are also used.

Cooperage wood is generally rich in phenolic compounds. It is also one of the sources of potentially toxic elements and other metals that may be transferred to alcoholic beverages during the maturation process. Although it is known that many flavonoids can form chelate complexes with metal ions, studies on the relationship between specific phenolic compounds and elements have not frequently published so far. In this work, different wood species commonly used in Balkan cooperage were studied. The aim was to investigate the correlations between mineral composition, total phenolic content, antioxidant capacity and specific phenolic compounds present in wood samples. Total phenolic content was determined by the Folin-Ciocalteu method, while antioxidant capacity was determined by the DPPH method. The mineral composition of wood is determined by inductively coupled plasma optical emission spectrometry (ICP-OES), while the content of phenolic compounds is determined by ultra-high performance liquid chromatography-diode array detector-triple-quadrupole mass spectrometer (UHPLC–DAD MS/MS). Multivariate statistical analysis was applied to obtain correlations between the elements and phenolic compounds present in wood samples. Conclusions were made according to the statistically significant correlations.

Acknowledgments

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SCFM OP 01

Characterization of lithiation-induced changes in anatase TiO_2 nanotubes: microstructural, electrical and optical insights

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Research in the field of nanotechnology has experienced expontential growth over the past few decades, with a particular focus on semiconductor materials [1]. Titanium dioxide (TiO_2) one such material, has garnered significant attention due to its low cost, low toxicity, long cycling life in Li-ion batteries, and high photo- and electrocatalytic activity. However, its low electrical conductivity and inability to utilize visible light severely limit its applications in Li-ion batteries and photocatalytic hydrogen production. Consequently, various strategies have been developed to overcome these obastacles [2]. Herein, anatase TiO_2 was prepared in the form of nanotubes (NTs) and subsequently lithiated to different extents at two different temperatures, 25 and 55 °C. The objective was to investigate the microstructural, electrical and optical properties of both pristine and lithiated TiO_2 NTs. Microstructural properties were examined using scanning and transmission electron microscopy (SEM and TEM), while changes in chemical composition, which occured due to lithiation, were analyzed with X-ray photoelectron spectroscopy (XPS). Electrochemical impedance spectroscopy (EIS) measurements revealed reduction in charge transfer resistance with lithiation, and four-point probe measurements showed an increase in specific electrical conductivity. Diffuse reflectance spectroscopy (DRS) demonstrated a decrease in energy gap from 3.04 eV for the as-prepared TiO_2 NTs to approximately 2.81 eV for the sample lithiated at 55 °C. Photoluminescence (PL) measurements indicate that lithiation suppresses deep-level trap states within the bandgap, while promoting shallow defect states. This observation was further confirmed by open-circuit photovoltage decay (OCVD) measurements. Moreover, enhanced performance of lithiated TiO_2 NTs towards hydrogen evolution reaction (HER) suggests that they could serve as noble or rare earth metals decorated substrates.

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SCFM OP 02

Investigation of the water stability of postmodified zirconium-based metal-organic frameworks with 4-nitrobenzaldehyde

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In this study, synthesis and characterization of imine-containing porous coordination polymers also known as metal-organic frameworks (MOFs) were performed. Specifically, UiO-67 based MOFs **1** and **2** incorporating two different ligands (2-amino-[1,1′-biphenyl]-4,4′-dicarboxylic acid and 2,2′-amino-[1,1′-biphenyl]-4,4′-dicarboxylic acid, respectively) were synthesized (Fig. 1). Post-synthetic modification of both types of MOFs with 4-nitrobenzaldehyde was carried out to form Schiff bases. The hydrolysis of the postmodified UiO-67-NH_2 (**1a**) and UiO-67-$(NH_2)_2$ (**2a**) MOFs was monitored using UV-Vis spectroscopy, SEM and EDS. All the obtained compounds were characterized by PXRD, TGA, NMR, and FTIR spectroscopy.

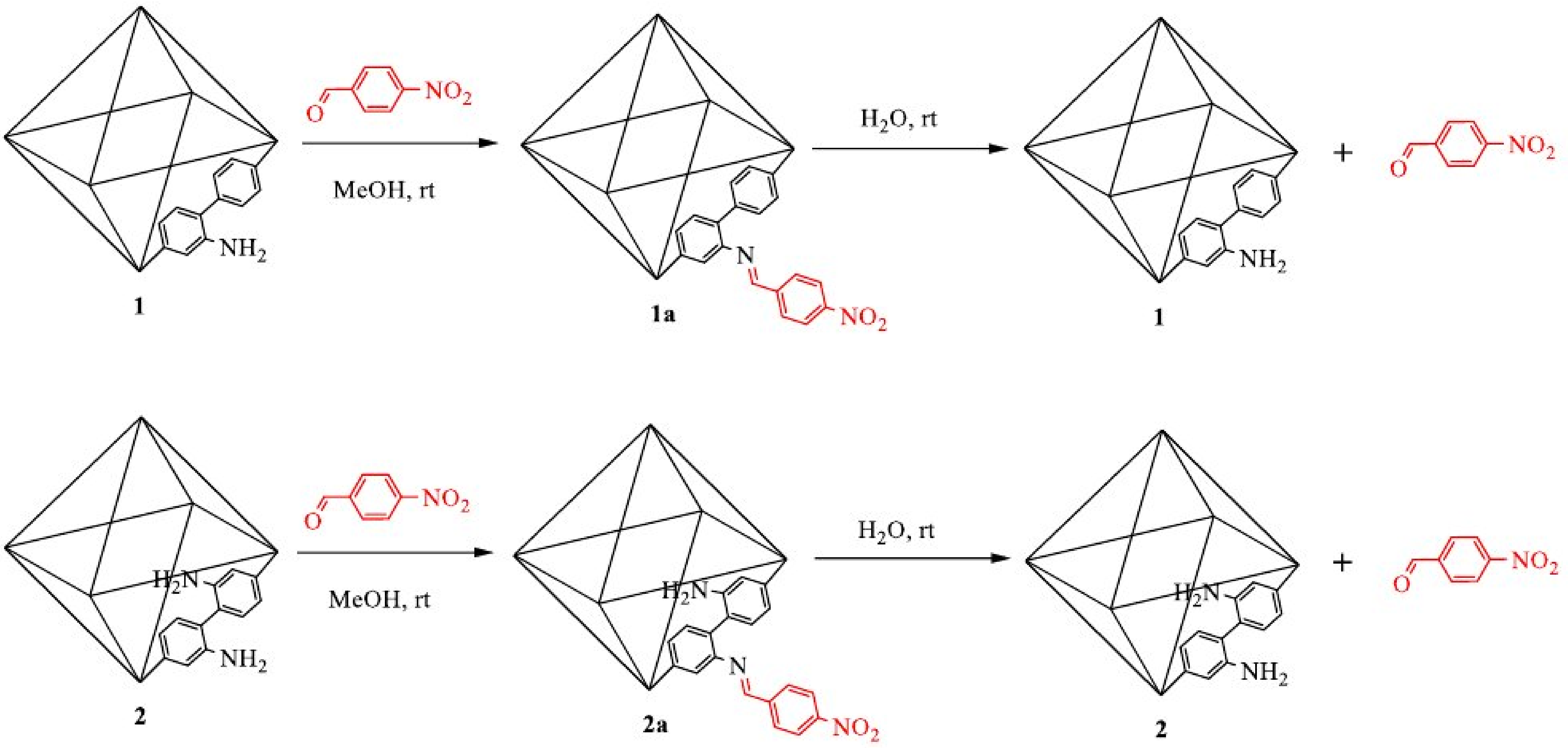

*Figure 1. Synthetic pathway to **1a** and **2a** from MOFs **1** and **2** via postmodification with 4-nitrobenzaldehyde and hydrolysis of postmodified **1a** and **2a**.*

Acknowledgments

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Flash Presentations

CB FP 01

Influence on iodine to the cytotoxicity of furofuranone compounds

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This abstract presents the synthesis and biological evaluation of a new C-5 goniofufurone analog (**1**, Figure 1). [1] The synthetic steps involved the reaction of D-ribose with Meldrum's acid, and the substitution of the primary hydroxyl group with iodine to obtain compound **1**. Antiproliferative activity was tested against eight human tumor cell lines and one non-cancerous cell line. Analysis of iodine group influence on cytotoxic activity of this type of compound was investigated and *in silico* ADME analysis of compound **1** to search and design novel analogs that will have improved antiproliferative activity and acceptable pharmaco-kinetic properties.

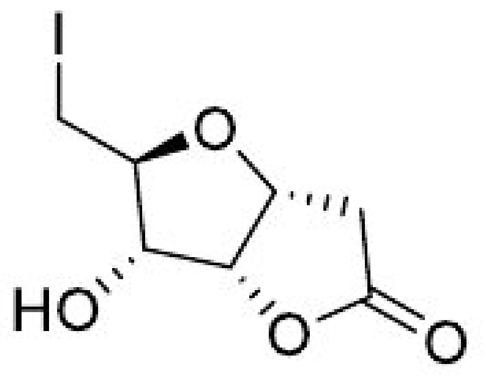

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Figure 1. Structure of novel C-5 goniofufurone analog (**1**).

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CB FP 02

Synthesis and cytotoxicity of novel furofuranone analog

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Herein, the synthesis of furofuranone compound (**4**, Figure 1) containing iodine moiety is presented. Firstly, we did cyclocondensation of D-ribose with Meldrum's acid [1], where the amount of Meldrum's acid, base, temperature, and reaction time were optimized to obtain compound **1** as the main product (Scheme 1). Then, the substitution of the hydroxyl group with iodine [2], within the optimization of reaction conditions, has been done to afford iodine **4** in better yield (Figure 1).

In addition to synthesis, the cytotoxicity of the obtained compounds was evaluated, and the *in silico* ADME test provided preliminary insights into their pharmacokinetic properties.

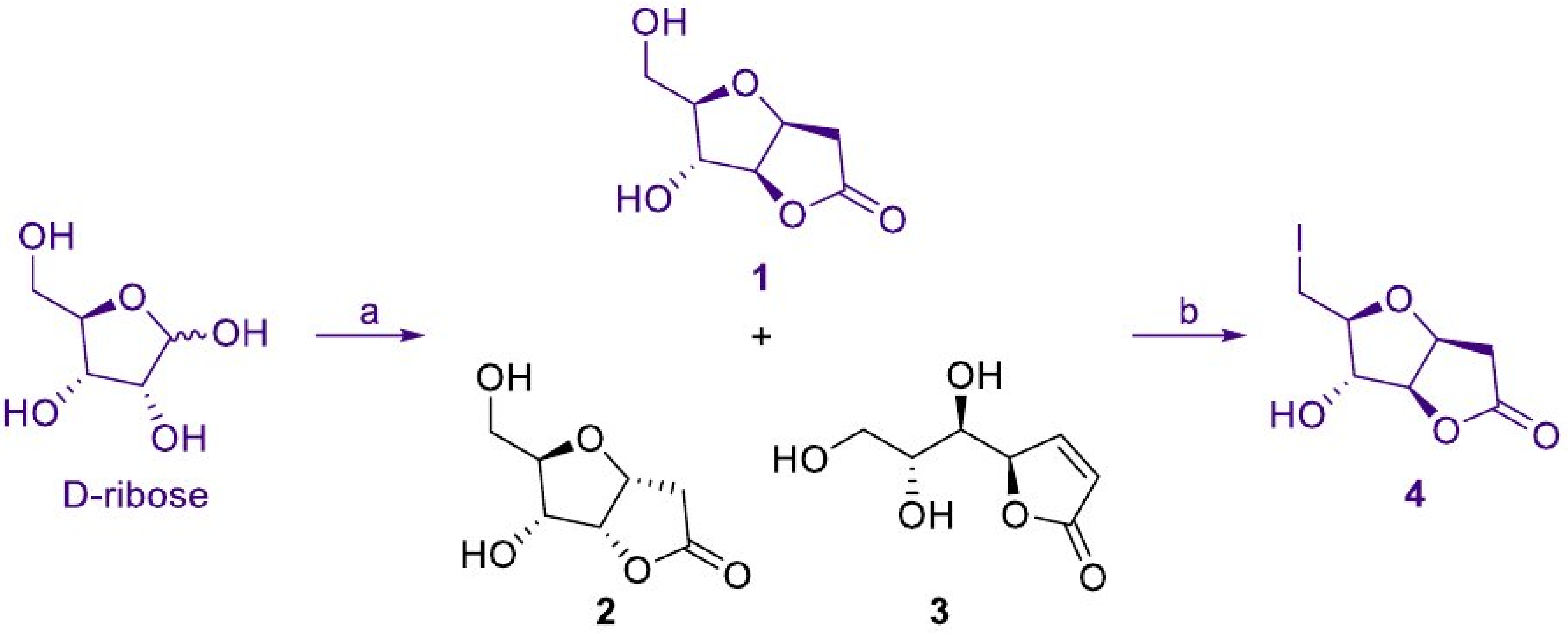

Figure 1. (a) Meldrum's acid, Et_3N, dry DMF; (b) I_2, imidazole, Ph_3P, dry THF.

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CB FP 03

Effects of different pre-processing methods on the outcome of partial least squares regression in infrared spectra obtained with DoE

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Attenuated Total Reflectance Fourier Transformation Infrared Spectroscopy (ATR-FTIR) is a spectroscopic technique that has been increasingly used in the field of metabolomics for its low cost, informative data and ease of use. Design of Experiments (DoE) is an umbrella term for mathematical operations aimed at predicting outcomes and optimizing processes with several changing variables. The Box-Behnken design is one of DoE's most popular models today. After optimisation, it is possible to collect infrared spectra from the samples obtained with DoE. Acquisition of spectral data is succeeded by pre-processing which can impact final results. In this work, the impact of different processing software solutions on the outcome of Partial Least Squares (PLS) regression was explored. The potential use of spectral data obtained was also investigated. The obtained Results showed that pre-processing methods significantly influence the Figures of Merit of the PLS models, as well as the ineptitude of this model to cope with spectral data obtained with Box-Behnken design.

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PCC FP 01

Energy decomposition analysis of cation-π interactions of sandwich compounds

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Ion-π interactions are prevalent in numerous chemical and biological systems. Within our recent interest in ion-π interactions of organometallic (half-)sandwich compounds [1], we have performed the Xiamen Energy Decomposition Analysis (XEDA) [2] of cation-π interactions of sandwich compounds. B3LYP(-D3)/def2-TZVP energies of cation-π interactions between six cations (Mg^{2+}, Ca^{2+}, Li^{+}, Na^{+}, K^{+}, NH_4^{+}) and six sandwich compounds (ferrocene, ruthenocene, osmocene, bis(benzene)chromium, bis(benzene)molybdenum, bis(benzene)tungsten) were decomposed into four physically meaningful components: electrostatic, polarization, exchange/repulsion and electron correlation/dispersion. XEDA reveals that in all cases the polarization component is the most responsible for remarkable strength of cation-π interactions. The observed dominance of polarization over electrostatic component is particularly pronounced for interactions of alkaline earth cations (Fig. 1).

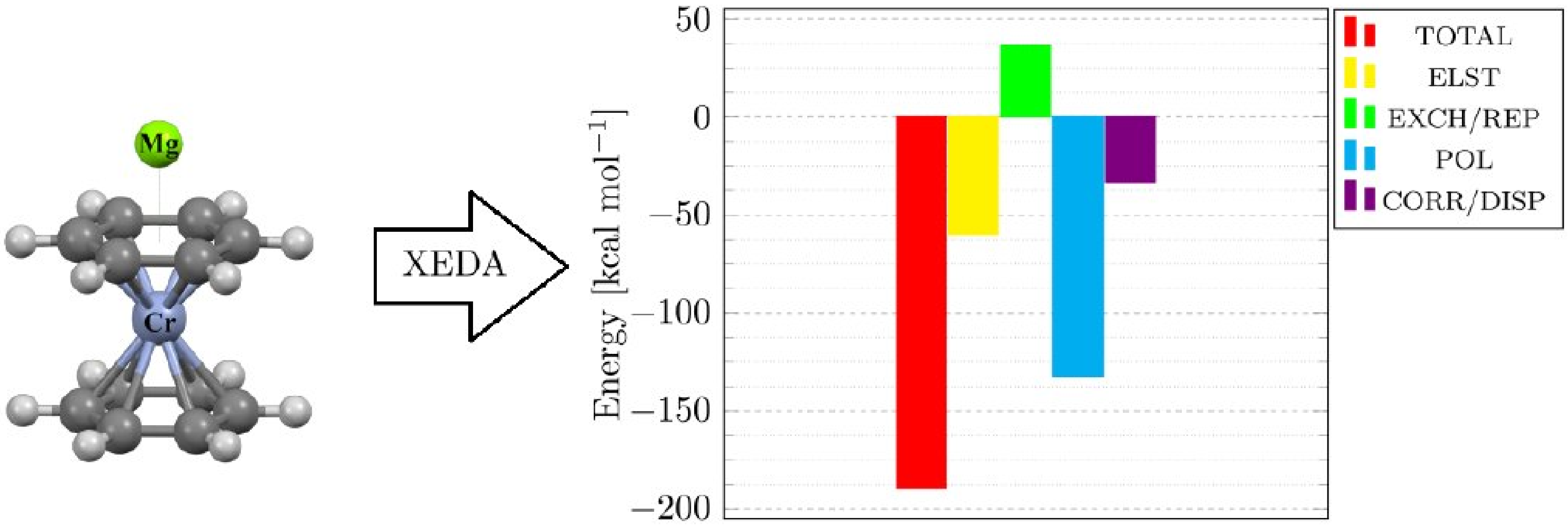

Figure 1. XEDA decomposition of cation-π interaction between Mg^{2+} and bis(benzene)chromium.

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PCC FP 02

On the nature of O-H/M hydrogen bonds of chelate complexes – DFT and EDA study

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Transition metal complexes are emerging as systems capable of forming strong hydrogen bonds [1], which can be utilized for obtaining materials with interesting properties [2]. In this work we have studied the nature of O-H/M hydrogen bonds between water and chelate complexes of *acac*, *NacNac* and *SacSac* type by the means of density functional theory and energy decomposition analysis. Calculations performed at the ωB97xD/def2-TZVP level of theory have shown that both metal and ligand have a big influence on the strength of O-H/M hydrogen bonds, which decreases in the following orders: Pt > Pd > Ni > Cu > Zn, and *NacNac* > *SacSac* > *acac*. The strongest calculated hydrogen bond is formed by Pt(NacNac)$_2$ complex (Figure 1), with interaction energy of –5.43 kcal/mol. Decomposition of interaction energies using the Xiamen Energy Decomposition Analysis shows that the most dominant energy component of O-H/M hydrogen bonds is in general the dispersion-correlation component. However, we show that total interaction energies are in linear relationship with electrostatics component, which can solely be used to explain the relative strengths of the observed hydrogen bonds.

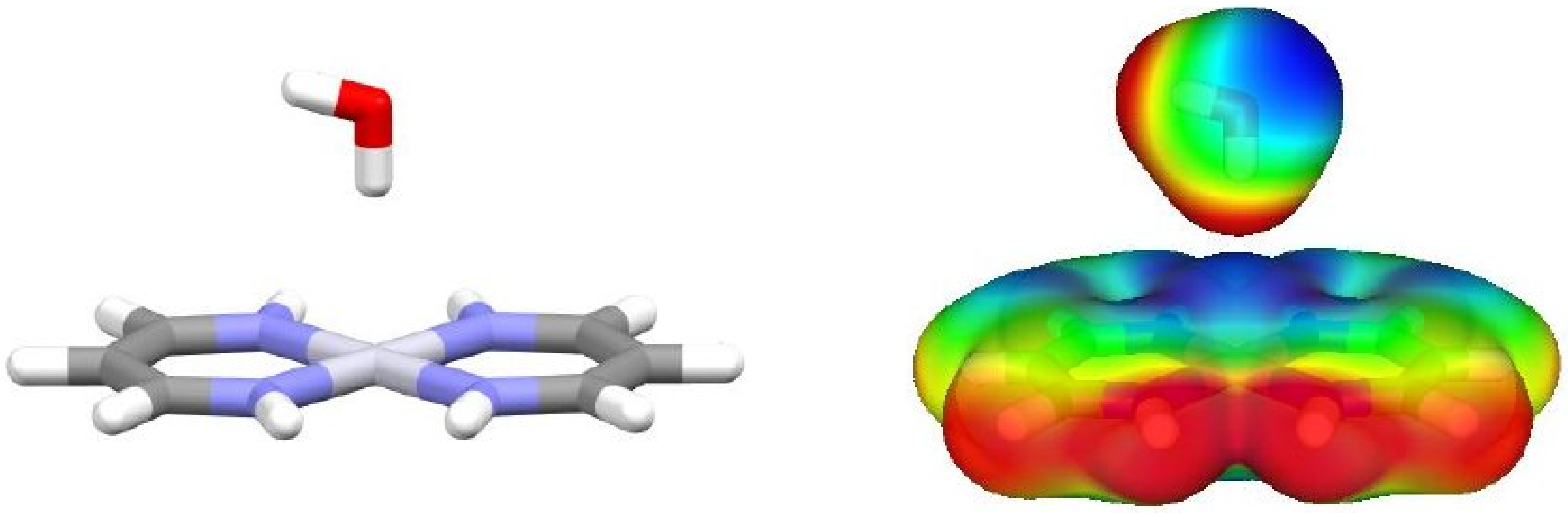

Figure 1. Electrostatic potentials of water and Pd(acac)$_2$ complex forming O-H/M hydrogen bond.

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PCC FP 03

Strong anion-π interactions between oxyanions and half-sandwich compounds – a DFT study

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Anion-π interactions are significant in many areas, ranging from crystal engineering and materials science to catalysis and receptor design, and they are typical for organic aromatic molecules with heteroatoms and/or electron-withdrawing substituents.[1] However, it was recently shown that halide anions can engage in very favorable anion-π interactions with organometallic half-sandwich compounds containing aromatic molecules without substituents or heteroatoms.[2]

In this work, we calculated the energies of anion-π interactions of several oxyanions – chlorate (ClO_3^-), perchlorate (ClO_4^-), nitrite (NO_2^-), nitrate (NO_3^-), sulfite (SO_3^{2-}), sulfate (SO_4^{2-}) and carbonate (CO_3^{2-}), with benzene and Cp ligands in half-sandwich compounds (Figure 1). The calculations were performed at the B3PW91-D3/def2-TZVP level of theory.

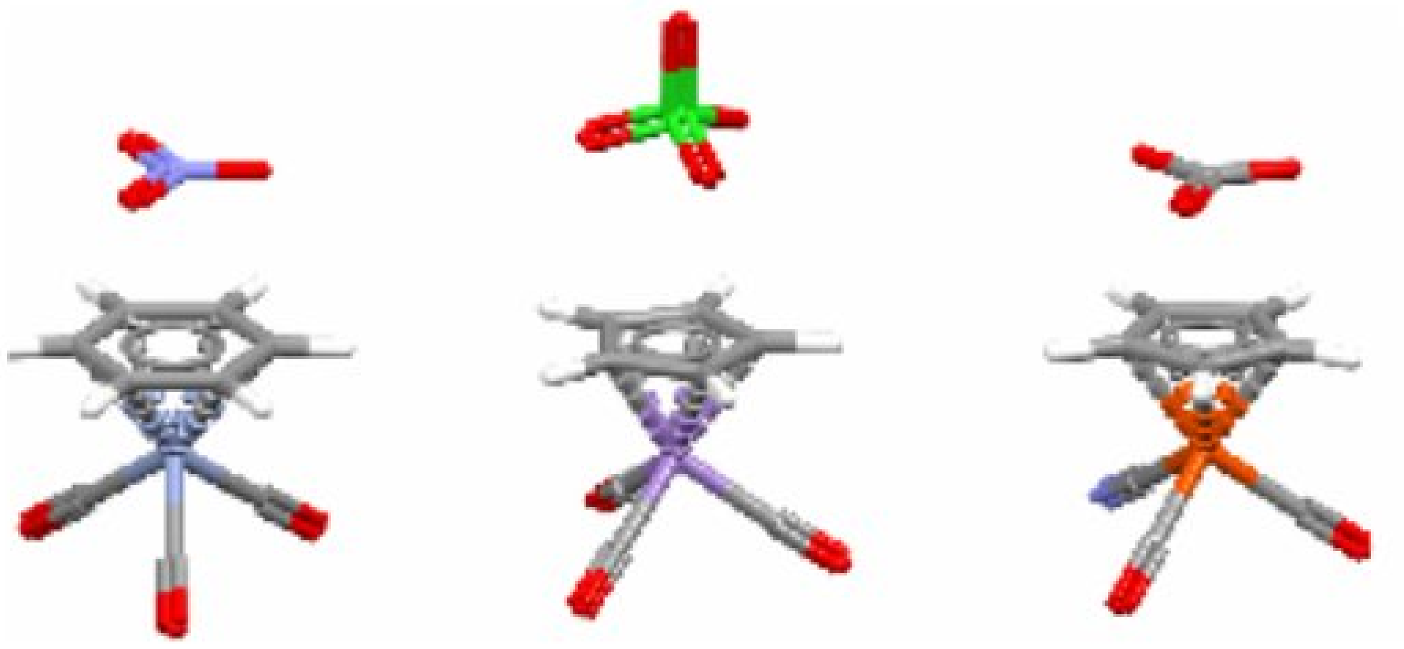

Figure 1. Anion-π interactions in Cr(benzene)$(CO)_3$/NO_3^-, MnCp$(CO)_3$/ClO_4^- and FeCp(CN)$(CO)_2$/CO_3^{2-} systems

The calculated interaction energies show favorable anion-π interactions, which are stronger for oxyanions with more negative charge. The strongest interactions are calculated for the Cp ligand in FeCp(CN)$(CO)_2$ with carbonate (–45.80 kcal/mol) and sulfate (–45.93 kcal/mol). The results show that half-sandwich compounds form significantly stronger anion-π interactions than organic aromatic molecules.

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Poster Presentations

Chemistry and Society (CS)

CS PP 01

Can the Android applications be successfully used in chemistry classes?

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The app *Chemical Substances* is great for two-way learning of chemical formulas of compounds. It also offers the possibility of checking answers, which makes it suitable for self-study. A special challenge is the time-limited level, which, in addition to knowledge, also requires the ability to think quickly.

High school students encounter a large number of compounds and their formulas, the mastery of which can be made easier and very interesting by this application. As for the application in elementary school, it could be a good choice for working with students who are particularly interested in chemistry. The application has several levels, which provides a chance to activate students from the initial stage of learning. After mastering one level, you move on to the next, then the next. Quick and constant feedback that students receive can be stimulating and motivating.

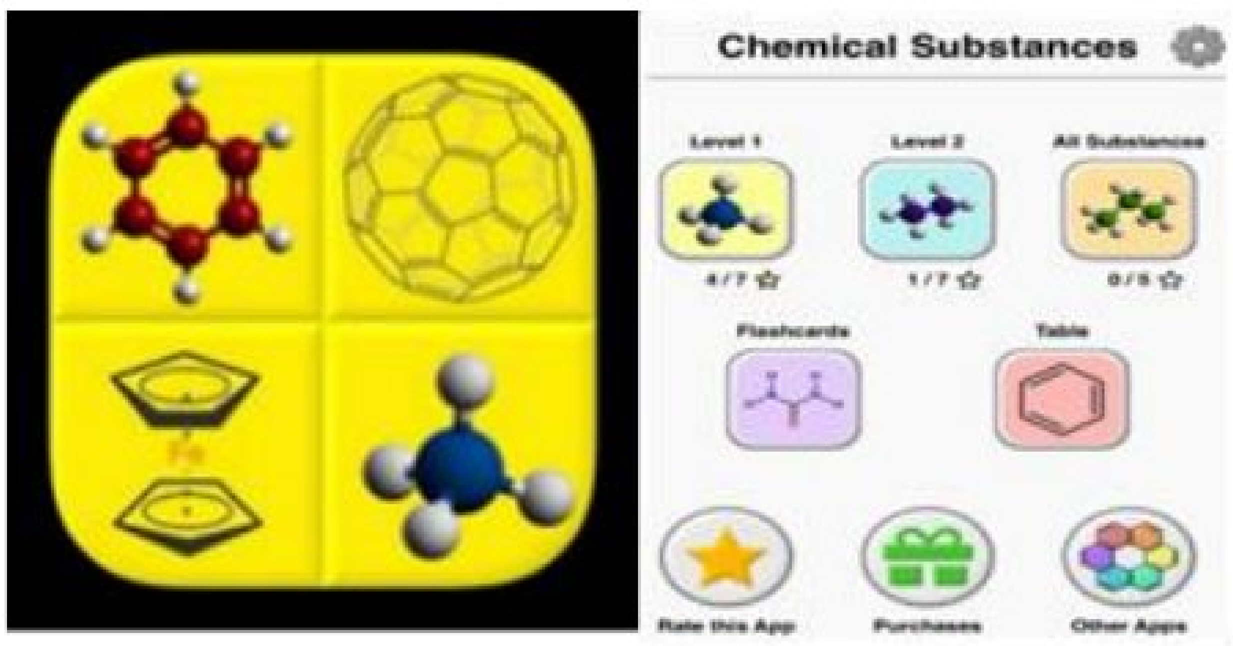

Figure 1. Icon and options App. Chemical Substances

Keywords: chemistry classes; android applications.

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Acknowledgments

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CS PP 02

Chemistry educational outcomes and standards in Serbia and Montenegro. Analysis of the teachers' attitudes

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Standards and outcomes-based education led to significant adjustments in school organizations and contributed to the in-depth analysis of teachers' professional identity. The educational reforms based on standards and outcomes started in the 2000s in Western Balkan countries, and stemmed from the criticism of the then exisiting educational system as highly centralized, and the curriculum as extensive and abstract. Due to strong historical ties, education in Serbia and Montenegro is structurally similar. In Serbian and Montenegrin educational systems, outcomes have the same meaning and show the desired and expected results expressed in the form of skills and knowledge that the student possesses at the end of a certain school year. On the other hand, standards of achievements, in Serbia, define the required knowledge, skills and attitudes for solving different social challenges and they are expressed in terms of measurable students' behavior, whilst in Montenegro, educational standards and outcomes are used interchangeably. This research aimed to examine the chemistry teachers' attitudes in the context of the implementation of the educational outcomes and standards in educational policy and in the school practices. The research sample included four chemistry teachers (three female and one male) from two countries, Serbia and Montenegro, with 10-20 years of teaching experience. The data were analyzed qualitatively jointly for two countries using mixed-methods research and constant comparison of the data. There are no significant differences in teachers' attitudes between these two educational systems. All teachers emphasized the importance of learning outcomes and standards and confirmed that they help them in organizing lessons and monitoring students' assessments. However, interviewed teachers pointed out the need for support and consideration of teachers' opinions about implementing educational changes.

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CS PP 03

Becoming a lab detective: an introduction to qualitative chemical analysis

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The importance of qualitative chemical analysis can be effectively demonstrated to pupils through straightforward laboratory exercises [1]. The objective of the proposed exercise, designed for late elementary and early secondary school pupils, is to identify four substances using their 5% aqueous solutions: magnesium chloride ($MgCl_2$), citric acid (CitA), sodium carbonate (Na_2CO_3), and sodium phosphate (Na_3PO_4). In this laboratory task, pupils are required to identify these substances solely through their mutual mixing in test tubes, with the recommendation to mix no more than two solutions at once. To ensure the experimental task is completed successfully, it is important to direct pupils to use Table 1 as a tool for applying logical reasoning and the method of elimination [2].

Table 1. Reactions of selected compounds

Compound	**$MgCl_2$**	**CitA**	**Na_2CO_3**	**Na_3PO_4**
$MgCl_2$	/	no visible reaction	$MgCO_3$ white precipitate	$Mg_3(PO_4)_2$ white precipitate
CitA	no visible reaction	/	CO_2 gas generation	no visible reaction
Na_2CO_3	$MgCO_3$ white precipitate	CO_2 gas generation	/	no visible reaction
Na_3PO_4	$Mg_3(PO_4)_2$ white precipitate	no visible reaction	no visible reaction	/

This proposed laboratory exercise introduces students to the fundamental concepts of qualitative chemical analysis while emphasizing the importance of integrating theoretical knowledge with practical laboratory work. It also highlights the significance of logical reasoning in addressing real-world challenges in chemistry.

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CS PP 04

Efficient distribution ratio lab exercise for college students

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The distribution ratio of a substance in two-phase systems of immiscible solvents (D_r) is a crucial characteristic with extensive applications, not only in laboratory settings but also in various industrial processes [1]. The study is aimed to provide college students and teachers in the natural sciences with an effective laboratory exercise in this specific area.

Aliquots of 30 cm^3 of a 0.1 mol/dm^3 aqueous solution of elemental iodine (I_2) containing 20 g/dm^3 of potassium iodide should be mixed with 30 cm^3 of each of the following solvents, respectively: cyclohexane, amyl alcohol, and amyl acetate. The resulting mixtures must be shaken every 5 minutes during 30 minutes in a separating funnel, after which the layers should be separated. Subsequently, the I_2 content in aliquot of 25 cm^3 of both the aqueous and organic layers needs to be determined volumetrically using a standard solution of sodium thiosulfate ($Na_2S_2O_3$; 0.1 mol/dm^3) and starch as an indicator. The D_r value of I_2 in the organic solvent/water systems should be calculated using the formula: $D_r = V_{os} / V_{aq}$, where V_{os} is the volume of $Na_2S_2O_3$ used to titrate I_2 in the organic layer, and V_{aq} is the volume of $Na_2S_2O_3$ used to titrate I_2 in the aqueous layer. The obtained D_r values must be discussed with students, considering the polarities of the used solvents, as well as the polarity of elemental I_2 and the triiodide anion.

This exercise provides an effective laboratory procedure for determining the D_r value of I_2 in three organic solvent/water systems. The straightforward quantitative determination of I_2 content in the final fractions enables students to calculate the D_r value directly from the volumes of the titrant used, without requiring prior calculation of the amount or concentration of I_2.

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Chemistry meets Biology (CB)

CB PP 01

Studying the aggregation of antiviral porphyrins and their peptide conjugates by molecular dynamics and UV/Vis spectroscopy

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Porphyrins, a class of macrocyclic compounds, are crucial in biological processes and are applied in catalysis, solar energy conversion; and photodynamic therapy (PDT) due to their ability to produce reactive oxygen species (ROS), which is an effective treatment for some cancer types [1]. With the increasing problem of multidrug-resistant microbes and viral infection outbreaks, porphyrins' antimicrobial properties are receiving renewed interest [2]. However, their therapeutic potential is challenged by aggregation issues. Aggregation behavior of antimicrobial porphyrins, specifically protoporphyrin IX (PPIX) and mesoporphyrin IX (MPIX), and their conjugates with cell-penetrating peptide PepH3 (AGILKRW) was investigated. The study employed all-atom molecular dynamics simulations to elucidate the aggregation mechanisms and the effects of peptide conjugation. UV/Vis spectroscopy goals included determining the spectral changes indicative of aggregation. The peptide AGILKRW was synthesized using solid-phase peptide synthesis (SPPS) and its conjugation with PPIX was performed while still anchored on the solid support. Successful synthesis of the PPIX-PepH3 conjugate was confirmed by MALDI-TOF-MS and LC-MS. Spectroscopic studies of PPIX in dimethyl sulfoxide showed a Soret band at 408 nm, which split and broadened with increasing water content, indicative of aggregation. Notably, peptide conjugation reduced these changes to a slight blueshift which suggests that peptide conjugation can mitigate extensive aggregation. *In silico* simulations revealed that porphyrins primarily aggregate through π-π interactions, forming dimers and larger aggregates. The peptide's presence altered this behavior, leading to the formation of globular structures stabilized by additional electrostatic and hydrogen bonding interactions. Effects of peptide conjugation, and subsequently aggregation state, on serum stability was also investigated.

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CB PP 02

Synthesis and *in silico* ADMET testing of novel 10-propargyloxy estrane derivatives

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Chemical transformations of natural estrogen hormones are a very popular research topic because of their important biological roles. Formation of dienone system in A-ring and introduction of alkoxy group in the steroidal core can be achieved through A-ring dearomatization of estran structure, in order to obtain new biologically active synthetic steroid derivatives. With this in mind, we have synthesized new 10-propargyloxy estrane derivatives (Figure 1). For synthesized compounds *in silico* ADMET analysis was carried out using the online SwissADME tool [1] and ProTox virtual lab [2]. Both compounds showed optimal ADME properties through competing calculated physicochemical parameters with those set by Lipinski, Veber, Egan, Ghose, and Muegge. The prediction of toxicity by the ProTox tool indicates that compound **1** belongs to Toxicity Class IV of compounds that are harmful if swallowed. In contrast, compound **2** is predicted to be Toxicity Class VI or the non-toxic group. Also, a virtual screening was performed in order to determine the receptors or enzymes to which the obtained compounds would potentially bind, and therefore to predict their biological activity. This work resulted in detecting the proteins for which the synthesized compounds show the highest affinity. Based on results obtained by SwissTarget Prediction, both synthesized compounds show the highest probability of binding for cytochrome P450 19A1 enzyme.

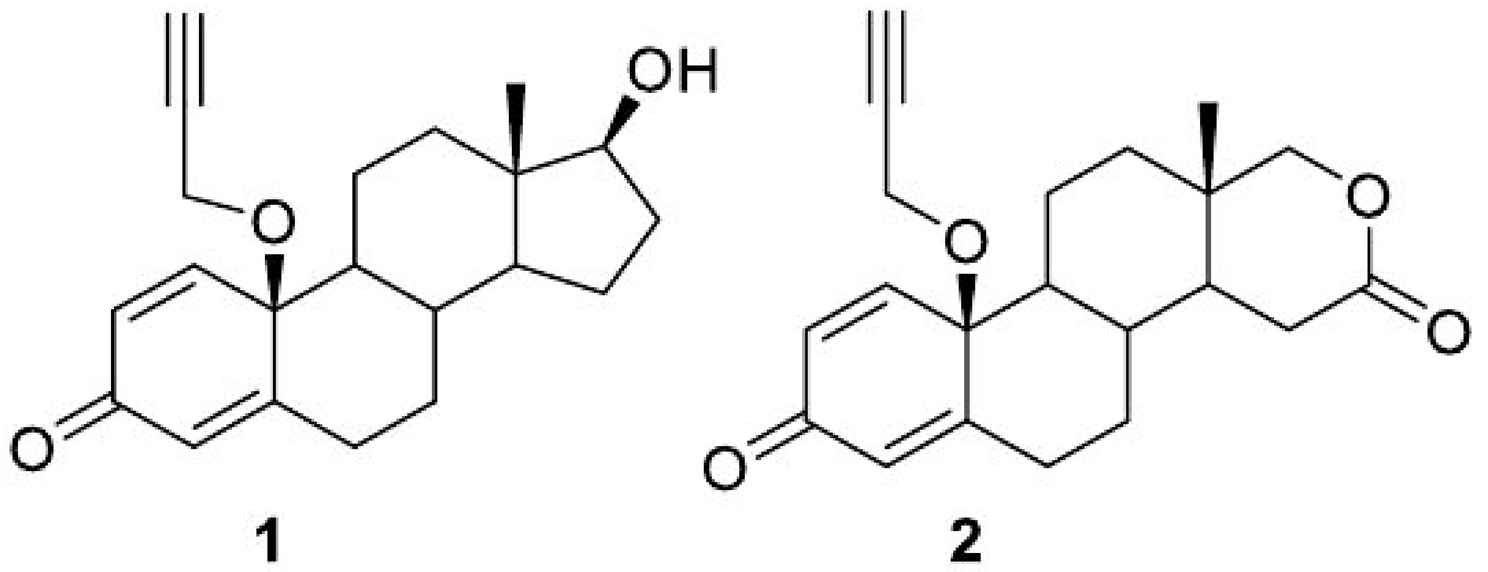

Figure 1. Structure of synthesized compounds ***1*** *and* ***2***

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CB PP 03

Synthesis, antimicrobial, antioxidant activities and BSA binding properties of some new Schiff's bases derived from benzylamine

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The synthesis of Schiff's bases derived from benzylamine and eight different aldehydes has been performed in absolute ethanol as a solvent. Bearing in mind that Schiff's bases are compounds with the wide range of biological activities, such as antifungal, antibacterial, anti-malarial, antiproliferative, anti-inflammatory and antipyretic [1], in this study, we presented the synthesis and characterization of eight novel imines and their antimicrobial and antioxidant activities. The required Schiff's bases were obtained in good yields. Antimicrobial and antioxidant assays of tested compounds showed potent antifungal activity, especially with compounds which incorporate quinoline or pyridine moieties. Those compounds have a better activity then standard drug Ketoconazole against *Penicillium italicum*. As the effectiveness of a potential drug depends on its ability to bind to a protein carrier and to be transported in bloodstream, the investigation of binding affinity of the most active imine to bovine serum albumin (BSA) was performed. Binding parameters as Ksv, Ka, k_q and n are calculated [2] and obtained values are in the favorable range which indicates the strong binding of examined compound to BSA.

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CB PP 04

Synthesis, chemical characterization, cytotoxic effect, and cellular localization of iridium(III) complexes

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Cancer is in second place as the deadliest disease after cardiovascular disease with a 2.74 million deaths in 2022. In the last decade, iridium(III) compounds have emerged as suitable substitutes for platinum complexes. As a transition metal, iridium exists in several oxidation states. Additionally, it was shown in a study from 2019 that various iridium(III) complexes in reaction with phenanthroline-type ligands exhibit a powerful cytotoxic activity toward gastric cancer cells and all complexes can generate reactive oxygen species (ROS).[1,2]

Here we present new nine Ir(III) complexes (C1 – C9) with general formula $[Ir(pyp)_2(L1\text{-}9)]PF_6$, where L1-9 are phenanthroline derivatives. All complexes were obtained in reaction using $[Ir(pyp)_2Cl]_2$ as the starting compound and the corresponding ligand in a mixture of methanol and dichloromethane with NH_4PF_6 as a counter ion. After 24 h all of them precipitated as an orange powder. All complexes were characterized with ^1H, ^{13}C NMR, IR spectroscopy, elemental analysis, and high-resolution mass spectrometry. Newly synthesized complexes expressed strong *in vitro* cytotoxic potential toward MDA-Mb-231 and HCT116 cancerous cell lines that were determined by MTT assay. Furthermore, a localization assay with confocal microscopy was performed on the most active Ir(III) complex on the MDA-Mb-231 cell line. This analysis revealed that the Ir(III)-complex is localized in mitochondria.

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CB PP 05

Molecular dynamics of peptide-based inhibitor targeting Aβ42 fibril formation in Alzheimer's

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Inhibiting amyloid-beta (Aβ) fibril formation is essential for Alzheimer's disease (AD) therapy [1]. This study examines the interactions between a newly designed peptide inhibitor [2], referred to as Peptide 2, and Aβ42 fibrils using molecular dynamics (MD) simulations over 100 nanoseconds. The MD simulations demonstrate that Peptide 2 stably interacts with critical residues Asp7, Tyr10, His14, Lys16, Leu17, Ile31, Gly33, and Leu34. These interactions involve hydrogen bonds and hydrophobic contacts, significantly stabilizing the Aβ42 monomer structure. The importance of these residues is further supported by prior structural studies and validated by recent research findings [1, 2]. The Root Mean Square Deviation (RMSD) and Root Mean Square Fluctuation (RMSF) analyses confirm that Peptide 2 effectively inhibits the conformational changes necessary for fibril growth. This study underscores Peptide 2's potential as a therapeutic agent for AD, laying the groundwork for the development of peptide-based inhibitors targeting amyloid aggregation in neurodegenerative diseases.

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CB PP 06

Disarming Parkinson's: targeting key residues in alpha-synuclein with VAQKTmV

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Alpha-synuclein, a critical protein implicated in Parkinson's disease, plays a central role in neurodegeneration through its aggregation into fibrils [1]. This protein is structurally divided into three regions: the N-terminal domain (Met1–Lys60), which contains amphipathic repeats facilitating membrane interactions; the central NAC region (Glu61–Val95), crucial for its aggregation; and the acidic C-terminal domain (Lys96–Ala140), essential for chaperone-like functions [1]. This study investigates the molecular dynamics of VAQKTmV, an innovative N-methylated peptide inhibitor designed from the Val77–Val82 sequence within the NAC region, specifically targeting alpha-synuclein aggregation [2]. Through molecular dynamics simulations, VAQKTmV was found to establish significant interactions with key residues such as Ser42, Lys80, Thr81, Val82, Ile88, Asp135, Tyr136, and Glu137. These interactions stabilize alpha-synuclein in non-aggregating conformations, thereby inhibiting its pathological aggregation. The observed interactions align with prior research that identified these residues as critical targets for effective inhibition of alpha-synuclein aggregation [1, 2]. This study provides valuable insights into the rational design of new, potent peptide inhibitors, highlighting the importance of targeting specific amino acids to combat Parkinson's disease.

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CB PP 07

Application of MIPAR Software in the Identification and Quantification of Novel Antifungal Agents

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In contemporary medicine, identifying and quantifying new antifungal agents is a critical challenge in combating fungal infections, which are increasingly prevalent and often resistant to existing treatments. Fluorine-containing compounds are known for their biological activities, and their antifungal properties are becoming increasingly significant in the context of fungal infection control. This study explores the application of MIPAR software, a powerful tool for data analysis in the fields of chemical and biomedical research. The discovery and evaluation of new antifungal agents and interpretation of complex biological data enables precise analysis of spectroscopic and other relevant data, thereby MIPAR enhances the efficiency of identifying potential candidates for new therapies. This work investigates the antifungal effects of ammonium fluoride against the pathogens *Aspergillus niger* and *Aspergillus flavus*, which are responsible for numerous diseases in humans and plants. Quantification of antifungal effects that impact growth rate and petri dish fungal surface coverage was performed using digital images analyzed with MIPAR software. The findings reveal significant differences in antifungal activity between *Aspergillus niger* and *Aspergillus flavus*. Our study revealed that *Aspergillus niger* was completely inhibited by ammonium fluoride, whereas the effects on *Aspergillus flavus* were less pronounced. These results highlight the potential of ammonium fluoride as an effective antifungal agent against *Aspergillus niger*, which may contribute to the development of new therapeutic strategies for fungal infection control. The use of digital imaging combined with MIPAR software represents an innovative approach to researching antifungal agents and can significantly enhance methodologies in this field. This study underscores how integrating software imaging technologies can improve research processes, reduce the time required for discovering new agents, and contribute to the development of more effective antifungal therapies. One of the future implementations for MIPAR software is using its machine learning capabilities and analyzing video frames as images form constant monitoring.

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CB PP 08

Design and synthesis of novel steroidal NRF2 activators

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Nuclear factor erythroid 2-related factor 2 (NRF2) is a pivotal regulator of cellular defense mechanisms against oxidative stress and inflammation, making it a prime pharmacological target for various non-communicable diseases, including inflammatory, neurodegenerative, metabolic, and cancerous conditions. Steroidal compounds, by virtue of their biologically privileged structure, have shown significant interactions with the NRF2 pathway. This is exemplified by natural products and FDA-approved drugs such as Ursodeoxycholic acid, which modulate physiological functions through NRF2 engagement [1].

Here, we aim to present the synthesis and preliminary results of biological activities of our NRF2 activators. The novel compounds are based on the bile acid steroidal skeleton with known electrophilic pharmacophores, the enone functional group, in the steroidal A and C rings (Fig. 1.). The reaction sequence starting from natural bile acid will be presented in detail.

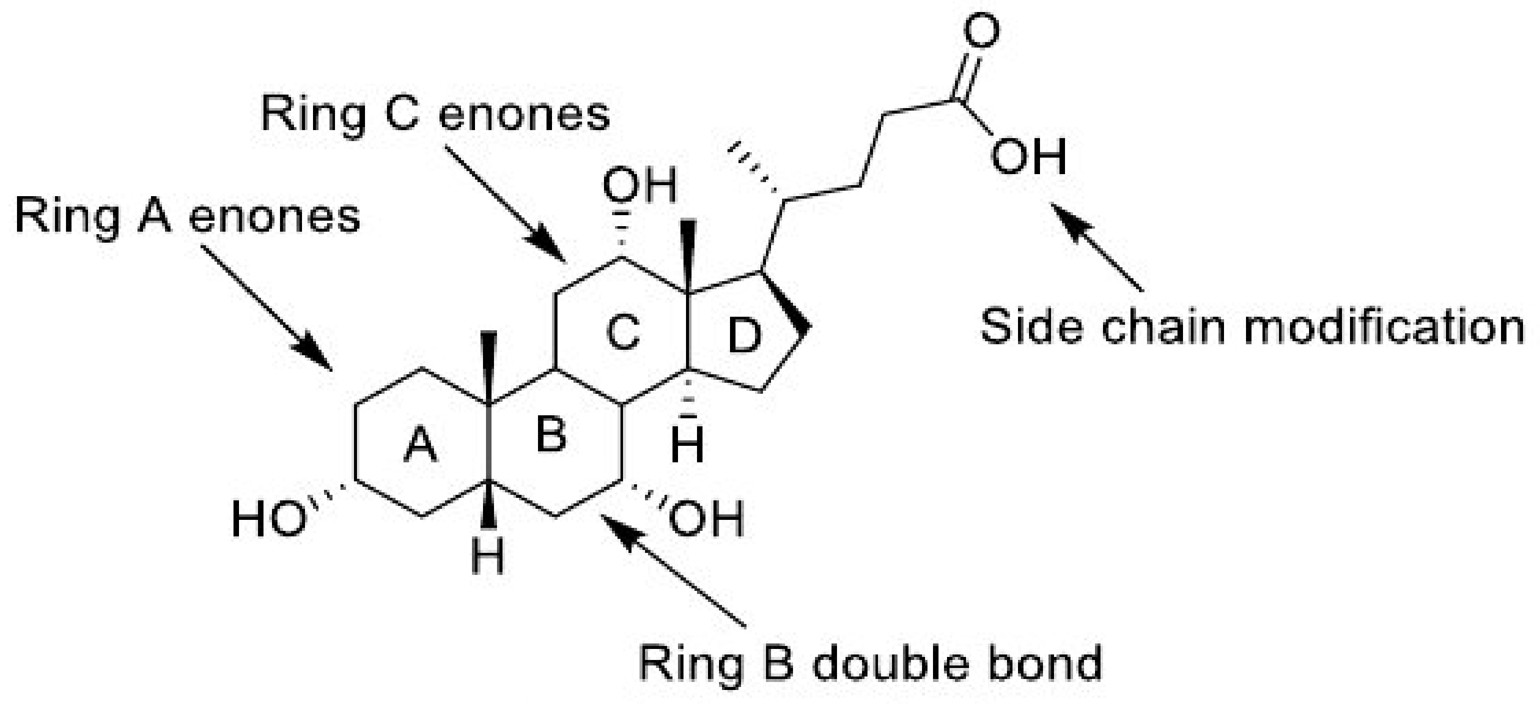

Figure 1. Cholic acid adjustments

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CB PP 09

Effect of pH on piroxicam interactions with Fe^{3+} ions in water

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Piroxicam (PRX) belongs to the oxicam class of nonsteroidal anti-inflammatory drugs (NSAIDs). It shows analgesic, antipyretic and anti-inflammatory effects [1]. PRX is amphiphilic, containing two ionizable groups (pKa 1.86 and pKa 5.46) [1], and heteroatoms available for coordination with different metal ions. In this study, interactions of PRX with Fe^{3+} ions were investigated in water at different pH values using UV-Vis spectroscopy and cyclic voltammetry (CV). The formation of a PRX-Fe^{3+} complex takes place at acidic pH values (pH 2, pH 4 and pH 5). In a neutral solution (pH 7) PRX is present in an anionic form favorable for coordination with metal ions, but its complex with Fe^{3+} is not formed due to the low solubility of Fe^{3+}. CV measurements were performed at pH 4 and pH 5 to study the redox properties of PRX in the presence of Fe^{3+} ions. At pH 4, the presence of Fe^{3+} ions stabilizes PRX towards oxidation, while at pH 5 the interactions with Fe^{3+} ions make PRX more prone to oxidation, and this difference can be attributed to the presence of a higher amount of doubly deprotonated (anionic form) of PRX at pH 5 (pKa 5.46). The change in Fe^{3+} reduction potential was also detected, additionally indicating the formation of the PRX-Fe^{3+} complex. It has been shown that coordination of NSAIDs to metal ions changes the effects of these drugs improving their biological activity [2]. According to this, further characterization of PRX-Fe^{3+} complexes and examination of their biological activity can be of interest.

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CB PP 10

Assessment of lipophilicity of thiocarbohydrazone by using thin-layer chromatography

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Thiocarbohydrazones have attracted the attention of scientists due to their potential biological activities including antifungal, antimicrobial, antibacterial, antiviral, antioxidant and even antitumoral properties [1]. One of the most important molecular descriptors indicating the potential biological activity of a compound is lipophilicity. In this study, the lipophilicity of thiocarbohydrazones was determined experimentally by using reversed-phase thin-layer chromatography in the mixtures of water and two organic modifiers, separately, as well as computationally by using appropriate software packages. The existence of a correlation between the obtained chromatographic parameters, R_M^0 and m, as alternative measures of lipophilicity, and the partition coefficient, log$P$, as the standard measure of lipophilicity, along with selected ecotoxicity predictors of the studied thiocarbohydrazones, was examined by using linear regression analysis.

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CB PP 11

The influence of the chemical structure on the antioxidant activity of acridine-1,8-dione derivatives

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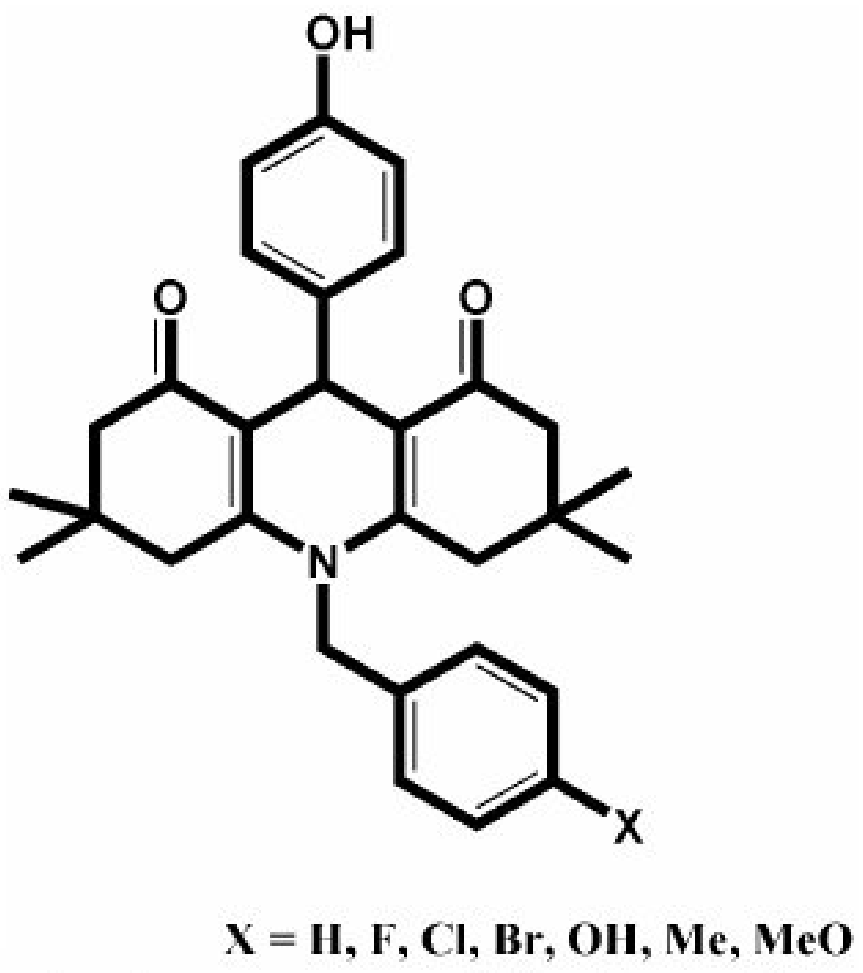
Acridine-1,8-dione derivatives are compounds with unique physicochemical and pharmacological properties and wide industrial applications. Thanks to their semiplanar structure and the ability to bind to various biological receptors, analogues of this condensed heterocycle are widely commercially available and as such have found application in the treatment of malaria (quinacrine), bacterial infections (acriflavine and proflavine) and cancer (amsacrine and nitracin) [1]. The influence of the chemical structure on the pharmacological potential of seven disubstituted derivatives of 3,3,6,6-tetramethyl-3,4,6,7,9,10-hexahydroacridine-1,8-dione (Figure 1) was evaluated using the "rule of five", Veber's, Egan's and Goz's empirical criterion, as well as by applying different *in silico* methods. In order to establish a correlation between the empirically estimated and experimentally determined pharmacological activity of seven disubstituted 3,3,6,6-tetramethyl-3,4,6,7,9,10-hexahydroacridine-1,8-diones, the potential antioxidant activity of the synthesized compounds was evaluated using ABTS (2,2'-azinobis-(3-ethylbenzothiazoline-6-sulfonic acid)) method and by determining the IC_{50} values of the most effective compounds.



X = H, F, Cl, Br, OH, Me, MeO

Figure 1. Chemical structure of the investigated compounds

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CB PP 12

Synthesis and biological evaluation of amodiaquine derivatives as inhibitors of human cholinesterase

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Alzheimer's disease (AD) is a complex neurological age-related disorder. Today, AD treatment is aimed mainly at increasing the level of the neurotransmitter acetylcholine by inhibiting acetylcholinesterase (AChE) and butyrylcholinesterase (BChE), the enzymes responsible for its hydrolysis. In this study, we explore the influence of different substituents in the quinoline part of the amodiaquine (AMQ) molecule on the inhibition of human AChE and BChE and evaluate the possibility of their use as drugs for the symptomatic treatment of AD. We synthesized AMQ derivatives that differ in the type and disposition of substituents on the quinoline ring (H-, Cl-, F-, CF_3-, NO_2-, CN-, CO_2H- or CH_3O- groups). Using *N*-(4-hydroxyphenyl)acetamide and diethylamine or 2-(ethylamino)ethan-1-ol in the Mannich reaction the key intermediaries were obtained, which were upon deacetylation put in the final coupling reaction with corresponding 4-chloroquinolines and provide the final products. Using 4-chloroquinoline-5-carbonitrile an unexpected product was obtained due to hydrolysis of CN-group, by neighbour activation through hydrogen-π interaction. Also, corresponding 5-F and 5-NO_2 derivatives were not obtained under the same reaction condition. All of the synthesized compounds were tested for their ability to inhibit the action of AChE and BChE, and for all of them, a reversible mode of inhibition was identified. The range of dissociation constant of the enzyme-ligand complex (K_i) for AChE was 0.025 to 7.6 µM and for BChE 1.7 to 21 µM. Molecular modelling was used to analyze the obtained kinetic results. In addition, metal chelating properties and antioxidative potential were determined and the drug-likeness of compounds was estimated *in silico*.

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CB PP 13

Lipophilicity assessment using the biomimetic immobilized artificial membrane chromatography

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The pharmaceutical companies use biomimetic and physicochemical measurements to assess the quality of newly synthesized drugs and their chance for clinical success in the earlier stages of drug design and development. It is recognized that the interactions in biomimetic chromatographic systems are analogous to the interactions that lead to the binding of drugs to their potential biological targets [1]. Immobilized artificial membrane (IAM) chromatography uses stationary phases that mimic the amphiphilic microenvironment of biological membranes, thus the corresponding retention mechanism shows good compatibility with drug pharmacokinetics [2]. Our research aims to examine the retention behaviour of structurally and therapeutically heterogeneous groups of compounds on the phosphatidylcholine (PC)-based IAM stationary phase. The chromatography analysis was performed by using the IAM.PC.DD2 HPLC column (10 µm, 100 x 4.6mm, Regis technologies), flow rate 0.8 ml/min, and UV detection at 220 nm. The optimal retention characteristics for all compounds were achieved using the mixture of acetonitrile and 10 mM ammonium acetate (pH 7), (30:70 v/v). The obtained values of the logarithm of the retention factor (log*k*) showed a high correlation with the lipophilicity of the investigated compounds ($r > 0.80$, $p < 0.05$) as well as with the *in silico* estimated binding to plasma proteins ($r > 0.83$, $p < 0.05$). The tested chromatographic system can be successfully used in the reliable prediction of the lipophilicity characteristics of tested compounds and their related analogs.

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CB PP 14

Biological activity of Zn(II) hydrazone complexes

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Three different Zn(II) complexes with (*E*)-2-(2-(1-(6-bromopyridin-2-yl)ethylidene)hydrazinyl)-*N*,*N*,*N*-trimethyl-2-oxoethan-1-aminium chloride (**HL**Cl) have been synthesized and characterized by single crystal X-ray diffraction, elemental analysis, IR and NMR spectroscopy. All complexes are mononuclear, with the ligand (L) coordinated in a deprotonated formally neutral zwitterionic form via NNO donor set atoms. Antibacterial and antifungal properties of these complexes were evaluated against two fungal strains, a yeast strain, and a panel of Gram-positive and Gram-negative bacteria. Notably, the selective antifungal activity of all three complexes is comparable to that of amphotericin B. Molecular docking studies predicted that geranylgeranyl pyrophosphate synthase, an enzyme important for sterol biosynthesis, is the most likely target for suppression by the tested complexes. Additionally, the cytotoxic activity of the complexes was tested against five human cancer cell lines (HeLa, A549, MDA-MB-231, K562, LS 174T) and normal human fibroblasts MRC-5.

Acknowledgments
This research was supported by the Science Fund of the Republic of Serbia, #7750288, Tailoring Molecular Magnets and Catalysts Based on Transition Metal Complexes ***TMMagCat***.

CB PP 15

Antioxidant properties of ferrocenyl cinnamoyl derivatives

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Cinnamic acid (CA) contains an α,β-unsaturated carbonyl moiety that acts as a Michael acceptor in drug design. Replacing the OH group in CA with an NHOH group produces the hydroxamic derivative CHA, which can coordinate metal ions and inhibit enzymes like lipoxygenase (LOX) [1]. Additional inhibition mechanism involves reducing the Fe^{3+} center in LOX. Incorporating ferrocene (Fc) enhances this inhibition; i.e. FcCOOH effectively inhibited human 5-LOX and reduced Fe^{3+} in the FRAP assay, while its phenyl analog was nearly inactive [2].

We present our findings on metal-based CA and CHA analogs, focusing on the Fc unit's impact on antioxidant activity. CA, CHA, and their Fc analogs (FcCA and FcCHA) were tested in the FRAP assay at 50 µM, using Trolox and FcCOOH as controls (Fig. 1). The Fc derivatives outperformed Trolox in reducing Fe^{3+} ions, while the phenyl counterparts showed no activity. FcCA exhibited a higher FRAP value than FcCOOH, suggesting that extended conjugation enhances antioxidant potential. Also, the hydroxamate group in FcHA improved its effectiveness. Future research will evaluate the anti-LOX activity of these derivatives.

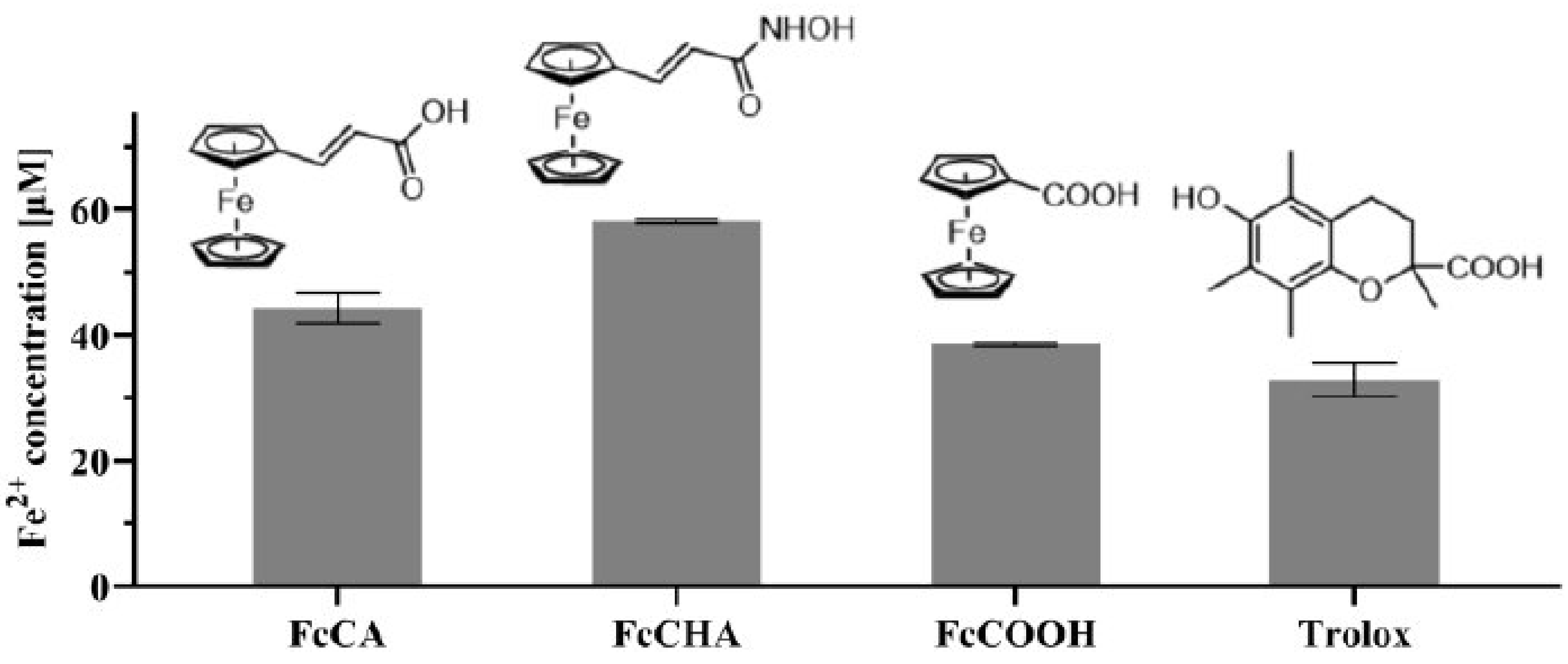

Figure 1. Results of the FRAP assay

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CB PP 16

Synthesis, *in vitro* hormonal activity and *in silico* analysis of new 17a-homolactone androstane carbamates

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Androgen (AR) and estrogen (ER) receptors belong to the steroid receptor subfamily and play a crucial role in the proliferation of hormone-dependent cancers, such as prostate and breast cancer [1]. Steroids represent a large class of biomolecules that exhibit a wide range of biological effects, including anticancer activity. On the other hand, carbamates are a large class of organic molecules that are part of many drugs used to treat various diseases, including cancer and Alzheimer's disease [2]. Since natural ligands for AR and ER play a significant role in the proliferation of cancerous cells, the aim of this research was to synthesize new steroidal D-homolactone androstane carbamates, evaluate their *in vitro* binding affinity for ERα, ERβ and AR ligand-binding domains, and conduct *in silico* ADME/T analysis. Based on a fluorescent screen in yeast, non of the new derivatives displayed affinity for androgen or estrogen receptors, suggesting negligible estrogenicity and androgenicity.

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CB PP 17

Efficient synthesis, ADME-Tox analysis and cytotoxic activity of benzoyl analogues of (−)-goniofufurone

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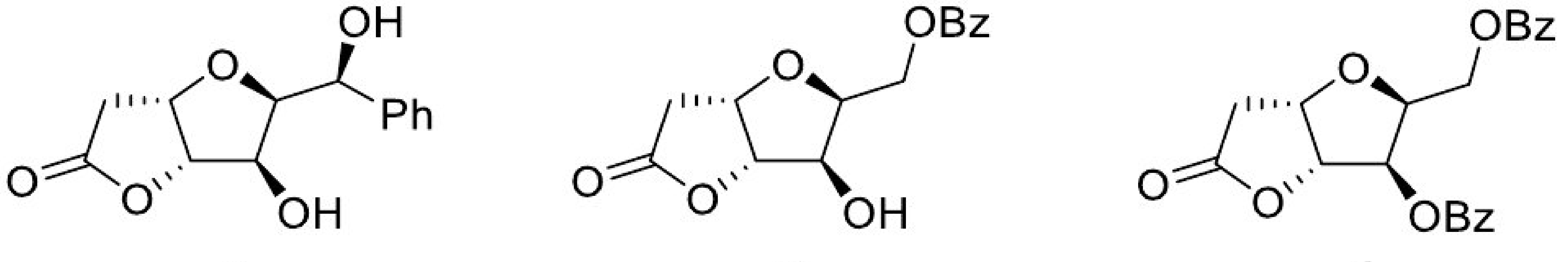
(–)-Goniofufurone (**1**) is the enantiomer of the naturally occurring cytotoxic lactone (+)-goniofufurone, which has previously demonstrated significant biological activity [1].

In this study, analogues of (−)-goniofufurone (**1**), compounds **3** and **4** (*Figure 1*), were synthesized from commercially available L-xylose. The benzoylation reaction was conducted under kinetically controlled conditions, resulting in obtaining mono- and di-benzoyl analogues (**3** and **4**). The synthesized compounds underwent *in vitro* testing against various tumor cell lines as well as normal fetal lung fibroblasts. In addition to antiproliferative activity, an ADME-Tox analysis was performed to evaluate the pharmacokinetic properties of novel dephenylated (−)-goniofufurone analogues.



1 **3** **4**

*Figure 1. Structures of (–)-goniofufurone **1** and new analogues **3** and **4**.*

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CB PP 18

Synthesis, ADME-Tox analysis and antiproliferative activity of new chloro analogue of (–)-goniofufurone

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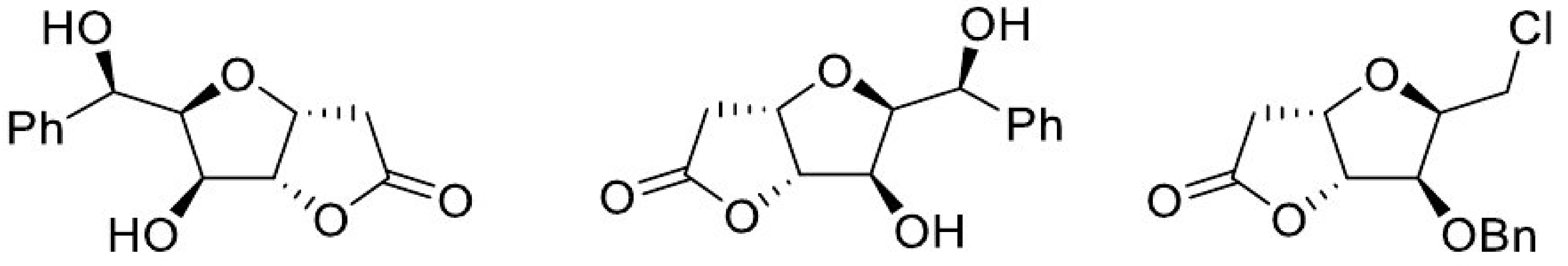
(–)-Goniofufurone (**1**) is a synthetic styryl lactone that exhibits significant antitumour activity [1] and is the enantiomer of the natural cytotoxic lactone (+)-goniofufurone (*ent*-**1**), which was isolated from the bark of the *Goniothalamus giganteus* tree in 1990 [2].

In this work, the efficient synthesis of a new dephenylated (−)-goniofufurone analogue (**5**) bearing a benzyloxy group at position C-5 and chlorine atom at position C-7 was achieved (*Figure 1*). Commercially available L-xylose was used as the starting compound. Additionally, the antiproliferative activity of the newly synthesized compound was examined and an ADME-Tox analysis was performed using the *SwissADME* tool to determine the pharmacological properties of the novel analogue **5**.



ent-**1** **1** **5**

*Figure 1. Structures of (+)-goniofufurone (ent-**1**), (–)-goniofufurone (**1**) and analogue **5**.*

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CB PP 19

Synthesis, characterization, antimicrobial activity of Cd(II) complex with a salicylaldehyde derivate

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Novel cadmium complex with methyl 3-formil-4-hydroxybenzoate (H**L**) has been synthesized and characterized by single crystal X-ray diffraction, IR and NMR spectroscopy. Crystal structure analysis shows that the formula of the complex is $[Cd(\mathbf{L})_2(H_2O)_2]$ and compound has octahedral geometry (Fig.1). Ligand was coordinated in a deprotonated form through the oxygen atoms of the phenolic and aldehyde groups. The antibacterial and antifungal activity of complex was evaluated *in vitro* on four Gram-negative and four Gram-positive bacterial strains, two fungal strains, and a yeast strain. Compound showed antibacterial activity towrds all bacterial strains. Antifungal activity of complex is comparable to the control compound amphotericin B.

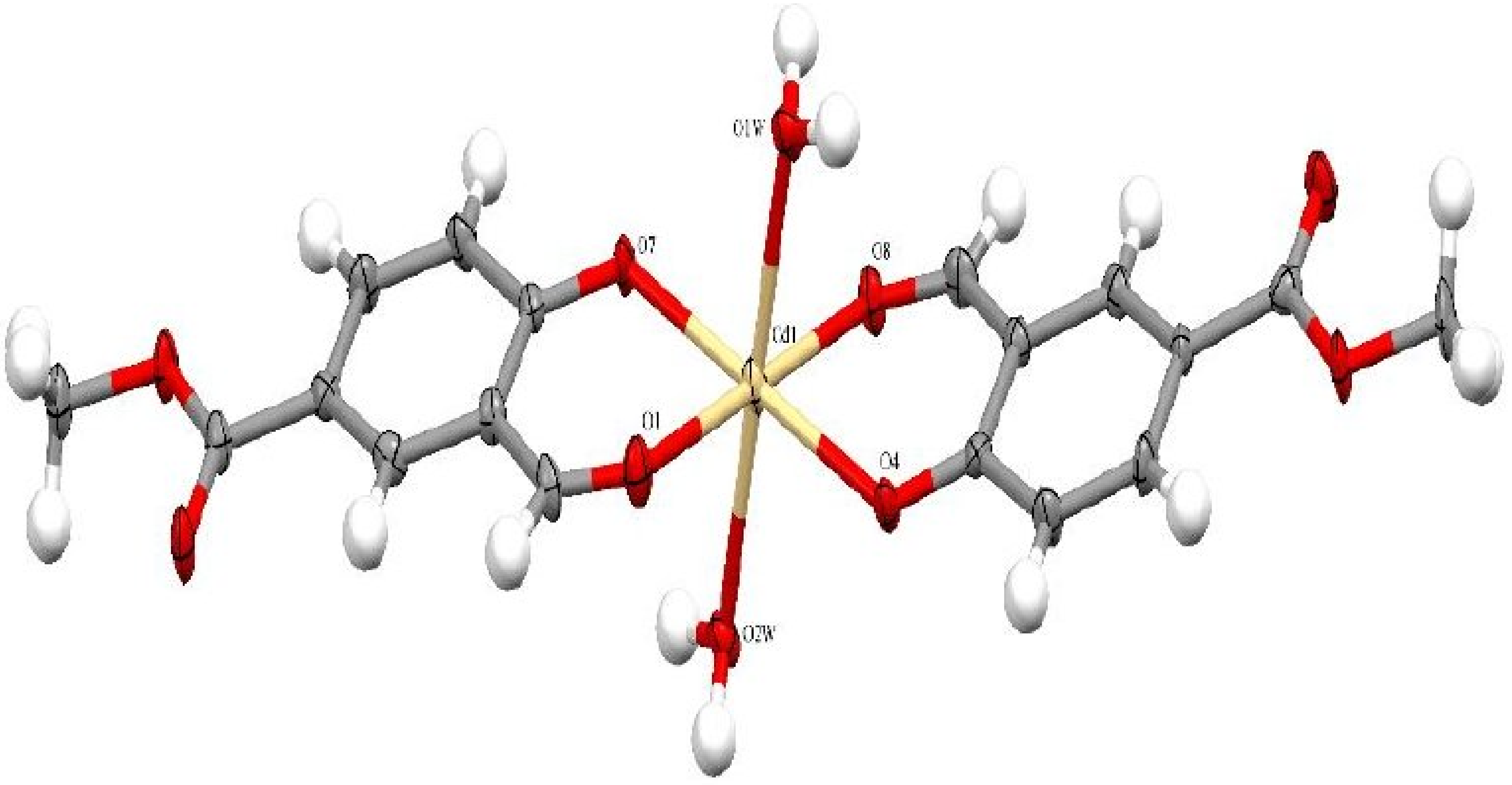

Figure 1. ORTEP representation of the $[Cd(\mathbf{L})_2(H_2O)_2]$ complex. Thermal ellipsoids are drawn at the 50 % probability level.

CB PP 20

Novel 4-aminoquinoline derivatives exhibit pro-ferroptotic activity in MIA PaCa-2 and PANC-1 cell lines

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Pancreatic ductal adenocarcinoma (PDAC) is a malignancy with an extremely high five-year mortality rate and highly resistant to conventional chemotherapeutic agents. Ferroptosis is a recently discovered caspase-independent programmed cell death caused by intracellular iron-driven membrane lipid peroxidation. Ferroptosis-inducing compounds, such as erastin, have been proposed as potentially effective against treatment-resistant tumors. Chloroquine, a quinoline derivative, exhibits anticancer properties, inhibiting cytoprotective autophagy. Our previous experiments have shown that 4-aminoquinoline derivatives induce apoptotic cell death and inhibit autophagy at low micromolar and nanomolar concentrations, which have been proven effective and non-toxic in zebrafish as animal models.

This study investigated the pro-ferroptotic properties of 4-aminoquinoline derivatives in 2D cultures of two PDAC cell lines, MIA PaCa-2 and PANC-1. Changes in mitochondrial membrane potential, caspase activity, and the expression of crucial ferroptosis- and autophagy-regulating proteins indicate that the 4-aminoquinoline derivatives tested induce caspase-independent cell death in both cell lines. Moreover, these compounds sensitize MIA PaCa-2 cells, which are resistant to erastin-induced ferroptosis, to ferroptosis. They also enhance ferroptosis in PANC-1 cells compared to erastin alone. These results demonstrate the promising potential of 4-aminoquinoline derivatives in ferroptosis-mediated anticancer therapy; they should be further examined in combination with other therapeutics in this field.

Acknowledgments

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CB PP 21

Optimization of sample preparation for short peptide sequencing by tandem mass spectrometry

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Tandem mass spectrometry plays a crucial role in proteomics for the identification and characterization of proteins. In bottom-up proteomics, complex proteins are initially fragmented into peptides through either chemical and/or enzymatic digestion before undergoing mass spectrometry analysis. Simple peptides, on the other hand, might not need harsh preparation conditions in order to provide results. In this study, we evaluated three preparation protocols of short peptides for MS. A control and a treatment sample were used, where total proteins were extracted using a 50 mM K-phosphate buffer, pH 7.5. Total protein samples were treated with an organic solvent in order to precipitate larger proteins, leaving only those with the size of 30 kDa or less in the supernatant. The three tested protocols were as follows: A) Single digestion – where samples were dried in a vacuum centrifuge, digested with trypsin in the presence of urea as a denaturation agent and desalted using Pierce C18 Spin Columns; B) Double digestion – where previously dried samples were treated with a LysC + trypsin proteinase mix followed by only trypsin in the presence of Rapigest™ as a mild protein denaturant and desalted using C18 columns; C) Desalting only – where samples underwent direct desalting using C18 columns immediately after organic solvent treatment. LC-MS/MS measurements were performed on a Cyclic QTof mass spectrometer (Waters™, USA) where 20 µg C protein was injected from each sample. The results were analyzed using the Byonic™ MS/MS Search Engine alongside an in-house peptide database. A total of 44 peptides were identified, with the Single digestion protocol showing the most hits – 40 in the control sample and 41 in the treatment sample. Double digestion had fewer hits, 24 and 17, while drying only proved to be the least effective with 17 and 14 hits from the in-house database. These findings underscore the importance of optimizing sample preparation techniques to enhance protein identification accuracy and reliability. As a result, the insights gained from this research will inform future experimental designs and contribute to improved methodologies in proteomic analyses, ultimately advancing our understanding of complex biological systems.

Acknowledgments

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CB PP 22

Crystallographic, quantum-chemical, protein-, and DNA-binding properties of two novel copper(II)–pyridoxal-aminoguanidine complexes with differing counterions (SO_4^{2-} and NO_3^-)

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New Cu(II) complexes with pyridoxal-aminoguanidine (PLAG) ligands and different counterions (SO_4^{2-} and NO_3^-) were prepared and their crystal structures were solved by the X-ray crystallography. Their molecular diagrams are presented in figure 1. The geometries of the obtained complexes significantly depended on the counterions, leading to the square-pyramidal structure of $[Cu(PLAG)NO_3H_2O]NO_3$ (complex 1) and square-planar structure of $[Cu(PLAG)H_2O]SO_4$ (complex 2). The intermolecular interactions were examined using the Hirshfeld surface analysis. The theoretical structures of these complexes were obtained by optimization at the B3LYP/6-311++G(d,p)(H,C,N,O,S)/LanL2DZ(Cu) level of theory. The Quantum Theory of Atoms in Molecules (QTAIM) was applied to assess the strength and type of the intramolecular interactions and the overall stability of the structures. The interactions between the complexes and transport proteins (human serum albumin (HSA)) and calf thymus DNA (CT DNA) were examined by spectrofluorometric/spectrophotometric titration and molecular docking. The binding mechanism to DNA was assessed by potassium iodide quenching experiments. The importance of counterions for binding was shown by comparing the experimental and theoretical results and the examination of binding at the molecular level.

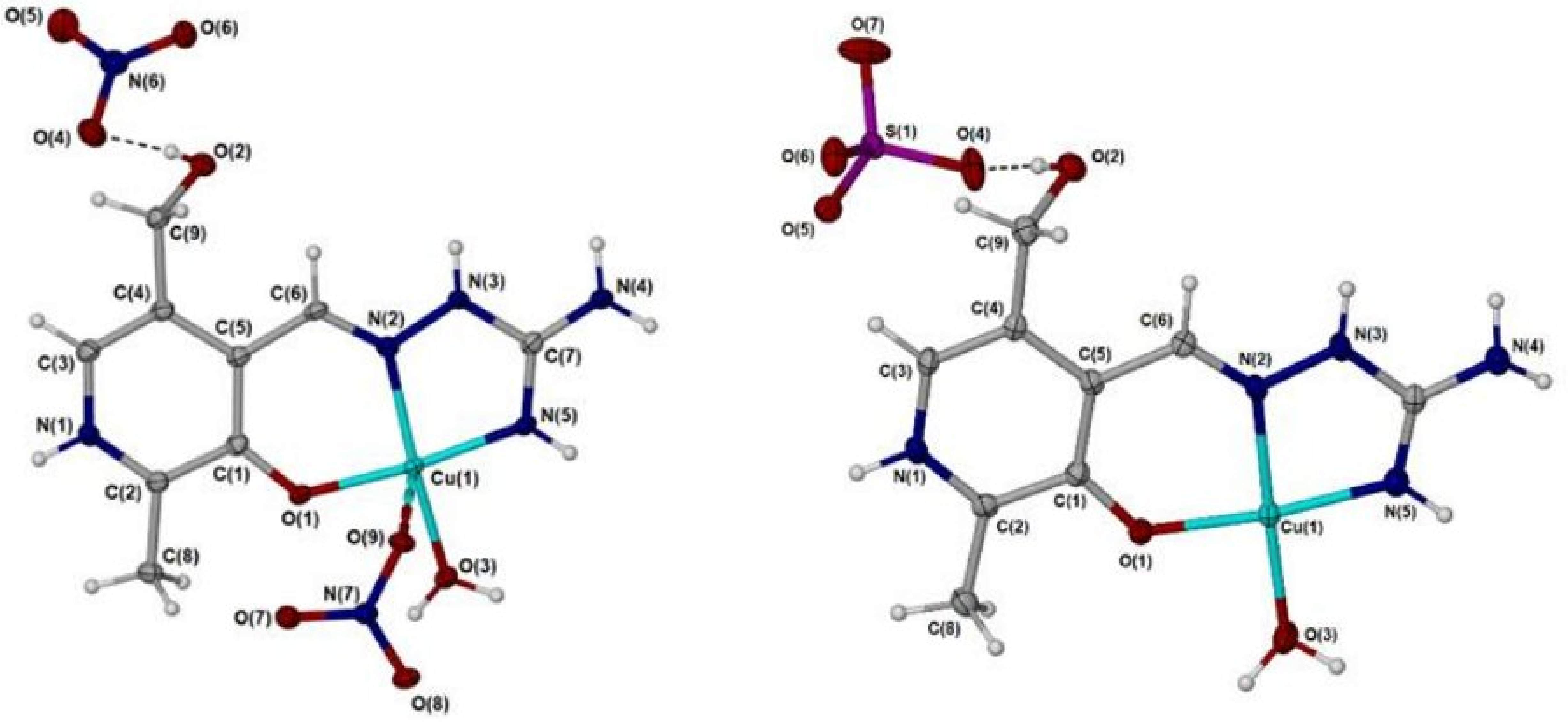

Figure 1. Molecular diagram of $[Cu(PLAG)(NO_3)(H_2O)]$NO3 (left) and $[Cu(PLAG)(H_2O)]SO_4$ (right) (PLAG=$C_9H_{13}N_5O_2$) with non-hydrogen atoms represented by 50% displacement ellipsoids and hydrogen atoms as spheres of arbitrary size.

CB PP 23

Assessing stem cell viability and redox potential using electrochemical and EPR techniques

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Stem cells and stem cell-conditioned media contain a complex array of bioactive molecules, including growth factors, cytokines, and extracellular vesicles. Because of this, they serve as promising alternative treatment modalities in regenerative medicine and have shown successful outcomes in some diseases [1]. The aim of this study is to determine the viability of stem cells using electrochemical methods and electron paramagnetic resonance (EPR) spectroscopy. To confidently differentiate between live and non-viable cells, dental pulp stem cells (DPSCs) were subjected to multiple freeze-thaw cycles

Electrochemical methods used to assess cell viability include cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS). While CV did not exhibit a predictable trend that could confirm cell viability, the results from EIS were more successful. The obtained Nyquist plots for viable and non-viable cells show a clear distinction. At lower frequencies, viable cells display characteristic capacitive behavior, which can be attributed to the intact cell membrane. In contrast, treated cell samples deviated from this behavior.

The EPR technique was used to detect the redox activity of cells against the stable free radical TEMPONE. EPR results show that cells scavenge radicals differently based on their viability. Dead cells exhibit a slower rate of EPR signal reduction compared to live cells, indicating that DPSCs in the medium have strong redox characteristics. In addition to their potential use in wound regeneration, they can also be applied to scavenge radicals generated by inflammation.

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projects from the Serbian Academy of Sciences and Arts (Grant No. F-130).

CB PP 24

Synthesis of 8-((2-aminoethyl)amino)-caffeine and investigation of its inhibitory effect on chymotrypsin and pepsin

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Chymotrypsin and pepsin are enzymes involved in protein digestion. Biosynthesis of these enzymes in appropriate amounts is important for maintaining homeostasis in cells. In order to treat diseases in which excessive secretion of proteases occurs, it is necessary to synthesize inhibitors that can be used as drugs for these diseases. Caffeine is a natural alkaloid and the most widely used psychoactive substance in the world. In addition to being used to improve physical and cognitive performances, it is also used as an inhibitor. C-8 substituted caffeine derivatives have been shown to be effective enzyme inhibitors.[1,2] Accordingly, the compound 8-((2-aminoethyl)amino)-caffeine was chosen for testing the inhibitory effect on chymotrypsin and pepsin. IC_{50} values were found to be 3.12 mM for pepsin and 6.80 mM for chymotrypsin. This compound was shown to be twice as good an inhibitor of pepsin as compared to chymotrypsin. Although the IC_{50} values are high, this is promising lead structure, considering the widespread usage of its precursor, *i.e.* caffeine.

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CB PP 25

Synthesis, characterization, antimicrobial activity of Zn(II) complex with a salicylaldehyde derivate

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In this work we are presenting the synthesis, characterization, and antimicrobial activity of a new mononuclear zinc(II) complex with methyl 3-formil-4-hydroxybenzoate (H**L**). The complex was obtained in the reaction of methyl 3-formil-4-hydroxybenzoate and $Zn(BF_4)_2 \cdot 6H_2O$ in a molar ratio of 1:1. Characterization was achieved by spectroscopic methods (IR and NMR). Crystal structure analysis shows that the coordination formula of the compound is $[Zn(\mathbf{L})_2(H_2O)_2]$ (Fig. 1). Antimicrobial activities of complex, corresponding Zn(II) salt and ligand H**L** were studied *in vitro* by examining the minimum inhibitory concentration (MIC) on four Gram-positive and four Gram-negative bacterial species, two fungal strains, and a yeast stain. Amikacin, ampicillin, and amphotericin B were used as the standard drugs. Zn(II) complex exhibited stronger antibacterial and antifungal activity than its precursors.

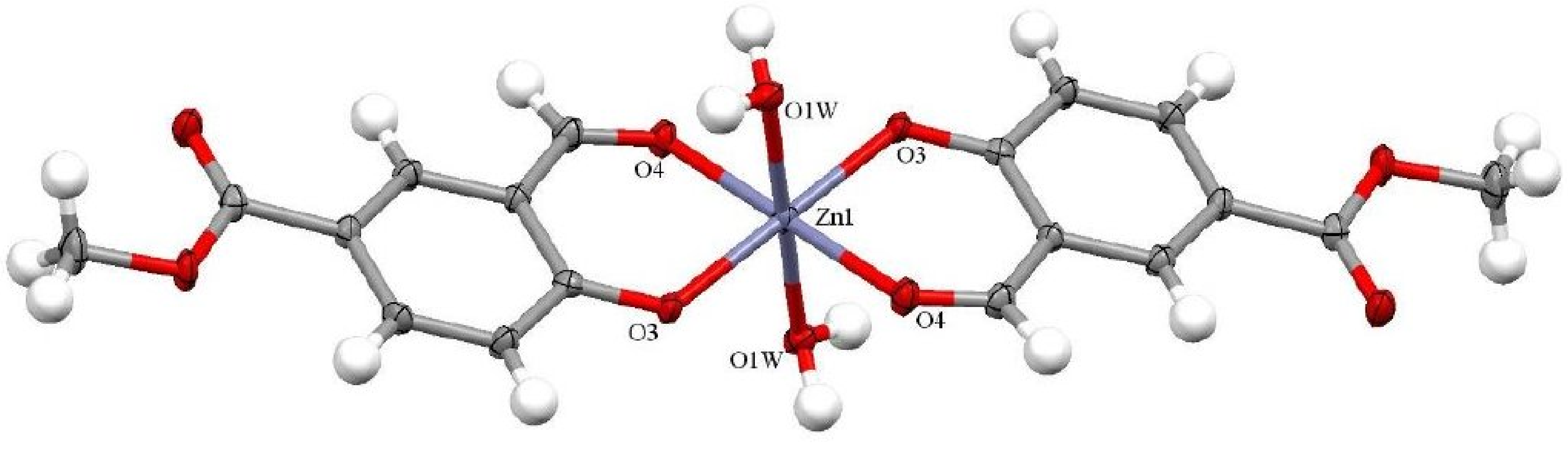

Figure 1. ORTEP representation of the $[Zn(\mathbf{L})_2(H_2O)_2]$ complex. Thermal ellipsoids are drawn at the 50% probability level.

Acknowledgments

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CB PP 26

Changes in histone acetyltransferase activity in ageing honey bees (*Apis mellifera* L.)

Jelena Spremo[1], Srđana Đorđievski[1], Tatjana Čelić[1], Elvira Vukašinović[1], Danijela Kojić[1], Jelena Purać[1]
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The honey bee (*Apis mellifera* L.) is a key model organism for research on ageing and longevity of eusocial insects due to extreme lifespan differences between and within castes. This seasonal variation is reflected in the life expectancy of summer (up to 8 weeks) versus winter, diutinus worker bees (over 6 months) [1]. The underlying processes responsible for this lifespan plasticity are still unclear [2]. In this study, we examined the effect of honey bee ageing on histone acetyltransferase (HAT) activity. Numerous studies have shown the role histone acetyltransferases play in the ageing process, where inhibition of these enzymes has been linked to an accelerated ageing process in organisms. The first sampling (groups S0 and W0) in both bee generations (summer and winter, respectively) consisted of newly hatched bees, while the remaining groups consisted of bees of a specific age. In each generation, three separate hives represented biological triplicates from which samples were taken biweekly in the case of summer bees (groups S2 and S4) and bimonthly in the case of winter bees (groups W2 and W4). To determine HAT activity, nuclear fraction from each group was isolated and the activity of HAT in the samples was determined using the Histone Acetyltransferase Activity Assay Kit (Abcam, ab65352) according to the manufacturer's instructions. The results showed that the level of total HAT activity in summer bees was not significantly different, while in winter bees, it was significantly increased in the W2 group. These findings provide an excellent starting point for further investigations into age-related changes and can serve as a basis for developing strategies to improve the health and longevity of bees.

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CB PP 27

Synthesis and *in silico* analysis of new iodinated furodioxol epimer

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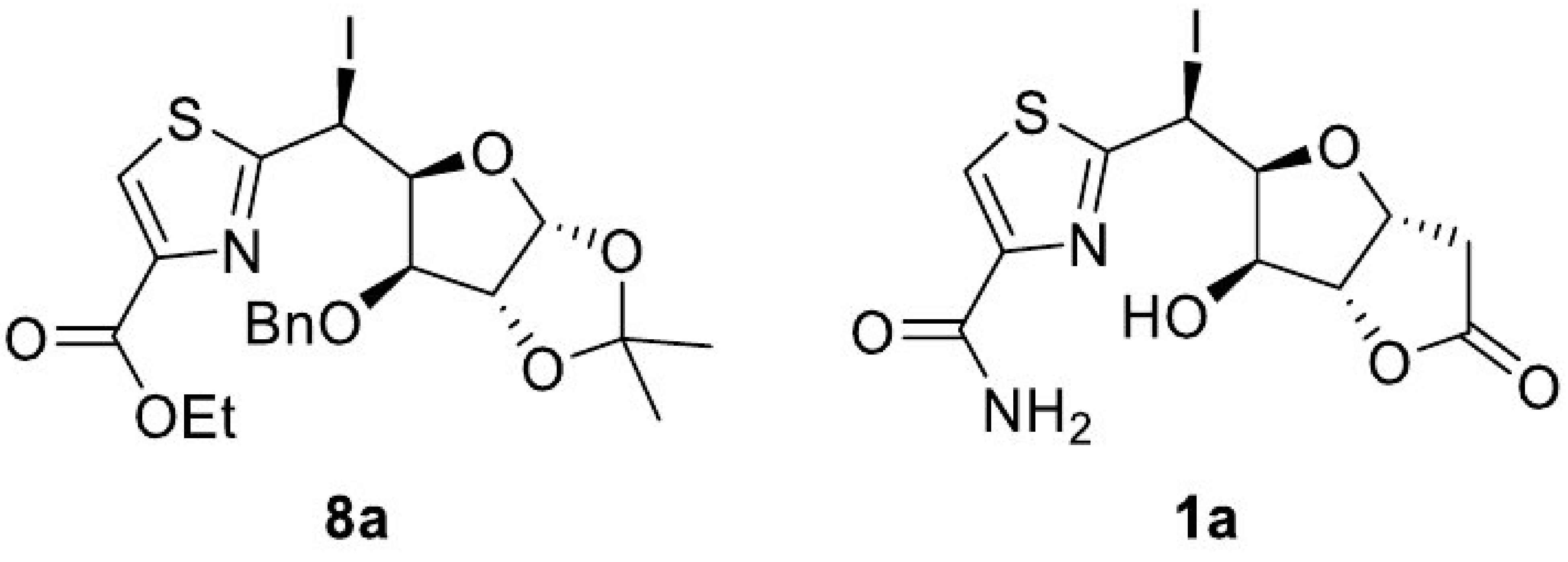
The synthesis of new iodinated derivative (**8a**) of D-glucose in seven stages is described. The synthesized furodioxol epimer is an intermediate in the path to the target compound, an iodinated hybrid of the C-nucleoside tiazofurin and the natural styril-lactone (+)-goniofufurone (**1a**, Scheme 1). *In silico* analysis was performed using the Pharmmapper server, through which potential targets for the newly synthesized compound were identified. Molecular docking of **8a** to the identified targets was than performed using AutoDock Vina tool, and the obrained results were subsequently compared with those ftom previous, metodologically different approach, potential indicating the accuracy of the methods applied.



Scheme 1. Obtained (8a) and target (1a) compound

Acknowledgments
This research is funded by the Ministry of Education and Ministry of Science, Technological Development and Innovation, Republic of Serbia, Grants: No. 451-03-68/2022-14/200125 as well as a research project from the Serbian Academy of Sciences and Arts (Grant No. F-130).

Developments in Chemical Synthesis (DCS)

DCS PP 01

Synthesis and crystal structure of a Ni(II) complex with a novel Schiff base of 2,6-diacetylpyridine

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University of Novi Sad – Faculty of Science, Novi Sad, Serbia

Among over 2500 of known 2,6-diacetylpyridine Schiff bases and their complex compounds, there are 133 nickel(II) complexes [1]. This work describes the synthesis and structural characterization of a new Ni(II) complex with a novel type of this Schiff base.

In the reaction of a warm suspension of the ligand 2,6-diacetylpyridine-adamantane-1-carbohydrazide (L) in methanol and a warm acetone solution of nickel(II)-trifluoroacetate, in the presence of lithium-acetate, in a molar ratio 1:1:1, the red stick crystals of a new dinuclear complex, $[Ni_2(L{-}H)_2]{\cdot}MeOH$, were obtained.

The X-ray diffraction on a single crystal confirm that the Schiff base in the newly synthesized compound acts as N_3O_2 pentadentate ligand. In this way, eight five-membered and one four-membered metallocycles are formed (Fig. 1). Both metal centers are located in the octahedral environment of the ligand donor atoms. The distance between two Ni(II) is 3.1147(7) Å, and the bond length of the metal–ligator atom bond is in the range of 1.960(3) – 2.437(3) Å.

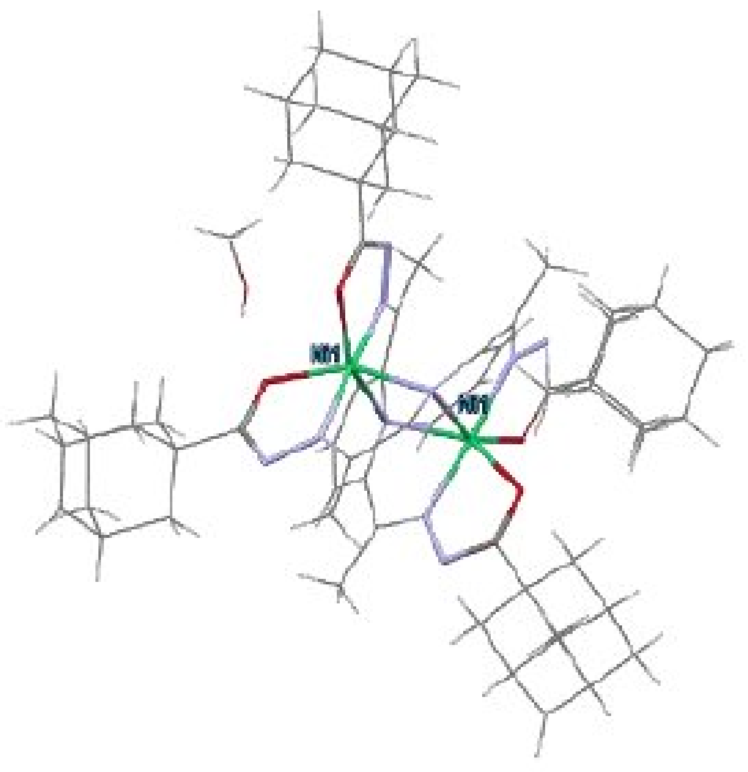

Figure 1. The molecular structure of novel Ni(II) complex

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DCS PP 02

Synthesis and electrochemical properties of a series of pyrazolines containing a ferrocenyl group

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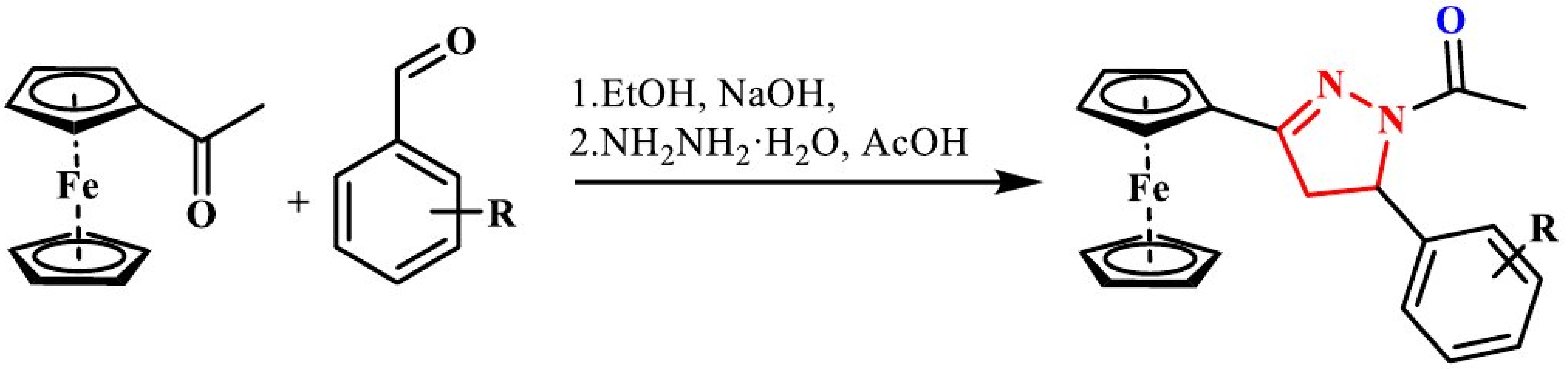
Pyrazolines are the core structure of numerous molecules which possess interesting biological features such as antibacterial, antimalarial, anti-inflammatory, monoamine oxidase inhibitory, as well as antioxidant activity [1]. Therefore, the synthesis of these heterocycles is of considerable interest to organic and medicinal chemists. Here we report the synthesis, spectral and electrochemical characterization of a new series of ferrocene-containing 1-acetylpyrazolines. The synthesis was achieved in two steps (Fig.1). In the first step, 1-ferrocenyl-3-arylprop-2-en-1-ones were obtained by Claisen-Schmidt condensation of acetylferrocene and the corresponding benzaldehydes [2]. The obtained chalcones were treated with hydrazine hydrate in acetic acid giving 1-acetyl-4,5-dihydro-1*H*-pyrazoles in good to high yields (58-88%).



R = 2-CH_3; 3-CH_3; 2,4,6-$(CH_3)_3$; 2-Br; 3-OCH_3

Figure 1. Synthesis of ferrocene containing 1-acetyl pyrazolines.

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DCS PP 03

Platinum(II) complex with promethazine: Synthesis, crystal structure and DNA/BSA binding affinity

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Previous research has indicated that various phenothiazine derivatives exhibit a wide range of antibacterial, antifungal and anticancer activities [1]. Considering this, a phenothiazine derivative, promethazine (pmz), was used as a ligand for the synthesis of a new platinum(II) complex, [$PtCl_3$(pmzH)]. The reaction of $PtCl_2$ and promethazine hydrochloride was performed in a 1 : 2 molar ratio in acetonitrile under reflux for 5 h. The complex obtained was characterized by different spectroscopic and electrochemical methods, while its crystal structure was determined by single-crystal X-ray diffraction analysis. In this complex, the protonated pmz is monodentately coordinated to the Pt(II) center through the sulfur atom, while the remaining coordination sites are occupied by the three chlorido ligands resulting in a square-planar geometry around the Pt(II). Moreover, the interactions of [$PtCl_3$(pmzH)] complex with calf thymus DNA (ct-DNA) and bovine serum albumin (BSA) were studied by fluorescence emission spectroscopy.

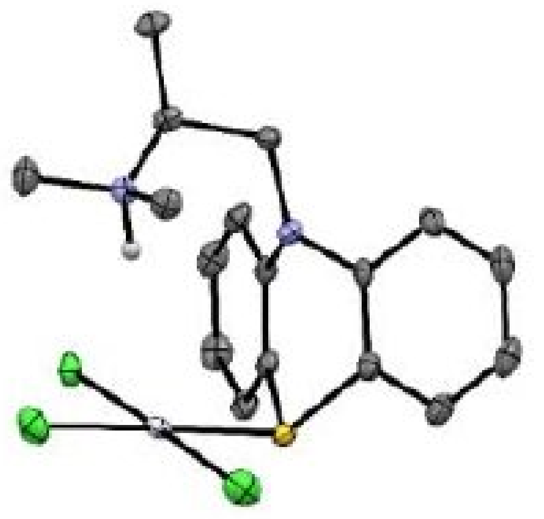

Figure 1. Crystal structure of [$PtCl_3$(pmzH)] complex.

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DCS PP 04

New palladium(II) complex with promethazine and its interaction with biomolecules

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The design of palladium(II) complexes with antitumor activity is of great importance due to increasing occurrence of tumors resistant to the clinically used cisplatin [1]. Moreover, phenothiazine derivatives occupy a prominent position in medicine as antihistaminic agents [2]. Considering this, in the present study, we reacted phenothiazine promethazine (pmz) with $PdCl_2$ in a 1 : 2 molar ratio in acetonitrile to obtain a palladium(II) complex, $[PdCl_3(pmzH)]$. The crystal structure of the complex was determined by single-crystal X-ray diffraction analysis, and the complex was characterized by different spectroscopic and electrochemical methods. The X-ray analysis showed that the complex has a square-planar geometry with monodentately coordinated protonated pmz ligand to the Pd(II) ion through the sulfur atom. We have also investigated the binding affinity of the $[PdCl_3(pmzH)]$ complex to calf thymus DNA (ct-DNA) and bovine serum albumin (BSA) by fluorescence emission spectroscopy.

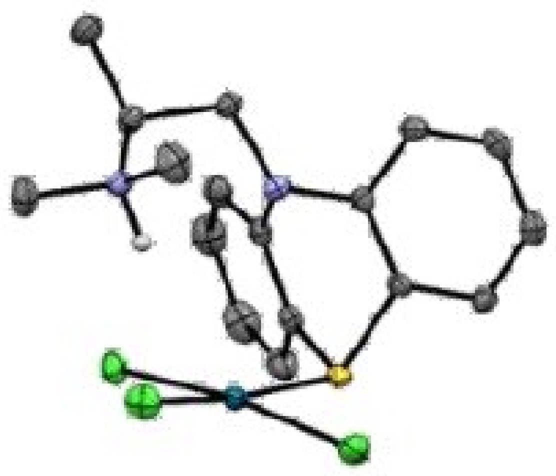

Figure 1. The crystal structure of $[PdCl_3(pmzH)]$ complex.

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DCS PP 05

Synthesis and structural characterization of a copper(II) complex with antifungal tebuconazole

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Tebuconazole (tbcz) is an azole fungicide used in agriculture due to its high bioactivity and acceptable toxicity profile [1]. Long-term use of this fungicide leads to the development of resistance, which can have environmental consequences. It is known that the presence of metal ions is necessary for many biological processes in living organisms, such as metabolism, respiration, photosynthesis, growth and reproduction, muscle contraction and transmission of nerve signals [2]. Therefore, a combination of biologically active organic compounds with metal ions can be a strategy for overcoming antifungal resistance. In this study, we synthesized and structurally characterized a copper(II) complex with tebuconazole. It was synthesized by reacting $CuCl_2 \times 2H_2O$ with tebuconazole in a 1 : 2 molar ratio in ethanol at room temperature. Upon slow evaporation crystals of the complex formed and X-ray structural analysis showed that the complex has a metal-to-ligand ratio of 1 : 4 with the formula *trans*-$[CuCl_2(tbcz)_4] \times H_2O$ The four tebuconazole molecules are monodentately coordinated to the Cu(II) ion through the N4 nitrogen atom of the triazole ring, while the remaining coordination sites are occupied by two chlorido ligands resulting in an octahedral geometry around Cu(II).

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DCS PP 06

A New, Selective, and Ratiometric Fluorescent Sensor for Zinc(II)

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[3]*University of Belgrade - Faculty of Chemistry, Belgrade, Serbia*

Due to the significance of zinc for human health, there is a great interest in developing methods for its detection. Ratiometric fluorescent sensing is particularly advantageous because it offers a self-calibrating mechanism [1]. In this study, a new excited-state intramolecular proton transfer (ESIPT) - based fluorescent ratiometric sensor for Zn^{2+} was synthesized by conjugating the respective motifs of derivatized tetramic acid and an N-heterocyclic compound (Fig.1.a.). Upon excitation, the sensor exhibits a strong emission band at 515 nm, while an additional blue-shifted emission maximum at 460 nm occurs only in the presence of Zn^{2+} ions. This is accompanied by a color change of the solution (Fig.1.b.). Through fluorescent titration, the limit of detection and the limit of quantification were determined to be 1.26×10^{-6} M and 3.81×10^{-6} M, respectively. The coordination of the sensor to Zn^{2+} ions was further confirmed in an NMR study.

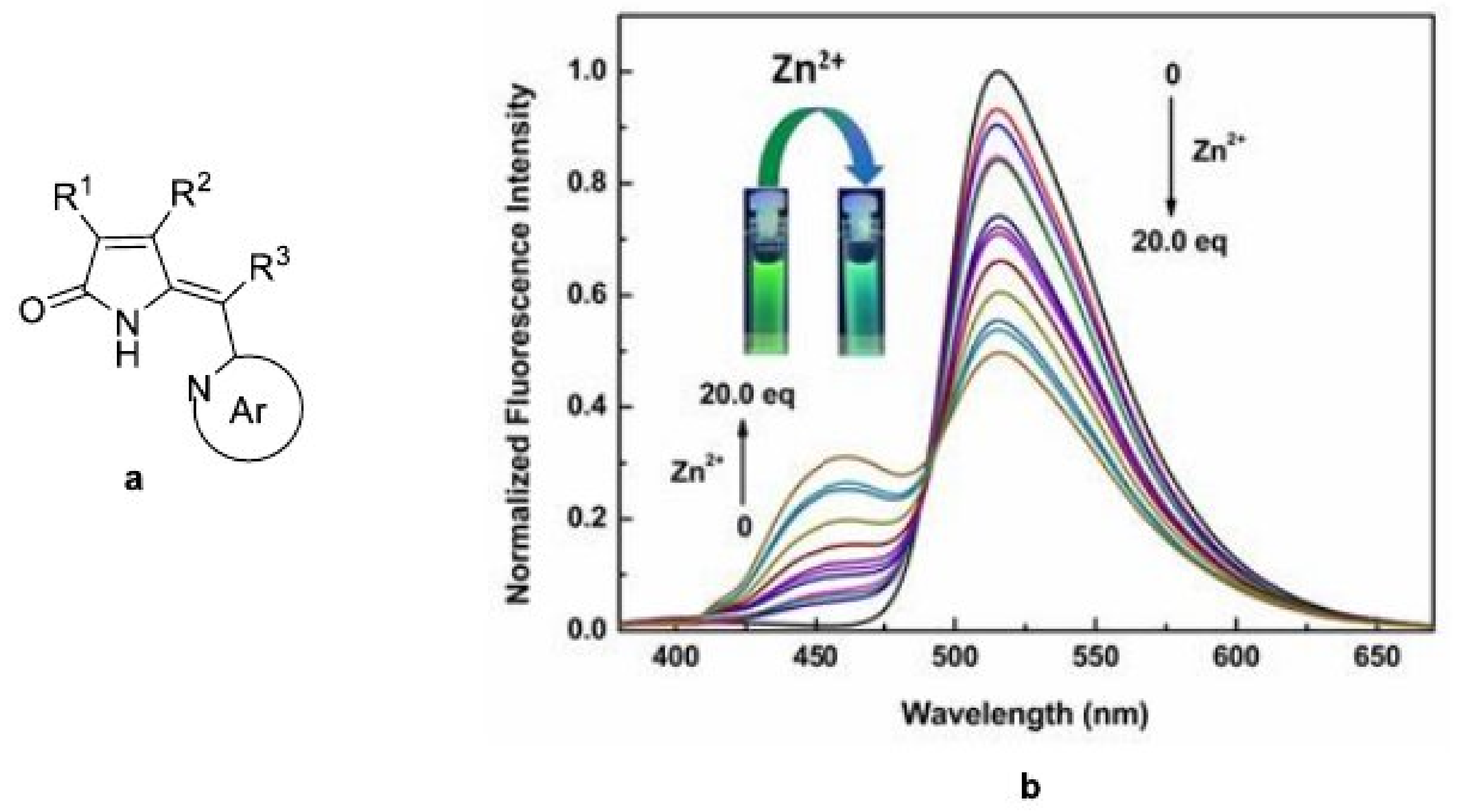

Figure 1. a. General structure of the sensor, b. Spectrofluorimetric titration of the sensor with the addition of $ZnCl_2$ (0-20 equivalents) and the appropriate color change under UV light.

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DCS PP 07

Synthesis, chemical characterization and X-ray analysis of rhenium(V) complexes with apigenin and its derivatives

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Apigenin is an aglycone of many natural glycosides and is known chemically as 4 ,5,7-trihydroxyflavone [1]. The biological and pharmacological activities of apigenin are diverse, including anti-inflammatory, antioxidant, anticancer, anti-proliferative and anti-spasmodic activities [2]. The chemistry of oxorhenium(V) complexes is receiving increasing attention because of the potential application in medical and catalytic chemistry.

Here we will present a new derivative of apigenin (L1) and its complex (C1), as well as a complex of apigenin with $ReOBr_3(PPh_3)_2$ (C2). The benzylated derivative of apigenin was obtained by the reaction of apigenin and benzyl bromide in DMF under reflux. The chemical structures of both complexes were confirmed using standard analitycal techniques, NMR and IR spectroscopy. Single green C1 and red C2 block-shaped crystals were obtained from acetone and their proposed structures were confirmed by X-ray analysis. The rhenium complexes exhibit distorted octahedral geometry with the apigenin ligand chelating the rhenium center through two oxygen atoms in an almost flat chelate. The oxido ligand is *cis* to two chlorido ligands and *trans* to the oxygen donor atoms of the ligand.

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DCS PP 08

Synthesis, chemical characterization and X-ray analysis of oxorhenium(V) complexes with picolinic acid derivatives

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Rhenium has a broad spectrum of oxidation states in coordination compounds and rhenium(V) complexes have been described in literature as good catalysts for the catalytic epoxidation of cyclooctene and perchlorate reduction [1].

Here we present five new Re(V)-oxo complexes (C1 – C5) with general formula $[ReOCl_2PPh_3(L1\text{-}5)]$, where L1-5 are 5-bromo, 6-bromo, 6-chloro, 6-fluoro and 5-hydroxo derivatives of picolinic acid. All complexes were synthesized starting with $[ReOCl_3(PPh_3)_2]$ and the corresponding ligand in acetonitrile. After 24 h of reflux, all of them precipitated as blue powder. All complexes were characterized with ^1H, ^{13}C NMR and IR spectroscopy and structures of two crystalized complexes were additionally confirmed by X-ray analysis. Blue crystals of those two complexes were obtained from acetonitrile solutions. Similar to literature data, crystal structure of those two complexes (C4 and C5) confirmed that two chlorido ligands are *cis* to each other, and the phosphine is *trans* to one of them. The rhenium complex exhibits a distorted octahedral geometry with the picolinate ligand chelating the rhenium center through the nitrogen atom and one oxygen atom of the carboxylic acid group in an almost flat chelate. The Re-oxido ligand bond length is similar to the Re-oxido complexes previously reported, with the oxido ligand *trans* to the oxygen donor of the ligand [1,2]. Complex C5 co-crystalized with a phosphine oxide molecule and the crystal structure showed an intermolecular hydrogen bonding between the hydroxy group and a phosphine oxide molecule.

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DCS PP 09

Synthesis and crystal structure of a new Ag(I) polymeric complex with 3-(pyrazol-1-yl)-L-alanine

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[2] *University of Novi Sad - Faculty of Sciences, Novi Sad, Serbia*

Pyrazole derivatives are important heterocyclic compounds capable of coordinating to metal centers and engaging in hydrogen bonding. Soft silver(I), with its d^{10} configuration and flexible coordination geometries, is often used in constructing varied polymeric complexes due to its tolerance for diverse structural arrangements [1]. In this work, we present the synthesis and structural characterization of the novel Ag(I) polymeric complex with ligand 3-(pyrazol-1-yl)-L-alanine (L) of the coordination formula $\{[Ag(\mu\text{–}L)]NO_3\}_n$.

The complex was obtained by the reaction of the aqueous solutions of $AgNO_3$ and the ligand in a 1:1 molar ratio. From the resulting colorless solution, whitish rod-like single crystals were filtered after a few days. The structure was confirmed by X-ray diffraction. The ligand exhibits an interesting tridentate O_2N coordination mode, where the pyrazole nitrogen atom and one carboxyl oxygen atom chelate one Ag(I) center, the latter atom ligator also coordinates another Ag(I), and the remaining carboxylic oxygen coordinates the third metal center (Fig. 1). This way of coordination results in formation of fused six-membered bimetallocycles with metal centers in a destorted tetrahedral environment with τ_4 parameter having the value of 0.67.

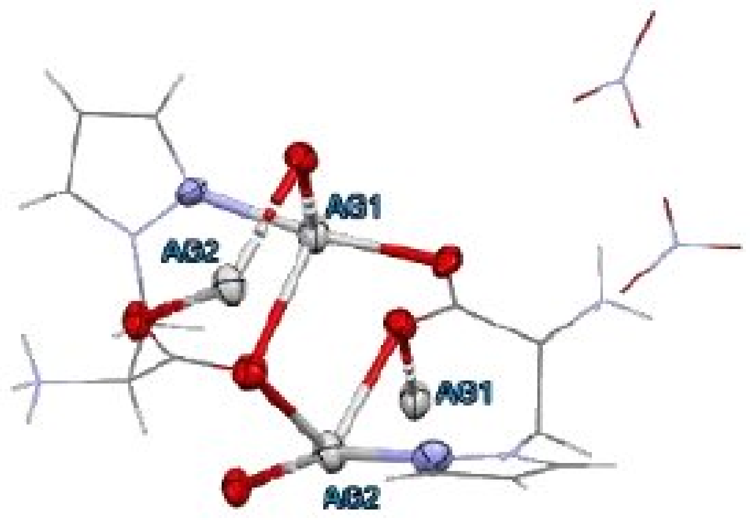

Figure 1. The coordination environment in $\{[Ag(\mu\text{–}L)]NO_3\}_n$.

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DCS PP 10

Synthesis and characterization of a Ni(II) complex with asymmetric Schiff base of 2,6-diacetylpyridine

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An important class of disubstituted pyridines are the 2,6-disubstituted derivatives, which are mainly obtained through derivatization of 2,6-diacetylpyridine, a significant precursor for further syntheses, to which the development of one-pot synthesis has certainly contributed [1]. This paper describes the synthesis and characterization of a Ni(II) complex with the asymmetric Schiff base of 2,6-diacetylpyridine.

The Ni(II) complex was obtained by the template reaction of $NiCl_2 \times 6H_2O$, the chloride salts of mono-2,6-diacetylpyridine-thiosemicarbazide and phenyl-hydrazine (1:1:1), in methanol. The complex [Ni(L-2H)], L – 2,6-diacetylpyridine-thiosemicarbazide-phenyl-hydrazone, was obtained in the form of dark-red needle-like single crystals. Its structure was confirmed by single-crystal X-ray diffraction. The ligand coordinates as an NNNS tetradentate, where the donor atoms are the pyridine nitrogen, azomethine nitrogen, and sulfur from the 2,6-diacetylpyridine thiohydrazide part, as well as the hydrazine nitrogen atom from the phenylhydrazone part of the ligand (Fig. 1). The Ni(II) ion is situated in a square-planar environment of donor atoms, and is elevated from the plane by approximately 0.017 Å.

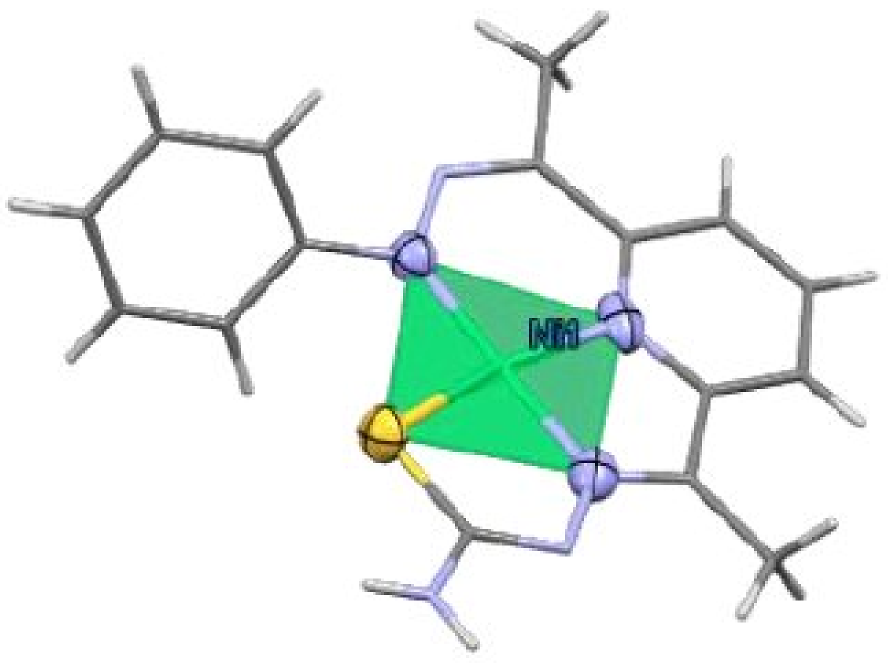

Figure 1. The molecular structure and coordination plane of [Ni(L-2H)]

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DCS PP 11

Novel atom-efficient photocatalyst-free visible light-induced approach to the synthesis of 2-methyl-4-(phenylsulfonyl)butan-2-ol

Branka R. Krnjaja, Nikola G. Knežević, Ana D. Popović, Dimitrije M. Gligorovski, Aleksa P. Vulićević, Bojan Z. Vulović
University of Belgrade - Faculty of Chemistry, Belgrade, Serbia

Sulfones serve as essential building blocks in organic synthesis. Notably, the synthesis of 2-methyl-4-(phenylsulfonyl)butan-2-ol has been patented due to its significance as a precursor in the production of vitamin D3 [1]. Herein, we report a new approach to visible-light-induced synthesis of 2-methyl-4-(phenylsulfonyl)butan-2-ol. This atom efficient transformation is performed under mild conditions and tolerates a wide range of solvents. Higher yields are obtained under argon atmosphere, and, interestingly, the reaction can also be performed under air. Mechanistic experiments indicate the reaction has an induction period.

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1. International Patent Classification: C07C 401/00, A61K 31/59

Acknowledgments

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DCS PP 12

Synthesis and structural characterization of a novel trimethyltin(IV) complex with 3-(4-methyl-2-oxoquinolin-1(2*H*)-yl)propanoic acid

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As the effectiveness of cisplatin and platinum-based drugs is limited due to their high toxicity, resistance and severe side effects, the discovery and development of new chemotherapeutic agents with enchanced properties than the clinically used drugs is of great importance. In recent years, organotin(IV) compounds have received considerable attention as promising non-platinum chemotherapeutics. These compounds are widely available, exhibit lower toxicity than platinum-based drugs, and induce cell death at low doses, thus avoiding the development of resistance [1]. Herein, we present the synthesis (Fig. 1) of novel (3-(4-methyl-2-oxoquinolin-1(2*H*)-yl)propanoato)trimethyltin(IV) compound (**Me_3SnL**), obtained in the reaction of deprotonated 3-(4-methyl-2-oxoquinolin-1(2*H*)-yl)propanoic acid (**HL**) and trimethyltin(IV) chloride. The compound was characterized by elemental microanalysis, FT-IR and multinuclear (^{1}H, ^{13}C and ^{119}Sn) NMR spectroscopy.

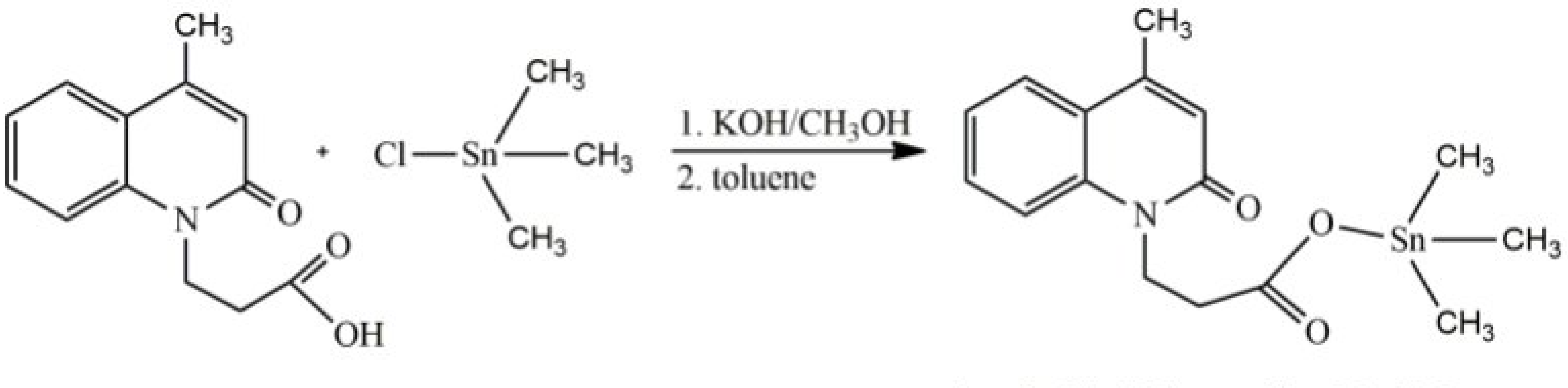

Figure 1. Synthesis of the ***Me_3SnL***

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DCS PP 13

Selective mono-alkylation of a primary amine

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Secondary amine is an important functional group found in many natural products, bioactive compounds and synthetic intermediates. The main methods for preparing secondary amines from primary amines include reductive alkylation with aldehydes and ketones, and alkylation by alcohols, halides or their equivalents [1]. However, alkylation often suffers from overalkylation even when excess amine is used. In continuation of our effort to make syntheses as simple as possible [2], we present the selective monoalkylation of a primary amine, which is achieved only by mixing the reactants in a molar ratio of 3:1 (amine/bromide) and allowing them to stand at room temperature, or by heating in a laboratory oven. As preliminary results, we show that biologically important tryptamine (solid) reacts with non-functionalized and functionalized primary, secondary and tertiary bromides (liquids) to give secondary amines in 36-64% yields, with selectivity ranging from 84:16 to 100:0 (Figure 1).

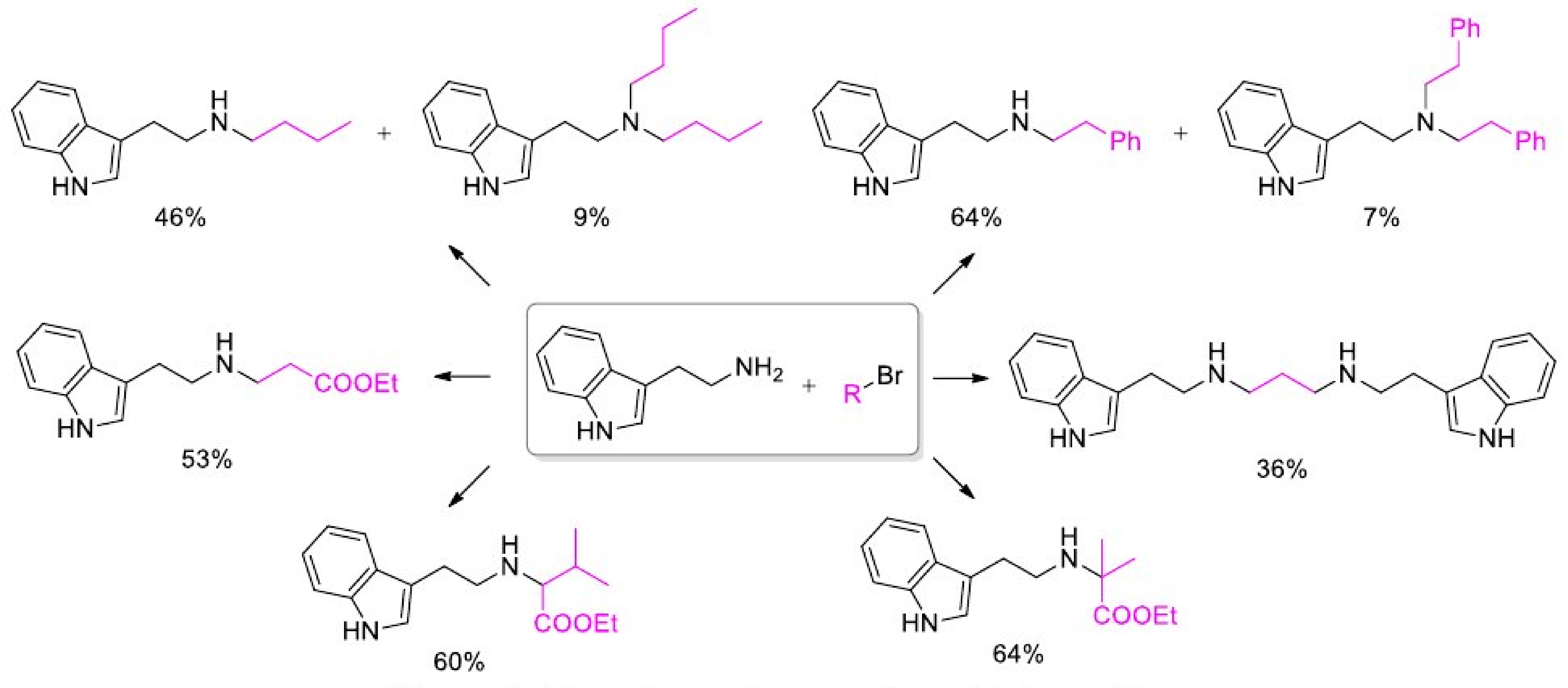

Figure 1. Reactions of tryptamine with bromides.

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DCS PP 14

A novel synthesis route to high-entropy spinel oxides

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High-entropy spinel oxides (HESOs) are a class of complex oxides, composed of five or more metal cations, arranged in a spinel crystal structure. Their composition provides enhanced structural stability and tailored physical properties, making them suitable for various applications, such as Li-ion batteries, solid oxide fuel cell components, tuneable magnets, microwave absorbers, catalysts, and gas sensors. Thus far, HESOs were synthesized using different methods, but the quest for new efficacious synthetic routes continues. In the present study, HESOs of eight different compositions, i.e. $(Co_{0.2}Cr_{0.2}Fe_{0.2}Mn_{0.2}Ni_{0.2})_3O_{3.6}$, $(Mg_{0.2}Cr_{0.2}Fe_{0.2}Mn_{0.2}Ni_{0.2})_3O_{3.6}$, $(Mg_{0.2}Co_{0.2}Fe_{0.2}Cr_{0.2}Mn_{0.2})_3O_{3.6}$, $(Mn_{0.2}Zn_{0.2}Fe_{0.2}Ni_{0.2}Cr_{0.2})_3O_{3.6}$, $(Co_{0.2}Mn_{0.2}Zn_{0.2}Fe_{0.2}Cr_{0.2})_3O_{3.6}$, $(Co_{0.2}Mn_{0.2}Ni_{0.2}Zn_{0.2}Cu_{0.2})Al_2O_4$, $(Co_{0.25}Mn_{0.25}Zn_{0.25}Ni_{0.25})Al_2O_4$, and $(Mg_{0.25}Mn_{0.25}Co_{0.25}Ni_{0.25})Al_2O_4$, were synthesized through a high-temperature synthesis activated by self-propagating room temperature reaction starting from nitrates. The stoichiometric amounts of nitrates, necessary for a particular HESO, and NaOH were hand-mixed in an alumina mortar for 5 minutes, facilitating a rapid reaction at room temperature. The resulting mixtures were dried at room temperature for 24 hours, then suspended in distilled water in order to remove $NaNO_3$ and centrifuged at 4000 rpm for 10 minutes. This process was repeated three times with distilled water and twice with ethanol. Upon completing five centrifugation cycles, the samples were dried at 70 °C for 24 h and calcined at 1000 °C in air for 3 h. The obtained products were XRD and SEM/EDS characterized. Based on XRD, all the products crystalized in spinel structure and *Fd*-3*m* space group with unit cell parameter of about 8.3 Å. Since all of the diffraction peaks can be indexed to the cubic spinel structure only, it can be concluded that all the cations were incorporated into the structure and that the resulting powders are single-phased high-entropy spinel oxides. This was confirmed by EDS mapping. In summary, the investigated synthesis route represents a novel, fast and simple way of obtaining high-entropy spinel oxides of various compositions.

Acknowledgments

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DCS PP 15

Anticancer evaluation, mechanism of action, and protein binding study of some Schiff bases: Molecular docking study

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To discover a new drug candidate for the treatment of life-threatening diseases such as cancer, we examined the antitumor potential of a small series of Schiff bases. We also conducted the same tests on a series of same-type compounds that we synthesized earlier [1]. The cytotoxic potential of the compounds was investigated on normal human embryonic lung fibroblast (MRC-5), human cervical adenocarcinoma (HeLa), human lung adenocarcinoma (A549), and human colon adenocarcinoma (LS174T) cancer cell lines, respectively. The obtained results were promising. Amongst all tested compounds, compound **C** showed excellent cytotoxic activity against malignant cell lines. In addition, compound **C** exhibited lower cytotoxic potential against MRC-5 compared to other cancer cell lines, pointing to very good selectivity, which is one of the crucial factors for a new antitumor drug candidates. Since they have shown good properties, the mechanism of antitumor action of these potential drugs was further examined. In order to better understand the binding mode of the tested compounds with biomolecules, a molecular docking study was performed. To conclude, all the results indicate the exceptional potential of these compounds for future use in clinical practice.

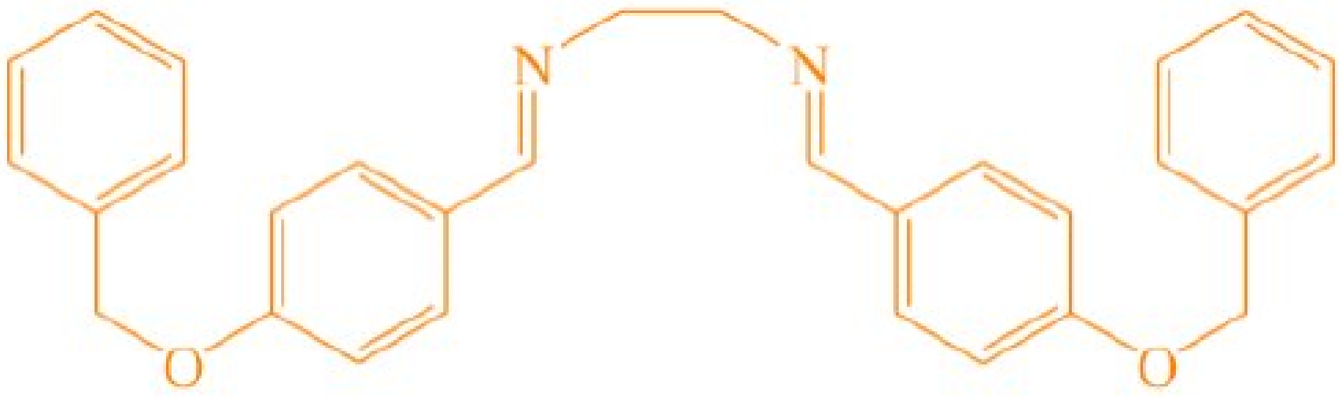

*Figure 1. Structure of compound **C***

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DCS PP 16

Synthesis of a new polymeric Zn(II) complex with bis(4-carboxybenzyl)ammonium chloride and *o*-phenanthroline

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The polymeric complex (Fig. 1) of the formula $\{[Zn(\mu\text{-}HL)(o\text{-}phen)]_2L\cdot 2H_2O\}_n$ was obtained in the reaction of zinc-chloride, *o*-phenanthroline (*o*-phen) and bis(4-carboxybenzyl)ammonium chloride (H_3LCl) in the mixture of DMF and H_2O (2:1), in the form of colorless block-shaped single crystals. The asymmetric unit comprises one zinc(II) ion, one HL^-, one half of L^{2-}, one *o*-phenanthroline and one water molecule split over two positions. The zinc atom is situated in a distorted octahedral environment, composed of two dicarboxylate ligands (HL^-), both having bridging role, coordinating in a tetradentate manner. Fifth and sixth coordination site is occupied by *o*-phen, which coordinates in a bidentate manner through the nitrogen atoms. The charge of the polymeric cations $\{[Zn(\mu\text{-}HL)(o\text{-}phen)]^+\}_n$ is balanced by L^{2-} anions which maximize electrostatic attraction of deprotonated carboxylic groups and protonated amino groups of bridging ligands. The compound is further characterized by PXRD, TG analysis and FTIR spectroscopy.

Selected crystallographic data and refinement details: $C_{72}H_{61}N_7O_{14}Zn_2$, $C2/c$, $a = 29.6874(6)$ Å, $b = 6.38976(18)$ Å, $c = 33.0314(6)$ Å, $\beta = 97.2495(18)°$, $V = 6215.8(2)$ Å^3, $Z = 4$, $R = 8.1$ % for 453 parameters and 7683 independent reflections.

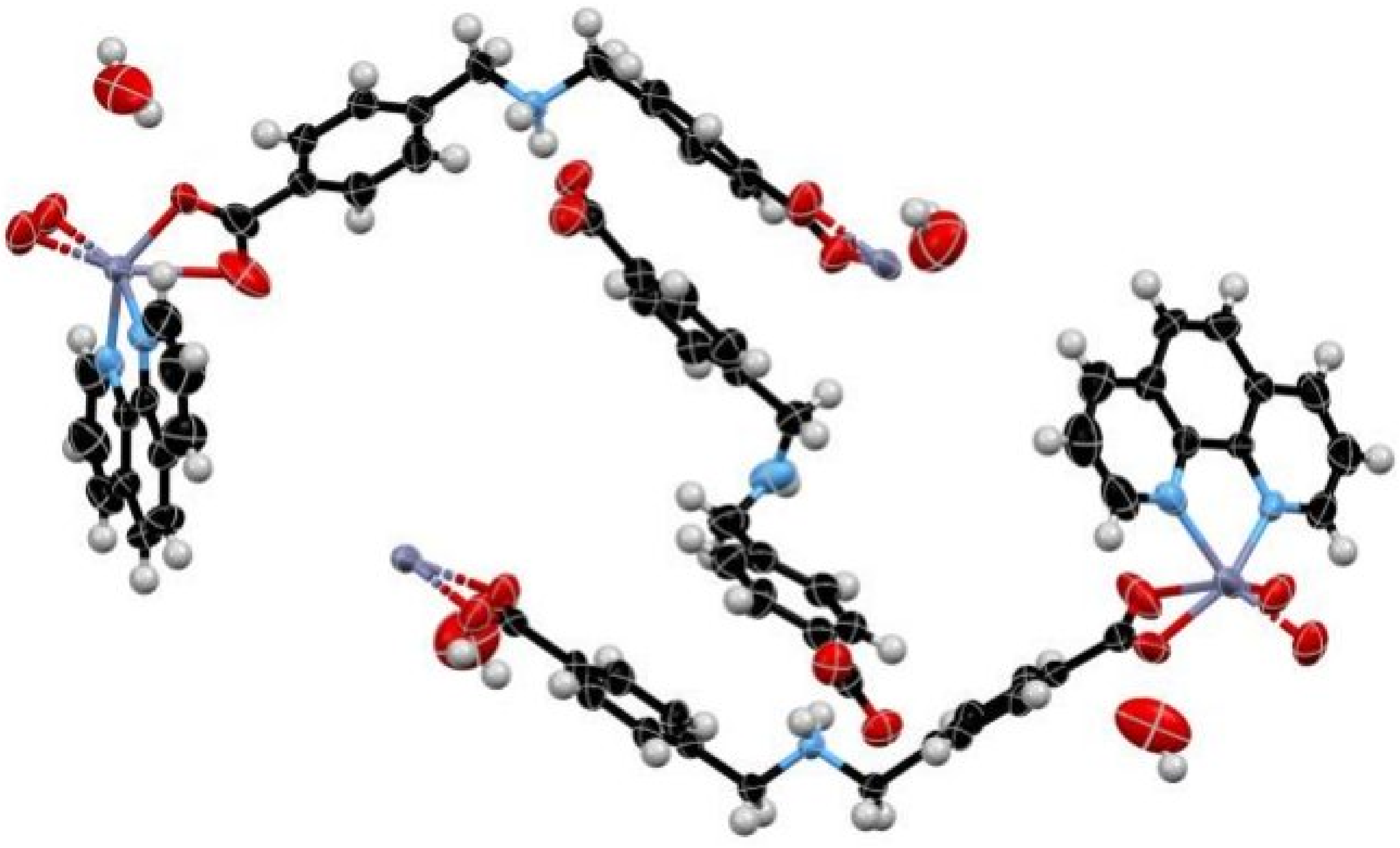

Figure 1. Polymeric structure of complex.

Acknowledgments
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Environmental Awareness (EA)

EA PP 01

Unveiling the reactive species involved in the photocatalytic degradation mechanisms of ciprofloxacin and sulpiride

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Pharmaceuticals, including antibiotics and antipsychotics, contribute significantly to environmental pollution. Despite low concentrations, their persistence poses serious risks to both aquatic and terrestrial ecosystems. For instance, the uncontrolled use of antibiotics can foster the development of antibiotic-resistant bacteria, while antipsychotics can disrupt the brain chemistry of non-target organisms. Thus, their presence and impact demands attention.[1] Heterogeneous photocatalysis offers a green and eco-friendly solution for the removal of organic pollutants from the environment. This process, which occurs in the presence of light and a catalyst, involves the generation of various reactive species – such as photogenerated holes, adsorbed and free hydroxyl radicals, superoxide radical anions and singlet oxygen. These reactive species actively contribute to the breakdown of persistent organic compounds.[2] Scavenger experiments were, therefore, conducted aiming to identify which of these species are predominantly involved in the photocatalytic degradation of one fluoroquinolone antibiotic (ciprofloxacin, CIP) and one benzamide class antipsychotic (sulpiride, SLP) under simulated solar irradiation using commercial zinc oxide as a photocatalyst. The findings indicate that adsorbed hydroxyl radicals and superoxide radical anions have the most important role in the photocatalytic degradation of CIP, whereas superoxide radical anions and positively charged holes are the driving force behind the photocatalytic degradation of SLP.

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EA PP 02

Impact of concentration of NaOH in alkali solution on the structural and radiological characteristics of alkali-activated material based on fly ash and metakaolin

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Alkali-activated materials can be used as alternative binders of Portland cements and can be producesed to have lower CO_2 emissions utilizing industrial residues. The main constituents of AAM are aluminosilicate precursors which are often waste-based materials such as fly ash [1]. The aim of this research was to study the impact of different concentration of sodium hydroxide, NaOH in alkali solution on the characteristics of alkali-activated metakaolin (MK) and fly ash (FA). Alkali activation solutions (A) were prepared from Na_2SiO_3 and two concentration of NaOH (4M and 12M), with volume ratio 1.5, and mass share of FA in the mixed sample of FA and MK was 10%. The concentration of radionuclide activity in the investigated materials for this examination reached radioactive equilibrium.

The structure properties of $AFA_{10}MK_{90}$ were studied by X-ray difraction (XRD) and diffuse reflectance infrared spectroscopy (DRIFT). XRD pattern of both materials showed the main crystal phase of quartz and in $A_{12}FA_{10}MK_{90}$ was formed a new crystal phase Fuajsite. DRIFT spectroscopy showed that the main vibration band at 1036 cm^{-1} of $AFA_{10}MK_{90}$ corresponds to Si-O-Si/Al-O-Si bands. Determination of radionuclide content was performed by means of gamma-ray spectrometry. Results showed that icreasing the concentration of NaOH in alkali solution led to a decrease in the activity concentration of radionuclides detected in the measured samples. External radiation hazard index (Hex) for $A_4FA_{10}MK_{90}$ and $A_{12}FA_{10}MK_{90}$ were 0,904 Bq/kg and 0,669 Bq/kg, respectively, and radium equivalent activity (Ra_{eq}) were 334,5 Bq/kg and 247,7 Bq/kg, respectively. The results of activity concentration measurements in $AFA_{10}MK_{90}$ indicate potential for safe application in building construction.

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EA PP 03

Analysis of sludge content from wastewater treatment plant for the presence of specific organic and inorganic compounds

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Sludge is an organic substrate generated at wastewater treatment plants, often containg nutrients, organic compounds, heavy metals and various other hazardous substances that can pose environmental risks if not properly managed. One of the key tehnologies used for sludge stabilization is anaerobic digestion [1]. In a recent analysis, the digested sludge from a wastewater treatment plant was examined for specific organic and inorganic compounds. After drying the sludge, the moisture content in the sludge was 55.87%, and the organic matter was 37.19%. Chemical oxygen demand was 424557 mg/kg, while biochemical oxygen demand was 283269 mg/kg. Analysis via inductively coupled plasma mass spectrometry (ICP-MS) revealed low concentrations of heavy metal: As 8.4 µg/g, Cu 13.1 µg/g, Cd 0.08 µg/g, Ni 2.6 µg/g, which was expected considering there are no industrial facilites near the wastewater treatment plant that would discharge effluents with heavy metals content. The values of heavy metals are not higher that the limit values provided by the Regulation on the method and procedure of sludge management from municipal wastewater treatment plants (Official Gazette of RS No. 103/2023) [2]. A significant observation was a high phosphorus content 130757 µg/g suggestion that the digested sludge holds potential for phosphours recovery, which could be used to produce artificial fertilizers. Additionally, polychlorinated biphenyls (PCBs) and polycyclic aromatic hydrocarbons (PAHs) were not detected. The obtained results can help in the further monitoring of sludge content and improvement of the process of sustainable sludge management.

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EA PP 04

A comparative analysis of the quality of tap water and yellow well water in Srbobran

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Water is a fundamental necessity for all living organisms and the human body requires water for daily survival. Moreover, water quality is also important, which is why it needs to be monitored. The properties and quality of drinking water have been documented in several regulations. In the Republic of Serbia, the legislation of the former state is still in effect, issued in 1998 under the title "Regulation on the Hygienic Safety of Drinking Water" which has been expanded several times ("Official Gazette SRJ", No. 42 from 28th August 1998, No. 44 from 25th June 1999, No. 28 from 17th April 2019). In the EU, it is defined by Directives 98/83/EC and 2015/1787[1]. Additionally, several organizations deal with both tap water and bottled water, such as the WHO (World Health Organization). The yellow water of Srbobran originates from an Artesian well, but its composition is currently unknown to the public. The aim of our research was to determine why the water is yellow and assess if it is rich in sulfur, which is believed to be responsible for its yellow color and distinctive smell. The comparison showed differences, primarily in organoleptic properties, bicarbonate and organic matter content, as well as in hardness and conductivity. Based on the existing results, the conclusion was that the yellow water of Srbobran is drinkable and not hazardous to health. The tests also managed to confirm that the yellow color of the water is not due to its sulfur content but rather its high organic matter content. This is evident from the fact that the water became colorless during the determination of oxidizability, which measures the amount of organic matter. Therefore, the yellow color likely originates from the presence of organic substances, which disappear during oxidation.

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EA PP 05

The role of quenching experiments in UV-based advanced oxidation processes

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UV-based advanced oxidation processes (AOPs) encompassing radical promoters such as hydrogen peroxide (H_2O_2), peroxydisulfate (PDS) or peroxymonosulfate (PMS) have been widely studied to remove organic contaminants during the water/wastewater treatment. Photolytic cleavage of oxidants under UV-C light (λ= 254 nm) leads to the formation of highly reactive oxygen species (ROS), which exhibit strong oxidative potential. Highly reactive radical species include free radicals such as hydroxyl radicals ($HO^{\bullet}$), sulfate radicals ($SO_4^{\bullet-}$) and superoxide radicals ($O_2^{\bullet-}$), as well as potent oxidizing molecules like singlet oxygen ($^1O_2$). Through complex electron exchange mechanisms, these ROS might decompose and mineralize organic pollutants [1]. Quenching experiments are a popular method for identifying the role of ROS in AOPs because of their simplicity, low cost and relatively reliable results. However, radical scavenging is sensitive to various factors, including water quality, the nature of the radicals, scavengers and organic compounds present, which can affect the accuracy of the quenching results. Choosing the appropriate scavenger is crucial for accurately reflecting the activity of specific radicals. In this study, the quenching experiments using methanol (MeOH) and *tert*-butyl alcohol (TBA) as scavengers were conducted to elucidate the degradation mechanism of UV filter 4-methylbenzylidene camphor (4-MBC) by UV/PMS processes. MeOH was employed as a scavenger for $HO^{\bullet}$ and $SO_4^{\bullet-}$ due to its high reactivity towards these species, whereas TBA was more effective for quenching the $HO^{\bullet}$ radical. The contributions to the degradation of 4-MBC in the UV/PMS process were approximately 31,5 % for $HO^{\bullet}$ and 68,5 % for $SO_4^{\bullet-}$, indicating that $SO_4^{\bullet-}$ was the dominant reactive species.

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EA PP 06

Removal of crystal violet from aqueous solution using *Ambrosia artemisiifolia* based biosorbent

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Industrial activities are leading contributors to water pollution and their wastewaters often contains numerous contaminants, including synthetic organic dyes such as crystal violet. Crystal violet (CV) is a cationic synthetic dye used in industrial dyeing, as an additive in poultry feed and as a dermatological agent, but it is toxic and persists in the environment for a long time [1]. Synthetic dyes can be harmful to living organisms, and it is essential to remove them from wastewaters. Biosorption is an efficient, cost-effective, and environmentally sustainable method, which uses biologically derived sorbents for wastewaters treatments [2].

The aim of this study was to investigate the efficiency of *Ambrosia artemisiifolia* based biosorbent for CV biosorption. The dye concentration was determined using UV/Vis spectroscopy (NOVEL-102S, COLOLab Experts, Slovenia). At a dye concentration of 20 mg/L, and a contact time of 1 h, a biosorption efficiency of 99% was achieved. The biosorbent was characterized by FTIR spectroscopy (Nicolet SUMMIT FT-IR Spectrometer) before and after biosorption, confirming the dye biosorption and the presence of functional groups in biosorbent structure, which enabled the successful binding of CV. The tested biosorbent demonstrated high efficiency in the biosorption of the cationic dye CV, providing a solid foundation for further research and improvement of its applications in the treatment of contaminated waters.

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EA PP 07

Efficient removal of bezafibrate using acid-modified hydrochar

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The growing presence of contaminants of emerging concern (CECs), such as pharmaceutically active compounds and pesticides, in water systems poses significant risks to ecosystems and human health. These pollutants, often not fully removed by conventional wastewater treatment processes, require innovative and sustainable remediation strategies. Various adsorbents, such as hydrochars, have proven effective in removing pollutants due to their specific properties. Hydrocarbon performance could be improved by application of acid/alkaline modification, thermal activation and metal ion doping. Each of these methods introduces specific changes to the hydrochar's surface properties, improving its adsorption capacity and efficiency for removing contaminants [1].

In this study, the efficiency of acid-modified hydrochar for the removal of bezafibrate, a representative from the group of pharmaceutical active compounds, was investigated. The results were compared with the efficiency obtained using pristine hydrochar. The hydrochar was produced from waste wood biomass under temperature of 300 °C, treatment time of 30 min, a solid-to-liquid ratio of 1:15, and autogenic pressure of 1168 psi. The modified hydrochar was produced using mixture of nitric and sulfuric acids under the same reaction conditions. The pollutant removal from the water was carried out using hydrochars in a concentration of 5 g/l. After 2 hours of treatment, the use of modified hydrochar achieves a higher degree of bezafibrate removal of 72%, compared to the application of pristine hydrochar at 60%.

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EA PP 08

Removal of polluting organic substances from aqueous solutions by adsorption on hydroxiapatite-enriched natural zeolite

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Municipal wastewater, as well as wastewater from arable land drainage, is a major source of organic pollutants such as insecticides. Intensive research is aimed at finding efficient, economically profitable, as well as environmentally acceptable adsorbents for their removal [1]. Zeolites are microporous crystalline aluminosilicates that show good adsorption properties in water purification processes [2]. The crystal lattice of zeolite is negatively charged and it does not have the ability to adsorb anions and nonpolar organic molecules. However, the zeolite surface can be adapted for the adsorption of organic molecules in different ways.

The aim of this work was the preparation of an adsorbent based on surfactant-modified natural zeolite and calcium hydroxyapatite (HAp) and an investigation of its potential application for the removal of acetamiprid (AC) from aqueous solution. The resulting powder was characterized before and after adsorption by X-ray powder diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), thermogravimetric analysis (TG/DTG) and scanning electron microscopy (SEM). The concentration of acetamiprid in the solution was determined by liquid chromatography-tandem mass spectrometry (LC-MS) technique. TG/DTG and FTIR analyses confirmed the binding of the surfactant to the zeolite surface, while SEM microscopy confirmed the presence of needle-like crystals of HAp. During the adsorption experiment, 0.6 mg AC per g (30%) was removed, while the equilibrium state was established after 90 min. The pseudo-second-order Lagergren model best described the kinetics of acetamiprid binding to the adsorbent surface.

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EA PP 09

Application of sodium stearoyl glutamate and polyacrylic acid mixture in cosmetic emulsions

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Cosmetic emulsions are certainly the most commonly used form of cosmetic products, and therefore they continuously attract the attention of researchers, especially in terms of developing safer and eco-friendly products. Accordingly, one direction of development is focused on the use of amino-acid based bio-surfactants, primarily due to their biocompatibility [1]. Sodium stearoyl glutamate (SSG) is, according to manufacturer specifications, an emulsifier suitable for stabilizing cosmetic creams and decorative cosmetic products and personal care products. However, our previous research has shown that SSG (AMISOFT HS 11P) has extremely low solubility in water, good foaming properties, but somewhat weaker emulsifying properties. For these reasons, this research was aimed at the application of a mixture of this emulsifier with polyacrylic acid (PAA), which is a common viscosity modifier in cosmetic products, with the goal of obtaining oil-in-water emulsions with satisfactory properties and stability.

The presence of PAA in aqueous solutions of SSG affected the reduction of surface tension to some extent. This effect was most pronounced in the concentration range of micelle formation of SSG (0.1-0.6%) and indicated a synergistic interaction between the polymer/surfactant mixture. The concentration of SSG significantly influenced the properties of the emulsions studied. As the concentration of SSG increased, the droplet size distribution narrowed and the droplet size in the emulsion decreased, resulting in more stable emulsions with better properties. The results of the dispersion analysis of 20% emulsions of Miglyol in water clearly showed that the presence of PAA in the continuous phase contributes to better dispersive properties of the emulsion and its sedimentation stability. The best properties were shown by the emulsion with 0.1% PAA and 2% SSG. The type of oil significantly affects the droplet size distribution and the stability of the emulsions. The best properties were obtained using grape seed oil and Miglyol as the oil phase. By examining the dispersive and rheological properties of 20% emulsions of Miglyol in water and grape seed oil in water, stabilized with 0.1% PAA and 2% SSG, it was found that emulsions with grape seed oil showed better properties. This vegetable oil could certainly be assessed the first choice when formulating cosmetic emulsions in the PAA/SSG system.

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EA PP 10

Leaching of antimony from water bottle materials

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Antimony oxide is frequently used as a catalyst in the production of polyethylene terephthalate (PET), which may result in the migration of antimony from packaging into bottled water. Considering the potentially toxic effects of long-term exposure to antimony, investigating its migration from packaging to water is essential.[1,2] This study focused on comparing antimony migration from PET and glass packaging in commercially available bottled waters. In July 2024, we analyzed five commercially available brands of bottled water (Knjaz Miloš, Voda voda, Rosa, Aqua viva and Life) in PET and glass packaging. The aim was to quantify and compare the concentrations of antimony and other elements (Ba, Cd, Cr, Cu, Li, Pb, Sb, Sr, B, Mn, K, Mg, Na, Ca) using inductively coupled plasma mass spectrometry (ICP-MS). The analysis confirmed the leaching of antimony from PET packaging into water, while the antimony concentration in water from glass packaging remains unchanged. This migration is linked to the use of antimony oxide as a catalyst in PET production, whereas glass packaging does not contribute to an increase in antimony levels.

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EA PP 11

Hansen solubility parameters as predictor of polymer compatibility for binding fluoxetine

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Polymers have shown great potential in improving drug delivery technology by providing controlled release of therapeutic agents in constant doses over long periods, cyclic dosage and tunable release of both hydrophilic and hydrophobic drugs [1]. In this study, we focused on selective serotonin reuptake inhibitors (SSRIs) such as fluoxetine. Despite the extensive use of these pharmaceuticals, their interaction with polymers remains insufficiently explored. The primary aim of this research is to investigate the binding capabilities of polymers with fluoxetine, which could lead to enhanced drug delivery systems by improving solubility, release profiles and bioavailability, while potentially reducing side effects.

Hansen solubility parameters (HSPs) are used in this study as a predictive tool to assess the compatibility of polymers with pharmaceuticals. HSPs quantify interactions based on dispersion, polar and hydrogen bonding forces [2], enabling the selection of polymers that exhibit optimal binding properties for experimental research. Based on the Ra values, preliminary findings indicate that poly(N-isopropylacrylamide) exhibits the highest compatibility with fluoxetine, with poly(methacrylic acid) as another potential option.

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EA PP 12

Decolorization of Indigo carmine dye with ozone

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Indigo carmine is an organic compound obtained by aromatic sulfonation of indigo. Sulfonation contributes to the solubility of compounds in water. Indigo carmine is also known as 5,5'-sodium salt of indigosulfonic acid, E132, Food Blue 1, C.I. Acid Blue 74 and Brilliant Indigo. The most famous application in medicine is as a diagnostic agent for kidney function tests, but it is also used for dyeing in the textile industry. In the textile dyeing industry, an average of 3–12 g of indigo dye is required to dye a pair of blue denim trousers, and various measurements have shown that up to 200 mg/L of dye can be found in wastewater. [1]

This research aimed to decolorize water polluted with this dye. The experiments were related to the optimization of the treatment time of certain dye concentrations (20, 40, 60, 80 and 100 mg/L). The treatment time intervals ranged between 30 and 300 s, with a sample taken every 30 s. The efficiency of the decolorization was monitored using a UV-VIS spectrophotometer, where a characteristic decrease in absorption at a wavelength of about 600 nm is observed. As a final result, complete decolorization was achieved at all dye concentrations tested, namely for a concentration of 20 mg/L of dye for 120 s, 40 mg/L for 150 s, 60 mg/L for 180 s, 80 mg/L for 210 s and 100 mg/L for 240 s.

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EA PP 13

Absorption of the Red F3B azo dye by humic acid

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The development of global industrialization and urbanization has led to extensive wastewater production. About 20% of textile dyes end up in aquatic ecosystems. The predominant type of dye, which is used in all industrial areas, is the azo dye. [1] The aim of this work was to investigate the ability of humic acids to remove azo dye Red F3B from aqueous solutions. Special attention was paid to determining the optimal amount of humic acid required for effective color removal from solution, with a focus on absorption conditions, such as the appropriate pH environment in which maximum color removal is possible. Two types of humic acids were used: commercial humic acid sodium salt purchased from Sigma Aldrich (purity greater than 50%) and extracted humic acid obtained from the company Center for New Technologies. In addition to research into the determination of the optimal amount of humic acid for the purification of dye-polluted water, a comparison of the efficiency of the mentioned two humic acids was also carried out.

In the experiment with commercial humic acid, the minimum content of humic acid for the removal of 300 mg/L aqueous dye solution was tested. 0.01 g, 0.05 g, 0.10 g, 0.15 g, 0.20 g, 0.25 g, 0.30 g, 0.35 g, 0.40 g and 0.50 g of humic acid was added to solution of the dye, where complete color removal was observed to be achieved with 0.10 g of humic acid. The extracted humic acid was also able to decolorize the same concentration of dye with 0.15 g of humic acid. Based on the experiments, it was determined that both humic acids are equally effective in removing the tested azo dye from water.

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We thank the Center for New Technologies that provided us with the extracted humic acids that were part of this research.

EA PP 14

Partitioning behavior of polyphenolic compounds in choline-based ionic liquid aqueous biphasic systems

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Polyphenols, known for their antioxidant properties, are abundantly found in food waste, making their extraction valuable [1]. Unlike traditional solvent extraction methods, which suffer from extended extraction times, lower efficiency and the use of organic solvents, an aqueous biphasic system (ABS) based on ionic liquids (IL) presents a promising alternative [2]. Cholinium-based ionic liquids in ABS, characterized by their low toxicity and biodegradability, offer an eco-friendly approach, especially when combined with pluronic copolymers [2]. In this study, an ABS composed of cholinium acetate [Ch][Ac] ionic liquid and the Pluronic copolymers PE6200 or L35 was utilized to extract and separate the polyphenolic compounds, vanillic acid and resveratrol from aqueous solutions. In the first system composed of [Ch][Ac] and PE6200, results demonstrated that resveratrol was preferentially extracted into the PE6200 copolymer phase, achieving an extraction efficiency of approximately 5% in the ionic liquid-rich phase. In contrast, vanillic acid was predominantly extracted into the ionic liquid-rich phase with an efficiency of 93%, enabling the successful separation of the two polyphenols. Furthermore, when Pluronic L35 was used, resveratrol exhibited a more balanced distribution, with about 50% partitioning into the polymer phase, while vanillic acid extraction into the IL phase remained high at 89%. This shift in partitioning behavior indicates that the choice of Pluronic copolymer significantly influences the separation efficiency, as the L35 system was less effective for achieving complete separation of both polyphenols. Overall, this study demonstrates the potential of biocompatible copolymer-ionic liquid-based ABSs as a sustainable platform for polyphenol extraction, with promising applications in the recovery of valuable compounds from real samples such as food waste.

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EA PP 15

Influence of Fe^{3+} ions and citrate in the photodegradation of levofloxacin in water solution at pH 5

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Levofloxacin (LVX) is an antibiotic from the fluoroquinolone family, often used to treat bacterial infections. Its extensive use can lead to environmental contamination, raising significant health concerns for both humans and ecosystems [1]. The influence of citrate and the presence of ferric ions on photosensitivity of LVX to UV-A and UV-B irradiation was investigated by UV-Vis and fluorescence spectroscopy in water at pH 5. Cyclic voltammetry was applied to examine the effect of coordination between Fe^{3+} ions and LVX on their redox properties in water at pH 5 in the presence of citrate. Results from UV-Vis and fluorescence spectroscopy demonstrated that significant spectral changes occur when the LVX:Fe:citrate 1:3:1 molar ratio, indicating the photodegradation of LVX. Understanding the stability of LVX can aid in the development of effective methods for its removal, which is crucial for reducing pollution and protecting the environment.

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EA PP 16

Development and application of electrochemical sensor for metol detection in adsorption studies

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Metol (4-(methylamino)phenol sulfate) is an organic compound that, in combination with hydroquinone, is used to develop black-and-white photographic films and papers [1]. It has an impact on humans, plants and animals, raising serious environmental concerns. The current scenario demands the development of a fast, cost-effective, precise and specific method for the detection of metol in environmental and biological samples. In this study, an electrochemical sensor was developed using an electrode modified with gold nanoparticles. The modified electrode shows exceptional selectivity, stability and reproducibility. The electrochemical sensor has a wide linear range (0.73 – 49.35 μM), a low detection limit and quantification limit (0.06 μM and 0.2 μM, respectively) and high sensitivity ($0.33\ \mu A\cdot(\mu M)^{-1}\cdot cm^{-2}$). The sensor's efficiency was confirmed through the analysis of aqueous solutions and the detection of metol residues after adsorption treatment on activated carbon material synthesized from sunflower agro-industrial waste.

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EA PP 17

Photodegradation of ciprofloxacin with zirconium-modified titan(IV)-oxide

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Ciprofloxacin (Figure 1) is a synthetic derivative of the fluoroquinolone class, extensively used in the treatment of bacterial infections in both humans and animals. Its broad-spectrum activity makes it highly effective against a wide range of pathogens, including both gram-positive and gram-negative bacteria. The mechanism of action involves inhibiting bacterial DNA gyrase and topoisomerase IV, enzymes essential for DNA replication, transcription, and repair, effectively halting bacterial growth. Due to its potency and versatility, ciprofloxacin is commonly prescribed for respiratory, urinary tract, skin and gastrointestinal infections However, the widespread use of ciprofloxacin not only raises concerns about antibiotic resistance but also makes it one of the three most commonly detected antibiotics in aquatic ecosystems. [1,2]. Therefore, in this study, we synthesized TiO_2 modified with Zr in three different molar ratios (0.5%, 1% and 2%) and applied it to the photodegradation of a ciprofloxacin infusion solution. The degradation process was monitored using UV-Vis spectroscopy over 240 minutes. Results indicated that the efficiency of $(Zr)TiO_2$ catalysts is approximately the same, but increasing the molar ratio of Zr in the photocatalyst slightly decreases the degradation efficiency.

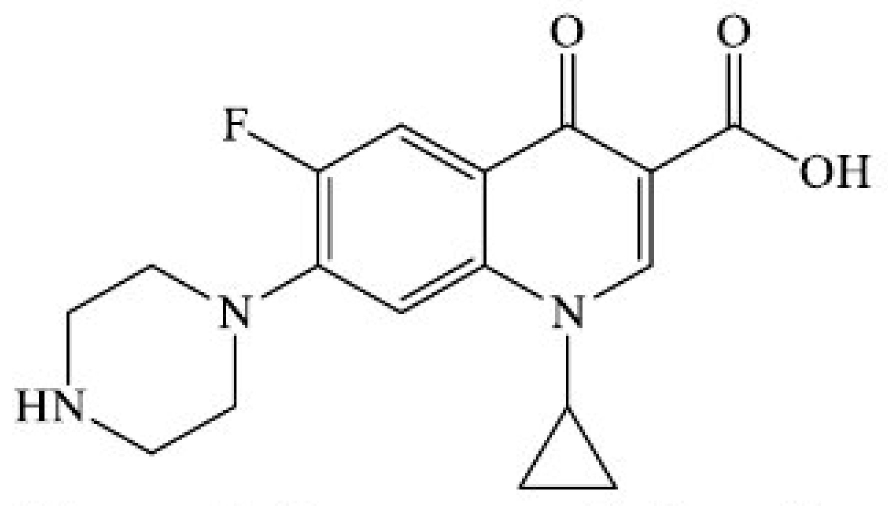

Figure 1. Structure of ciprofloxacin

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EA PP 18

Valorization of shells from the invasive river crayfish *Faxonius limosus:* Chitosan extraction and characterizartion

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Chitosan, a natural biopolymer from crustacean exoskeletons, is typically obtained from crabs and shrimp. *Faxonius limosus*, an invasive American crayfish species, has spread along the Danube River, disrupting biodiversity and harming native species. Due to its harmful effects, initiatives have been launched to harvest this invasive crayfish and explore its potential as a valuable resource. In addition to the use of the crayfish meat, byproducts, such as its shell are being extensively researched as source of valuable compounds [1]. This study aims to valorize the shells by using them to extract chitosan, applying different extraction procedures. Two methods were used to extract chitosan: conventional and modified chemical extraction. The modification reduced both demineralization and deproteinization from three steps to one, aiming to lower chemical use and wastewater without compromising the final product. Characterization included visual inspection, structural analysis, degree of deacetylation via FTIR, and molecular weight determination by viscometric method. The modified procedure significantly reduced chemical use (66% for HCl, 51% for NaOH) and wastewater by 45%. Both extraction methods produced structurally similar chitosan, with degrees of deacetylation at 79% and 75%, and molecular weights of 189 kDa and 146 kDa. This demonstrates the potential of utilizing Faxonius limosus shells to produce chitosan with desirable properties using the modified method.

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Acknowledgments

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Physical and Computational Chemistry (PCC)

PCC PP 01

Study of Nb_2CTx properties for application in microsupercapacitors

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MXenes represent a novel class of two-dimensional materials, first identified in 2011, with a number of potential applications. The distinctive characteristics of niobium MXenes, including high conductivity, hydrophilicity, and stability, make them suitable for use in energy storage devices [1]. Accordingly, this study proposes an investigation of the morphostructural and electrochemical properties of delaminated Nb_2CT_x, prepared from the MAX phase (Nb_2AlC) using the MILD method (LiF+HCl). The specific capacitance value of 161.58 mF cm^{-2} was reached at 5 mV s^{-1} in 1 M H_2SO_4 for the potential variation of 1 V (Fig. 1). The charge/discharge tests demonstrated that the material exhibits stability over 1000 cycles, with a charge retention of 105.03%, a power of 5 mW cm^{-2}, and an energy of 1.21 μWh cm^{-2}; such performance confirmed Nb_2CTx as a suitable material for electrodes in microsupercapacitor devices.

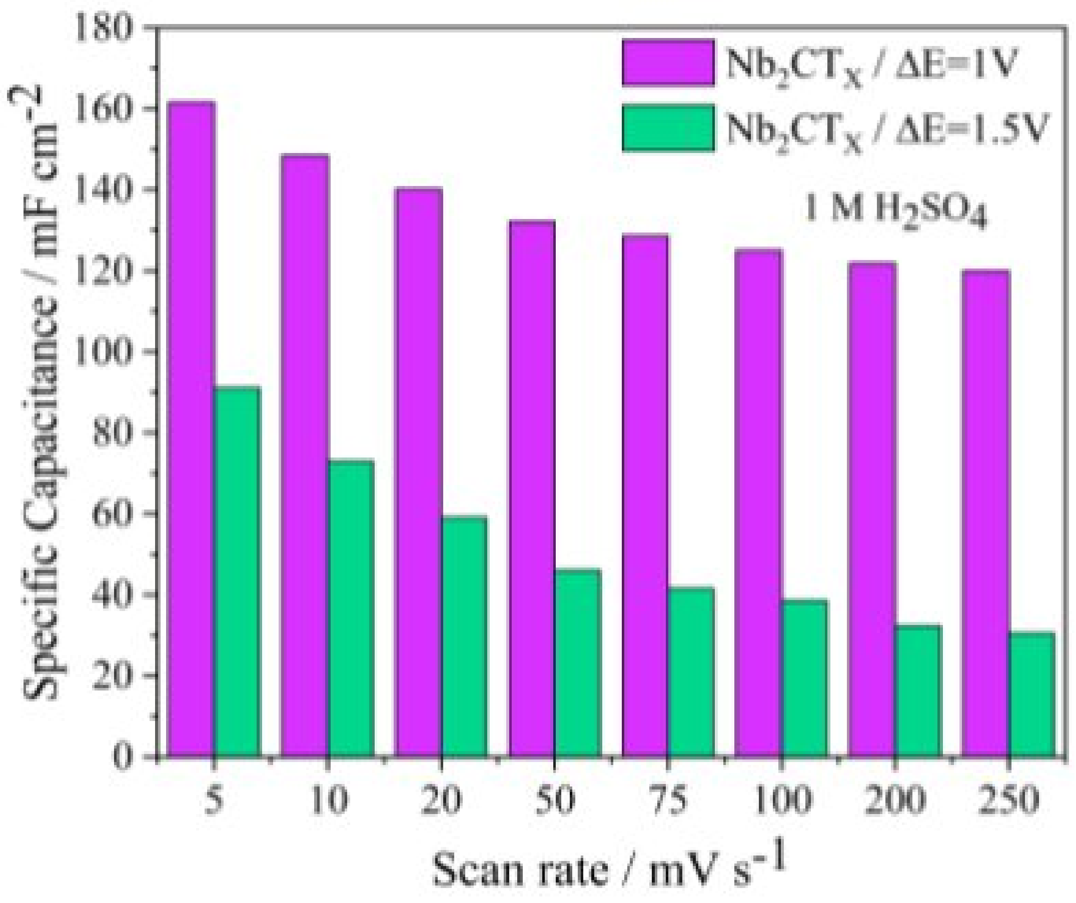

Figure 1. Specific capacitance values of Nb_2CTx in 1 M H_2SO_4 when cycling in two different potential windows.

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PCC PP 02

Designing a crown ether detector for Mg^{2+} ions

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Cyclic crown ethers can be used as ion traps because of the partial negative charge on oxygen atoms. Crown ethers with a bithiophene unit were synthesized and theoretically examined for Na^+ and K^+ ions [1,2]. In the present study, we focus on theoretically designing an optimal detector for Mg^{2+} ions. We have investigated 20 crown ethers with bithiophene units utilizing Density Functional Theory (DFT) at the M06-2X/6-311+G(p,d) level. All twenty candidates were optimized in vacuum, and as micro-solvated complexes with two molecules of water attached to Mg^{2+}. After analyzing the corresponding interaction energies and the geometric parameters, we were left with six possible candidates. These six crown ethers were then completely solvated with two solvation shells, and their time evolution was studied using Density Functional Theory based Molecular Dynamics (DFT-MD) at the BLYP(-D3)/DZVP level. After analyzing the dynamics of the chosen six crown ethers we found an optimal host for catching magnesium ions (Fig. 1).

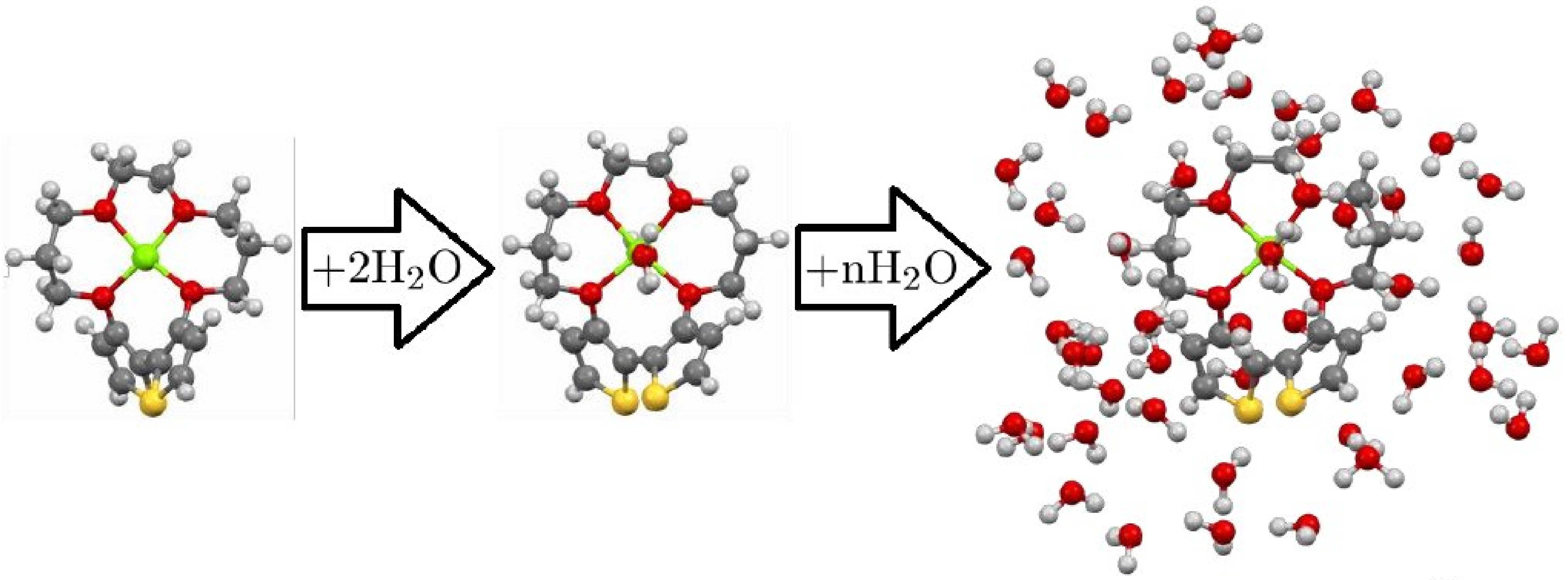

Figure 1. A quick overview of our methodology for finding the optimal detector for Mg^{2+} ions.

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PCC PP 03

Glassy carbon electrode modified by ZnO/GO composite for electrochemical detection of diclofenac

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In 2019, diclofenac (DCF) was classified as a substance of high priority for monitoring in order to protect aquatic environments [1]. Electroanalytical methods have numerous advantages compared to conventional instrumental methods when it comes to detection and monitoring of DCF in water, however, there is still a need for developing electrodes with sufficiently good analytical properties. Herein, a composite of zinc oxide (ZnO) and graphene oxide (GO) (0.005 wt % relative to ZnO) was characterized by XRD, Raman spectroscopy, and FESEM imaging, and used to prepare an ink that was applied to a glassy carbon electrode (GCE). After *in situ* reduction of GO, the obtained ZnO_0.005rGO@GCE electrode was tested for the detection and quantification of DCF in 0.1 M phosphate buffer (pH=7) by cyclic voltammetry (CV) (Fig. 1A) and differential pulse voltammetry (DPV) (Fig. 1B). It was found that the ZnO_0.005rGO@GCE electrode is active for detection of DCF by both CV and DPV method. Significant improvement in sensitivity, as well as lower limit of detection/quantification was achieved by DPV method.

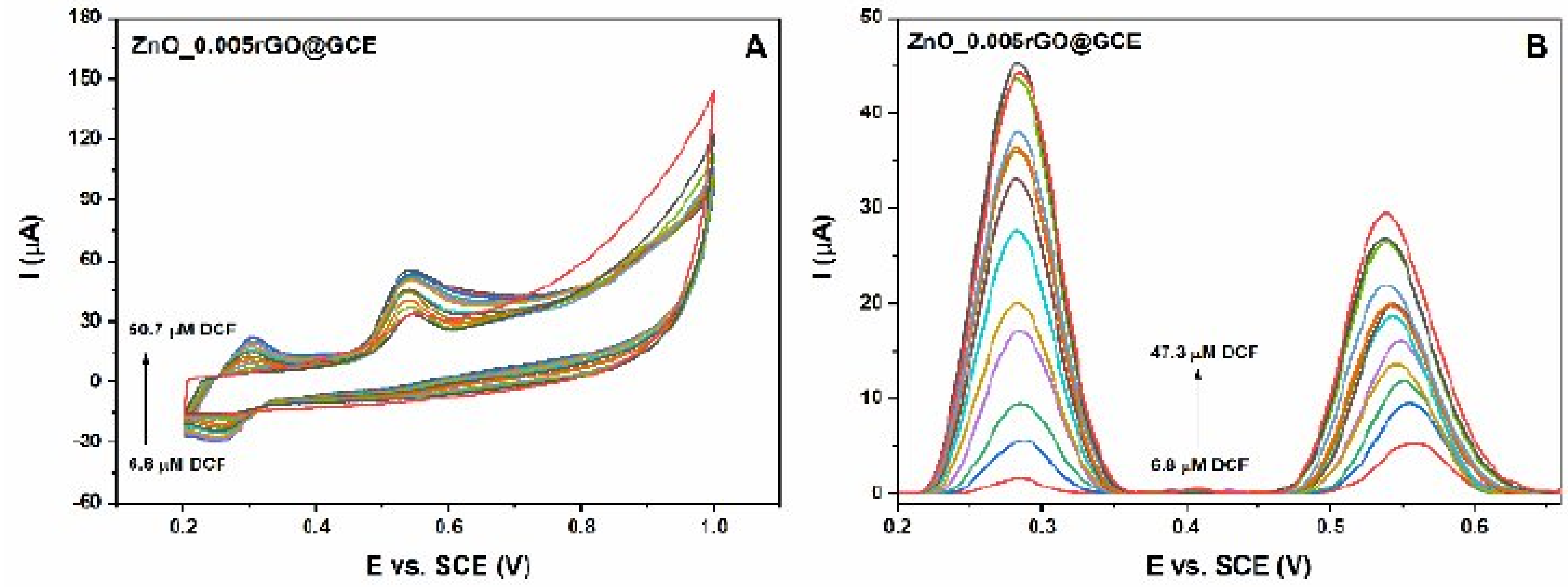

Figure 1. Cyclic voltammograms (A) and Differential pulse voltammograms (B) of ZnO_0.005rGO@GCE for different concentrations of DCF in 0.1 M phosphate buffer (pH=7)

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PCC PP 04

Zn/rGO nanosize electrocatalyst for oxygen reduction reaction in alkaline media

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The oxygen reduction reaction (ORR), a reaction of vital importance for the promising zero-carbon and effective electrochemical devices like metal-air batteries and fuel cells, can occur via a two- or four-electron mechanism, and due to this multi-electron transfer have sluggish kinetics [1]. Therefore, the development of efficient and low-cost ORR electrocatalysts is needed. Herein, zinc deposited on reduced graphene oxide (Zn/rGO) was proposed as nanosized electrocatalyst for ORR in alkaline media. Electrocatalytic activity of Zn/rGO towards ORR was examined in N_2- and O_2- saturated 1 M KOH solution (Fig. 1) by cyclic voltammetry. A well-defined ORR peak was observed at 0.65 V in the O_2- saturated solution, giving about 7.8 times higher current density than in the N_2- saturated solution. Zn/rGO exhibited catalytic activity for ORR, making it a potentially good replacement for costly state-of-the-art electrocatalysts for ORR.

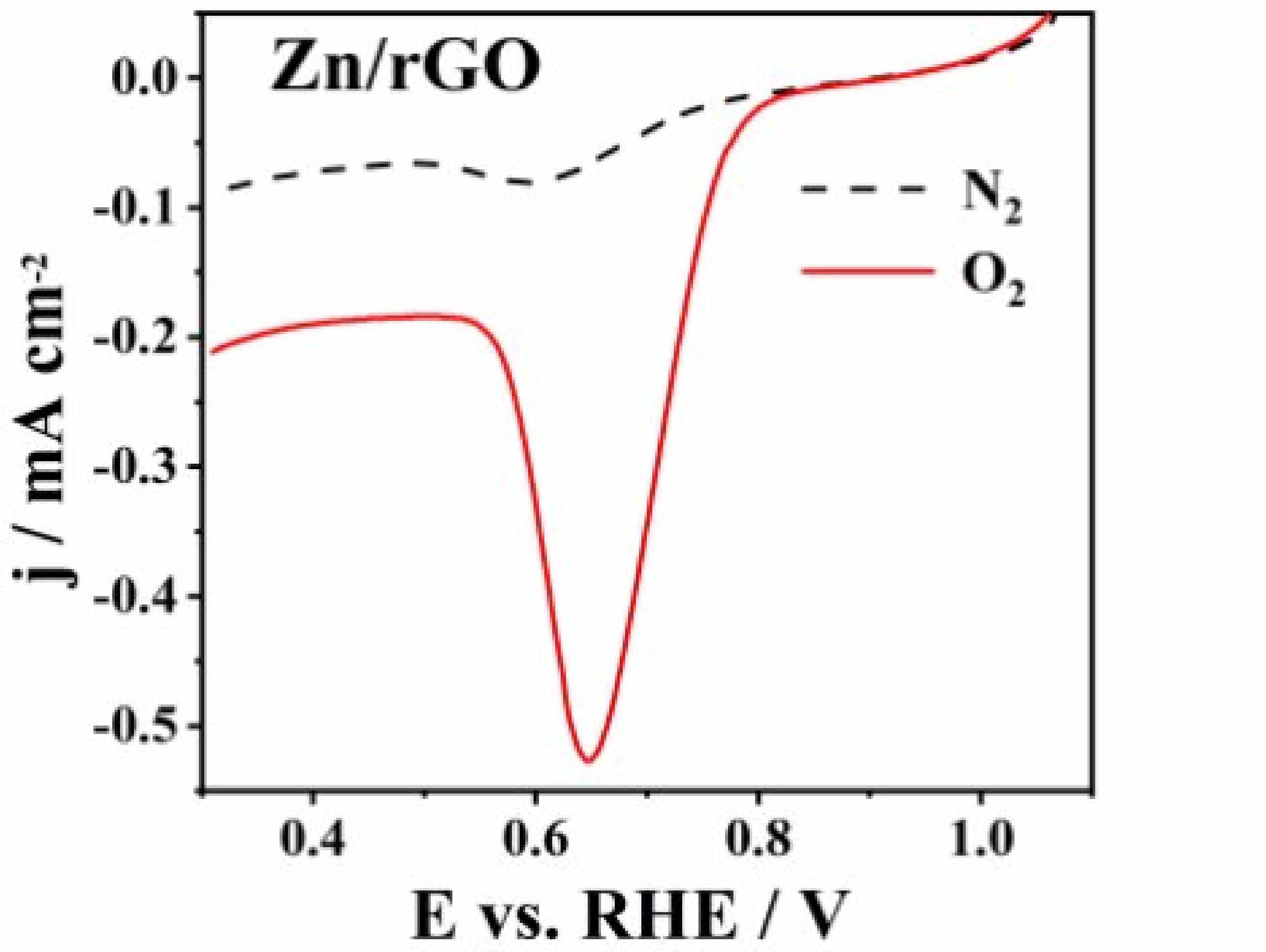

Figure 1. Cathodic scan of cyclic voltammogram of Zn/rGO at 5 mV s^{-1} in O_2-saturated 1 M KOH

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PCC PP 05

Analysis of trigger bond strength in nitroaromatic systems with intermolecular hydrogen bonding using Wiberg bond indices

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Previous studies have shown that hydrogen bonds can influence the sensitivity of nitroaromatic explosives in various ways.[1] For instance, the intramolecular hydrogen bonds typically deactivate C-NO_2 trigger bonds, thereby reducing the sensitivity of nitroaniline-based energetic compounds. However, the intramolecular hydrogen bonding in nitrophenol-based energetic compounds strengthens the *ortho*-C-NO_2 bond, while the lone pairs on the phenol group induce steric repulsion, leading to the activation of another neighboring nitro group.[2]

In this study, we utilized Wiberg bond indices (WBI) to identify trigger bonds and examine the role of intermolecular hydrogen bonds in the sensitivity of various nitroaromatic compounds. We compared the WBIs for the C-N, N-O and C-C bonds in both non-bonded and hydrogen-bonded nitroaromatic systems. Our findings indicate that intermolecular hydrogen bonds can either increase or decrease the strength of C-N bonds, depending on the position of the C-NO_2 bond within the molecular structure. Additionally, the resulting effects are influenced by the steric effects present in the molecule.

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PCC PP 06

Development and validation of QSRR models of 3-(4-substituted benzyl)-cycloalkylspiro-5-hidantoins

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A Quantitative structure-retention relationship (QSRR) analysis has been performed on the chromatography parameters of lipophilicity of some spirohydantoins. The chromatographic parameters of lipophilicity were determined by reversed-phase thin-layer chromatography. Chromatographic analyses were performed on C-18 modified silica gel with a two-component mobile phase consisting of water and organic solvent (ethanol, n-propanol, i-propanol, t-butanol, acetone, acetonitrile, tetrahydrofuran or 1,4-dioxane) in different ratios [1]. QSRR models were created for eight aqueous mobile phases. Molecular descriptors were calculated using several software packages: *Dragon*, *ChemDraw Ultra 7.0*, *Molinspiration*, and *ADMETlab*. Multiple linear regression (MLR) was applied to construct the QSRR models. The predictive ability of each model was evaluated using internal and external validation.

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PCC PP 07

The influence of solvent polarity on the kinetic and thermodynamic parameters of the reaction of substitution of methyl chloride with *p*-hydroxybenzoate anion

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This study investigates the influence of solvent polarity on the thermodynamic and kinetic parameters of the nucleophilic substitution reaction of methyl chloride with the *p*-hydroxybenzoate anion, which proceeds via the S_N2 mechanism [1]. The research aims to elucidate how various polar aprotic solvents, characterized by distinct dielectric constants, affect both the kinetics and thermodynamics of the reaction. The reaction was analyzed under vacuum conditions as well as in the presence of dimethyl sulfoxide (ε = 46.826), dimethylformamide (ε = 37.219), acetone (ε = 20.493), and tetrahydrofuran (ε = 7.426). Geometry optimization was done by using the M06-2X/6-311++G(d,p) theoretical model implemented in the Gaussian 09 software package, while the CPCM solvation model was applied to simulate the impact of the solvents [2]. By analyzing the reaction enthalpy (Δ_rH) and Gibbs free energy (Δ_rG), and calculating the reaction rate constant using Transition State Theory (TST) and Eyring's equation, it was determined that the substitution reaction became increasingly favorable, both kinetically and thermodynamically, with increasing solvent polarity. It is a consequence of the fact that polar aprotic solvents enhance the stabilization of both the transition state and the product complex. Symmetric polar aprotic solvents are highlighted as more suitable because their stabilization effect toward the product complex is higher. It is of significant importance when the leaving group is a small-volume anion, and then the stabilization of the product complex is enabled with the greater surface of the solvent's molecule positive charge.

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PCC PP 08

Effects of sulfuric acid on pig bone quality: Implications for forensic analysis

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The study examined the effects of sulfuric acid on pig shoulder bone quality through various analytical methods, including FTIR, LIBS, and AAS. In forensic practice, sulfuric acid is commonly used to destroy biological evidence, complicating the determination of cause and time of death, as well as victim identification. Pig bones serve as model bones in forensic investigations due to their similarity to human bones in lamellar structure, regeneration rate, cortical mineralization, mineral concentration, and density. Over a 14-day immersion in sulfuric acid solutions of varying concentrations (0.01 M, 0.1 M and 1 M), significant changes in the elemental composition and the collagen and phosphate content of the pig bone were observed. The study utilized deconvolution techniques to analyze spectral data, focusing on regions associated with protein structure and mineral content. Findings indicated that sulfuric acid is an effective demineralization agent that primarily targets hydroxyapatite while preserving the collagen matrix. The assessment of collagen maturity provided insights into the bone's structural integrity. Additionally, LIBS and AAS results revealed alterations in bone hardness and the ratios of calcium, phosphorus, and magnesium in the solutions post-immersion. Notably, an increase in acid concentration and immersion time led to an ionization change in calcium, suggesting a potential hardening of the bone due to calcium sulfate deposition, while the concentrations of calcium, phosphorus, and magnesium in the solutions exhibited varying trends with increasing acid intensity.

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PCC PP 09

Elucidating nonclassical hydrogen bonding between water and pyramidane molecule

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Tetracyclo[2.1.0.$0^{1,3}$.$0^{0,25}$]pentane (pyramidane) and its derivatives are distinguished by their nonclassical cage-like geometries.[1] We performed interaction energy calculations to evaluate the capability of the apex carbon in pyramidane and its derivatives to act as hydrogen bond acceptors. MP2/aug-cc-pVTZ quantum chemical calculations demonstrated that pyramidane and its derivatives with substituents R = H, CH_3, F, Cl, OH, and CN are capable to form strong hydrogen bonds. The computed interaction energy between the apex carbon atom and a water molecule was $\Delta E = -6.41$ kcal/mol (see Fig. 1), whereas the tetramethyl derivative exhibited the strongest interaction with an energy of $\Delta E = -7.40$ kcal/mol.

The interaction energy trend, ranging from −2.05 kcal/mol for -CN to −7.40 kcal/mol for -CH_3, indicates that electron-donating substituents enhance system stability, while electron-withdrawing groups result in the weakest interaction energies. SAPT2/aug-cc-pVTZ energy decomposition reveals that the electrostatic component is the dominant attractive force in all studied systems. These findings are crucial for advancing the understanding and identification of nonclassical hydrogen bonds.

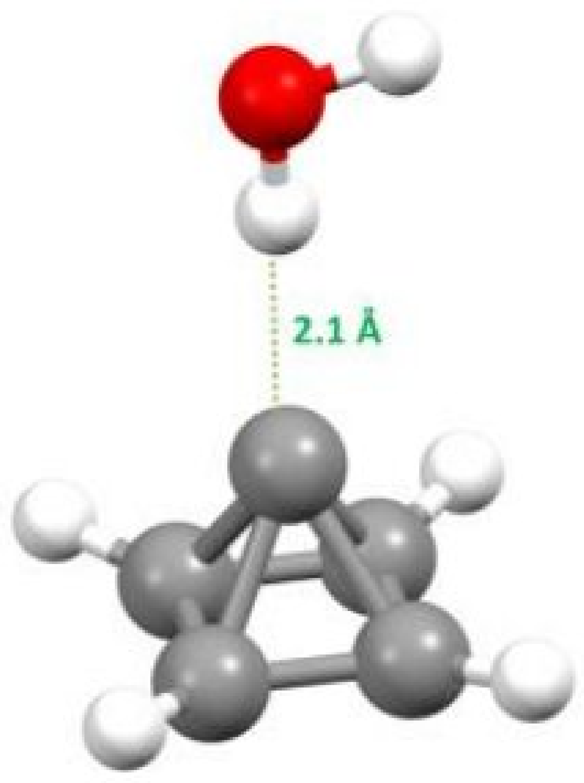

Figure 1. Geometry of the most stable hydrogen bond between pyramidane and a water molecule.

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PCC PP 10

Investigation of C-H/O interactions between series of some aromatic and anti-aromatic cyclic hydrocarbons and water

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Investigation of the CH/O interactions of aromatic CH donors has shown that linear geometry is not preferred for these systems, but the geometry depends on the type of atom in the *o*-position to the CH donor group. [1] Research done on benzene and other polycyclic aromatic molecules and water has shown that as the number of aromatic rings increases, so does the strength of the interactions. [2]

In this paper, the interaction energies between oxygen from the water molecules and hydrogens bonded to carbon ring of aromatic or anti-aromatic molecules were investigated. Also, bifurcated systems were considered (Fig. 1). Optimal geometries and interactions were calculated using MP2/cc-pVTZ level of theory and using Gaussian 09 program.

The results showed that there are attractive interactions in all systems included in the research. For most of them, bifurcated systems were not the most stable ones. The exceptions were phenantren/water and cyclooctatetraene/water systems. For them, interactions type 2 were favorable. The strongest calculated interactions were interactions type 1 between oxirene and water (-3,33 kcal/mol), while the weakest were interactions type 2 between cyclooctatetraene and water (-1,24 kcal/mol).

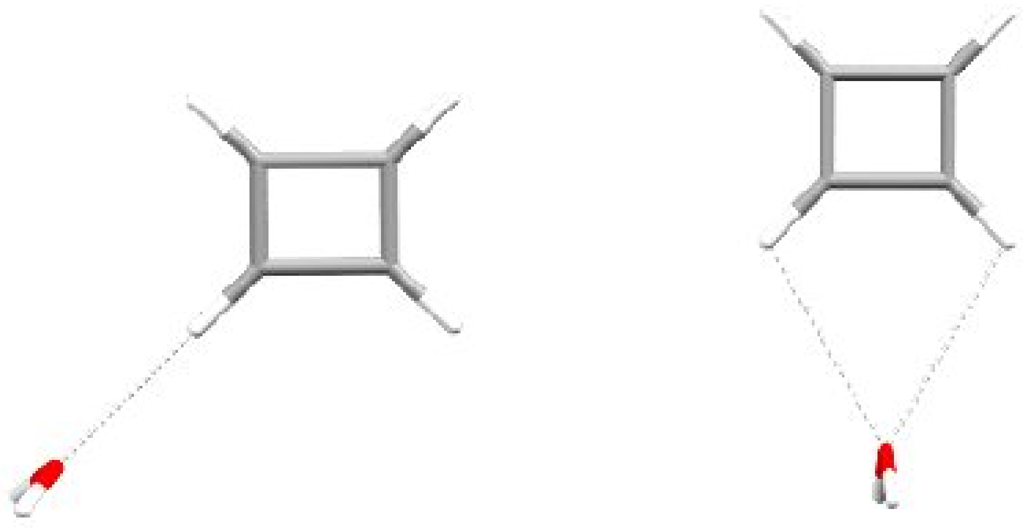

Figure 1. Geometries used in research: model system type 1 (left) and model system type 2 (right)

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PCC PP 11

Helical ladderanes – the first few steps

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Since their discovery in bacterial anammoxosome membranes in the early 2000s, ladderanes, polycondensed cyclobutanes, have inspired a number of papers focusing on their unique properties, synthesis and biological role. However, not much work has been done on those ladderane isomers and conformers which do not occur in biological systems. Here, to the best of our knowledge, we report for the first time the structures and selected electronic properties of all-syn ladderanes obtained through DFT calculations at the B3LYP/6-311+G(d,p)//M06-2X/6-31+G(d,p) level of theory. We found that all-syn ladderanes adopt a spiral structure with C_2 symmetry, a type of structure not commonly associated with alkanes, having approximately 6 cyclobutane rings per turn (see Fig.1). These configurations correspond to minima on the PES and their stability was further demonstrated using molecular mechanics. Calculated ^{1}H-NMR spectra of all-syn isomers show no great deviation from those of all-anti molecules, however, ^{13}C-NMR spectra of all-syn ladderanes are much more complex then those of their all-anti counterparts, exhibiting substantial variation of δ_C with atom's position in the helix. This indicates an unevenness in the electronic density distribution along the helix, which was corroborated using maps of electrostatic potential (MEP). It remains to be seen how this could influence interactions between ladderanes themselves and with other molecules. Furthermore, maximal and minimal MEP values per atom were tested as a means of separating all-syn and all-anti isomers in chemical space, and the preliminary results are promising. More work is needed to establish the general utility of this approach in areas such as machine learning for non-covalent interactions and soft-matter.

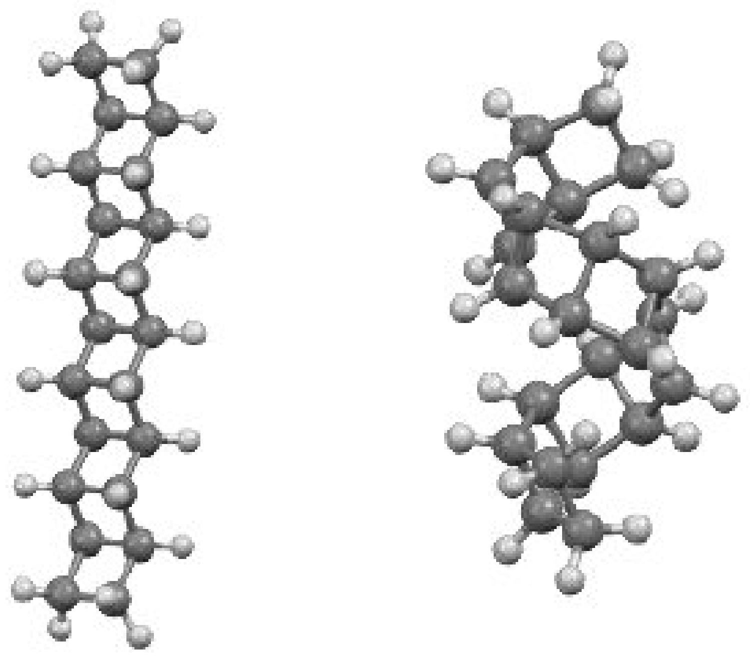

Figure 1. All-anti (left) and newly reported all-syn (right) [10]ladderane.

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PCC PP 12

Energy decomposition analysis of hydrogen bonds of coordinated glycine complexes with water

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Interaction energies between various glycine complexes and a water molecule had been evaluated using quantum chemistry calculations for three hydrogen bond types: NH/O of α-amino group, O1/HO involving oxygen coordinated to the metal ion (O1), and O2/HO involving α-carbonyl oxygen (O2). [1,2] Different transition metals and geometries were investigated, and their values compared: octahedral cobalt(III) and nickel(II), square pyramidal copper(II), and square planar copper(II), palladium(II), and platinum(II) complexes. [2] In this work, we analyzed the nature of these three hydrogen bond types by means of: symmetry-adapted perturbation theory (SAPT) and variational energy decomposition analysis (EDA) method (TPSS-D3/def2-TZVPP). The results show that the cheaper EDA variational method is in good agreement with the reliable SAPT2+3/def2-TZVPP and its total interaction energies are in good agreement with CCSD(T)/CBS values. Out of three attractive interaction terms, in majority of the systems, electrostatic is the strongest, followed by orbital relaxation, while dispersion is the weakest. However, for the weakest hydrogen bonds, all three attractive terms have very similar values. Comparing EDA values for the selected systems, the effects of changes in glycine complexes can be determined. Decomposition analysis results are very strongly affected by the change in complex charge, quite strongly by the metal oxidation and coordination number, and much weaker by atomic number changes in the complex. The strongest decomposition terms (electrostatics and exchange-repulsion) are influenced the most. The O2/HO hydrogen bond experiences the least fluctuations in interaction energy values, because of its location further away from the metal ion.

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PCC PP 13

Hydrogen bonds between aqua complexes – crystallographic and DFT study

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Hydrogen bond is arguably the most abundant noncovalent interaction and it is particularly important for systems containing water. Previous studies have shown that hydrogen bonds of water become significantly stronger if water coordinates to a metal. [1,2] In this work, hydrogen bonds between two coordinated water molecules were studied through data screening and density functional calculations. The screening of crystal structures deposited in the Cambridge Structural Database resulted in 1161 hydrogen bonds between two aqua ligands. The majority of these hydrogen bonds possess high degree of linearity, but they are slightly longer than hydrogen bonds between coordinated and free water due to the size of aqua complexes. Nevertheless, DFT calculations performed at B97D/def2-TZVP level of theory showed that these hydrogen bonds are stronger than hydrogen bonds between free and coordinated water, reaching interaction energies of –11.0 kcal/mol. Moreover, it was shown that aqua complexes tend to form multiple simultaneous hydrogen bonds that can reach remarkable interaction energy of –70.0 kcal/mol.

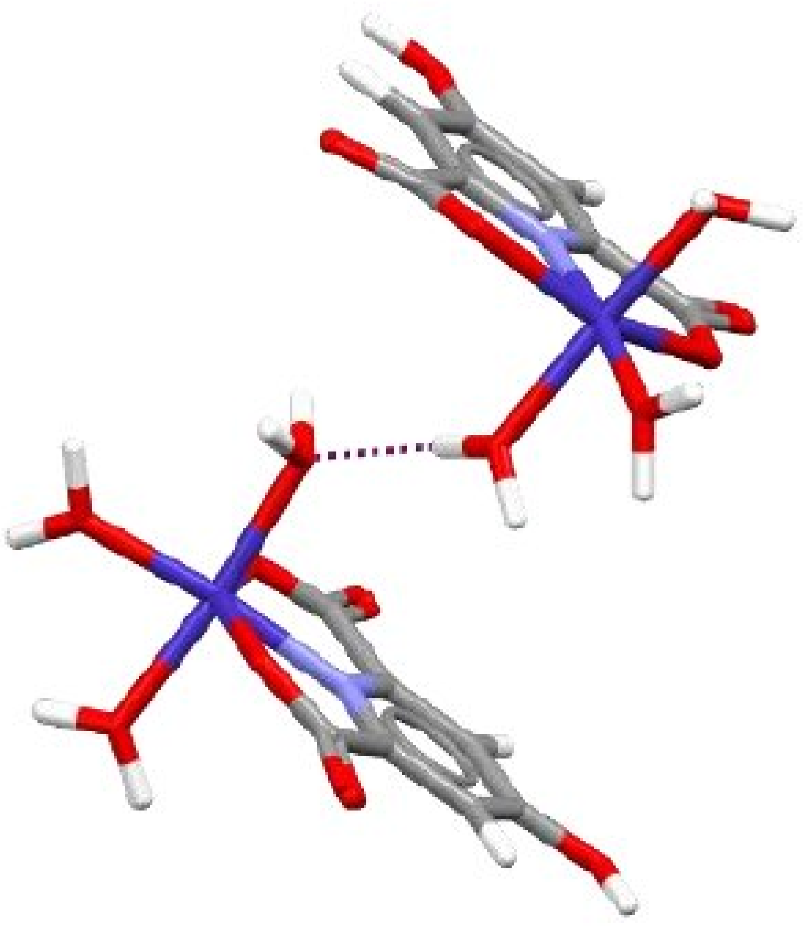

Figure 1. Hydrogen bond between two aqua complexes in crystal structure POCXIQ.

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PCC PP 14

Weak C-H/O hydrogen bonds become stronger upon transition metal coordination – a crystallographic and computational study

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In spite of being weak, C-H/O hydrogen bonds are omnipresent in many molecular systems.[1] Interesting case are interactions of aromatic C-H donors, which were shown to be bifurcated rather than linear, but nevertheless not exceeding the energy of –1.5 kcal/mol.[2] In our joined crystallographic and computational study, we have observed the aromatic C-H donors within sandwich and half-sandwich compounds. Our search of crystal structures deposited in the Cambridge Structural Database found 152 examples of C-H/O hydrogen bonds of benzene coordinated to transition metals. These hydrogen bonds are mostly linear, and they are shorter than hydrogen bonds of uncoordinated aromatic C-H donors, which implies that coordinated benzene forms stronger interactions than uncoordinated one. These findings were corroborated by performing the B3LYP-D3/aug-cc-pVDZ calculations, which showed that coordinated benzene is capable of forming C-H/O interactions that almost reach the energy of –4.0 kcal/mol. Our study indicates that transition metal coordination of aromatic molecules significantly increases the strength of their hydrogen bonds, upgrading them from weak to moderately strong.

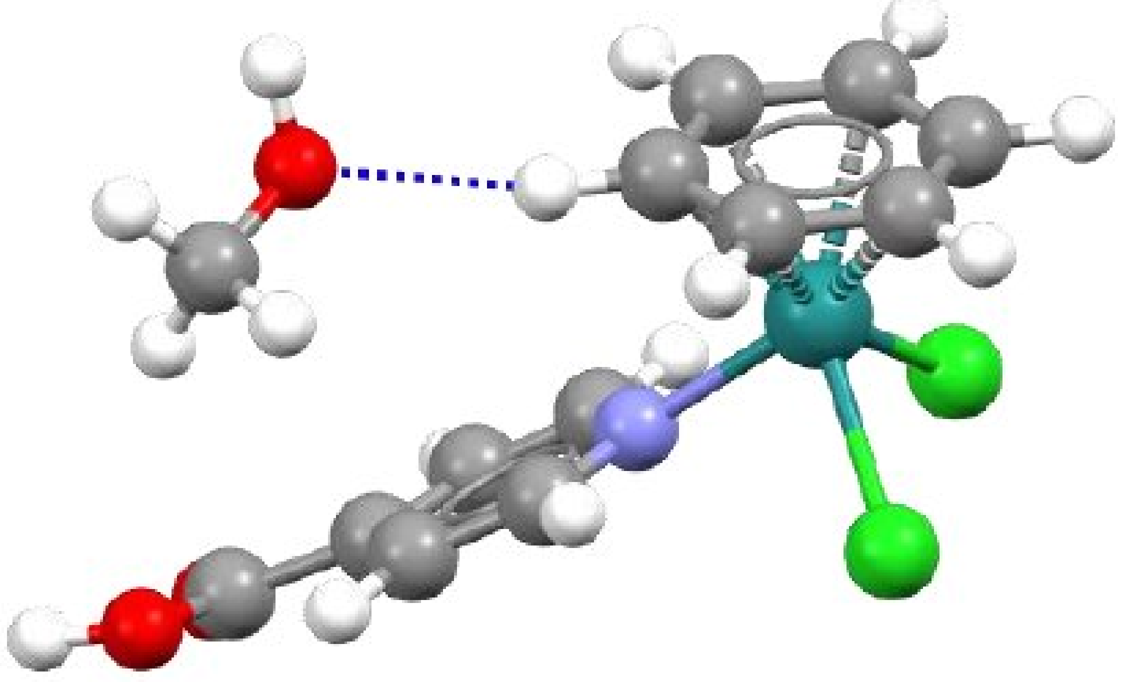

Figure 1. C-H/O interaction between coordinated benzene and methanol in the crystal structure SIVYOM

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PCC PP 15

Catalysis of oxygen electrode reactions using transition metal fluorides

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Bifunctional electrocatalysts are catalysts capable of catalyzing both the oxygen reduction reaction (ORR) and the oxygen evolution reaction (OER) in different modes of operation. Currently, the ORR benchmark are materials based on platinum (Pt), while the best electrocatalysts of the OER are oxides of noble metals iridium and ruthenium (IrO_2 and RuO_2) [1]. In order to find such electrocatalysts, five fluorides of transition metals: CoF_2, NiF_2, ZnF_2, CuF_2 and FeF_3, were tested. The electric double-layer capacitance and the electrochemically active surface, as well as the catalytic activity for the reaction of reduction and evolution of oxygen in an alkaline medium, were examined. The following electrochemical methods were used: cyclic voltammetry, linear scanning voltammetry with rotating disc electrode, chronoamperometry and electrochemical impedance spectroscopy. The lowest Tafel slope for the ORR of 112 mV dec^{-1} was determined for CoF_2. The number of exchanged electrons, determined by the Koutecky-Levich analysis, shows that the ORR reaction catalyzed by CoF_2 takes place by a favorable four-electron mechanism, with NiF_2, ZnF_2 and FeF_3 by a two-electron mechanism, while with CuF_2 there is mixed kinetics, that is, the ORR reaction takes place via both mechanisms simultaneously. The lowest onset potentials during OER was determined for CoF_2 (1.59 V) and NiF_2 (1.58 V). Moreover, CoF_2 showed a high OER current density (45.75 mA cm^{-2} at 2 V), two times higher than the reference OER electrocatalyst (IrO_2), and the lowest Tafel slope (137 mV dec^{-1}).

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PCC PP 16

Voltammetric determination of paracetamol using glassy carbon electrode modified with gold nanoparticles and molecularly imprinted polypyrrole

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In this study, a new electroanalytical method for the determination of paracetamol is developed. For this purpose, a glassy carbon (GC) electrode modified with gold nanoparticles and molecularly imprinted polypyrrole was used as the working electrode, which increased the detection limits and selectivity towards paracetamol. Gold nanoparticles (AuNPs) were electrodeposited on a GC electrode using cyclic voltammetry in a solution of chloroauric acid and potassium chloride. Electropolymerization of pyrrole was performed on the surface of a AuNPs modified GC electrode using cyclic voltammetry in the presence of paracetamol as a template (MIPppy), as well as without it (NIPppy). Qualitative data on the electrodes were obtained using cyclic voltammetry. The NIPppy/AuNPs/GC electrode gave the highest voltammetric response in paracetamol solutions, followed by the MIPppy/AuNPs/GC electrode. The performance of the MIPppy/AuNPs/GC electrode was evaluated by square wave voltammetry (SWV). A calibration curve was constructed, and a linear dependence between the peak current and the concentration of paracetamol was observed in the interval from 5×10^{-5} mol/dm^3 to 1×10^{-3} mol/dm^3. The concentration of paracetamol in the solution of the drug in the phosphate buffer was determined by the method of the calibration curve. Results obtained using SWV were compared with results obtained using high performance liquid chromatography.

Acknowledgments

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PCC PP 17

Half-sandwich compounds of heavier transition metals form the strongest anion-π interactions – a DFT study

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Anion-π interactions are an important class of noncovalent interactions which are achieved by introducing heteroatoms and/or electron-withdrawing groups into aromatic systems [1]. Another way this can be achieved is by transition metal coordination within organometallic half-sandwich compounds which results in strong anion-π interactions.[2] In this work, we have studied the effect of metals from different transition rows on the strength of anion-π interactions of their half-sandwich compounds.

DFT calculations were performed on anion-π complexes containing halide anions and M(arene)(CN)$(CO)_2$ half-sandwich compounds, where M = Fe, Ru, Os, and arene = Cp, Cp* and Ind (Fig. 1). The energies of anion-π interactions in these systems were calculated using the B3LYP method with D3 empirical dispersion and def2-TZVP basis set.

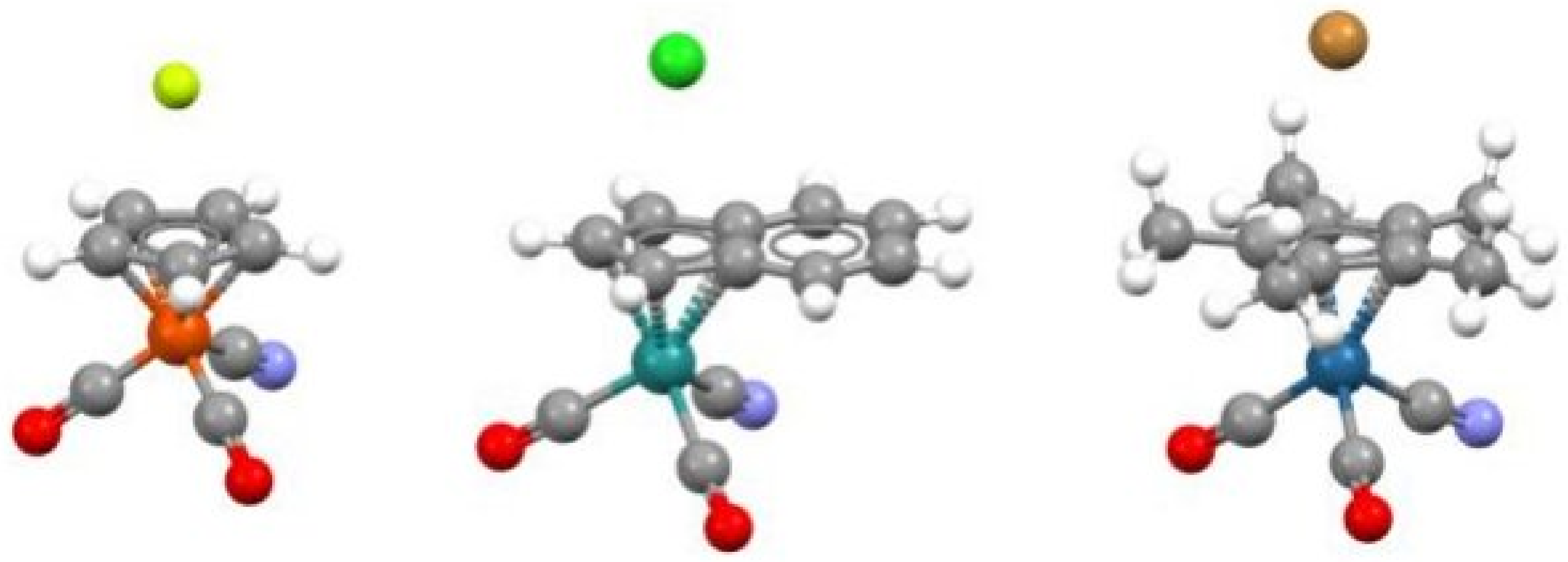

Figure 1. Anion-π interactions in the systems FeCp(CN)$(CO)_2$/fluoride, RuInd(CN)$(CO)_2$/chloride and OsCp(CN)$(CO)_2$/bromide*

Our calculations indicate that for all halides and aromatic ligands anion-π interactions are stronger for half-sandwich compounds of heavier transition metals, decreasing in the following order: Os > Ru > Fe, the strongest being the interaction between OsCp*(CN)$(CO)_2$ and fluoride (-28.80 kcal/mol) (Fig. 1). It is shown that the anion-π interactions of chloride and bromide are stronger for all Ru and Os half-sandwich compounds than for all observed organic aromatic molecules.[1]

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PCC PP 18

Influence of the nature of ligands in square-planar complexes on the electrostatic potential of iodine

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Electrostatic potentials (ESP) on the hydrogen atoms were calculated using the optimized 2,2'-bipyridine molecule. The results showed that the potential on the hydrogen atom increases from position C1 to C4. This organic molecule, acting as a bidentate ligand, was coordinated with palladium and platinum ions, while their coordination spheres were completed with different pairs of ligands. The electrostatic potentials were also calculated for coordinated 2,2'-bipyridine molecule and obtained values of potentials on the hydrogen atoms ($Vs_{,H}$) were more positive on molecules.

To observe change in ESP on halogen atoms attached to both free and coordinated 2,2'-bipyridine, the hydrogen atom was substituted with a polarizable iodine atom at positions C2 and C3. The results showed that the $Vs_{,I}$ values were generally higher (up to 10 kcal/mol) compared to the corresponding $Vs_{,H}$ values on hydrogens in the same positions. Considering coordinated molecules, the Vs values vary in complexes depending on the various other ligands used to complete the coordination sphere in the metal complex.

The interaction energies between the iodine atom substituted in 2,2'-bipyridine and an ammonia molecule were calculated. The obtained interaction energy values range from -5.3 kcal/mol to -6.8 kcal/mol, indicating that these interactions are quite strong, comparable with hydrogen bond between two water molecules.

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Phytochemistry and Food Chemistry (PFC)

PFC PP 01

Fatty acid profile of different avocado varieties

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The avocado (*Persea americana Mill.*) is a rich source of monounsaturated fatty acids (MUFA), particularly oleic acid, which accounts for approximately 60-70% of its lipid content. The unique fatty acid profile of avocados contributes to their nutritional benefits, including improved cardiovascular health, anti-inflammatory properties, and the ability to lower cholesterol levels [1]. In addition to oleic acid, avocados also contain other essential fatty acids such as linoleic acid (omega-6) and α-linolenic acid (omega-3), which play crucial roles in metabolic processes and cellular function [2]. Moreover, the balanced ratio of these fatty acids in avocados supports overall health by enhancing the absorption of fat-soluble vitamins and promoting optimal brain function [2].

In this study, gas chromatography was employed to analyze the fatty acid composition in pulp samples of three different avocado varieties. Results obtained showed that avocado pulp of Arad variety contains mainly palmitic acid (51.0%), followed by heneicosanoic acid (25.7%), elaidic acid (10.2%) and linoleic acid (9.2%). Avocado pulp of Pinkerton variety contained the highest percentage of palmitic acid (35.5%), followed by oleic acid (15.1%), linoleic acid (13.3%) and heneicosanonic acid (10.6%). It also contains some fatty acids in smaller quantities such as elaidic acid (6.3%) and palmitoleic acid (4.7%). The third sample was avocado pulp of the Hass variety and the results have shown that it contains large percentages of palmitic acid (26.8%), heneicosanoic acid (18.1%) and oleic acid (17.5%), but also significant amounts of elaidic acid (9.8%), linoleic acid (9.0%) and behenic acid (8.8%). These findings are consistent with previous literature and emphasize the high nutritional value of avocado fats, highlighting avocado's role as a significant source of health-promoting fats.

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PFC PP 02

Phytochemical profile and antioxidant activity of *Galium verum* L. monocomponent tea

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Galium verum L., known as lady's bedstraw, is a perennial herb native to Europe, Asia, and North Africa, recognized for its aromatic yellow flowers and long history of use in traditional medicine, particularly in Serbia. This herbaceous plant has been utilized in various forms, including decoctions, and teas for internal use, as well as topically as poultices, creams, and bath additives to address ailments such as skin conditions, digestive issues, and urinary tract problems. For the purposes of this research, the *Gali veri herba* monocomponent tea, sourced from the wild flora of the Rtanj mountain region, was obtained from the company *Adonis d.o.o*. The extraction was conducted using hot water to simulate domestic procedure and determine the phytochemical profile and antioxidant activity in tea prepared according to the provided instructions. The determination of total phenolic content (TPC), total flavonoid content (TFC), the total tannin content as well as the content of total hydroxycinnamic derivatives (HCAs) was conducted spectrophotometrically. In the same manner, the antioxidant properties were assessed using four assays: ABTS•+, DPPH•, ferric reducing power (FRP), *in vitro* phosphomolybdenum total antioxidant capacity (TAC), and cupric reducing antioxidant capacity (CUPRAC) The results were expressed on a dry weight (DW) basis. The TPC content was 27.01 mg/g GAE, whereas the TFC results indicated a value of 147.95 mg/g RE, and for HCAs 2.71 mg/g CGAE. Additionally, the total tannin content was measured at 14.81 mg/g TAE. Furthermore, the quencher assays, ABTS•+ and DPPH•, demonstrated antioxidant capacities of 27.78 and 71.17 µmol Trolox/g, respectively. Notably, the TAC assay revealed a value of 56.54 mg/g AAE, highlighting the extract's overall antioxidant potential. The FRP evaluation further demonstrated the sample's reducing ability, measuring 22.53 mg/g AAE. Similarly, the CUPRAC evaluation confirmed the antioxidant activity, yielding 53.92 mg/g AAE. These findings offer valuable insights into the potential health benefits and efficacy of lady's bedstraw tea as a natural remedy.

Acknowledgments
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PFC PP 03

Lavender: nutrients, chemical composition and bioactivity

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Lavandula, a genus within the Lamiaceae family, comprises 47 flowering plant species, with a widespread distribution from Southern Europe to India. This botanical diversity finds culinary utility as lavender flower extracts and oils enhance a variety of food products, from confectionaries and desserts to teas and sauces, enriching them with a distinct floral essence. This study aimed to compile literature data on the nutrients, chemical composition, and bioactivity of Lavandula species essential for comprehending their potential health benefits and guiding dietary and medicinal uses. Within the genus, significant variations in nutrient compositions were observed. Proteins, carbohydrates, and water are the most abundant components, ranging from 6.34% to 23.43%, 40.53% to 71.05%, and 59.99% to 64.91%, respectively. Additionally, the content of essential elements such as calcium (106.22 - 327.05 mg/kg) and potassium (103.03 - 164.02 mg/kg) is notable, highlighting their importance in the *Lavandula* species nutritional profile. Moreover, the content of iron, spanning from 119.50 mg/kg to 833.13 mg/kg, further contributes to the nutritional potential of the plant. The chemical composition of lavender essential oils reveals a plethora of unique and abundant compounds. From prevalent elements including linalool and linalyl acetate, which contribute to the pleasant aroma and therapeutic significance, to species-specific constituents like trans-carveol in *Lavandula bipinnata* (Roth) Kuntze. and carvacrol in *Lavandula canariensis* (L.) Mill. Furthermore, variations in terpene composition, the prevalence of β-bisabolene in *Lavandula multifida* L. and the exclusive presence of viridiflorol in *Lavandula stoechas* L., underscore the diverse and versatile nature of essential oils. The chemical composition of *Lavandula angustifolia* Mill includes phenolic and flavonoid compounds, phenolic acids (caffeic acid, ferulic acid, rosmarinic acid). These compounds exhibit an array of bioactivities, including antioxidant, anti-inflammatory, antimicrobial, neuroprotective, and cytotoxic properties suggesting its potential for enhancing both the flavor and health benefits of food.

Acknowledgments

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PFC PP 04

Photosynthetic pigments, carotenoids, phenolics and antioxidant properties of five microgreen species

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Microgreens are the shoots of vegetables, pulses and herbs picked just after the first leaves have developed. Due to increasing interest and demands of consumers for healthy food products ('super foods') with various benefits, more focus is put to growing microgreens. These miniature greens are good source of nutrients as well as biactive compounds and antioxidants, hence primarily used in culinary and in vegan nutrient-enriched dietary food [1]. In this work five microgreen species (Broccoli – *Brassica oleracea* var. *italica*; Daikon radish *Raphanus sativus* var. *longipinnatus*; Black mustard- *Brassica nigra*; Pea - *Pisum sativum*; Garden rocket - *Eruca sativa* Mill.) were grown in controled enivironment: in soil (S) and in high-purity cellulose (C) substrate systems. Fresh microgreens (FM) were analysed for selected chemical parameters: content of chlorophyls *a* and *b* (Chl *a*, *b*), content of caroteinoids (β-carotene and lycopen), content of phenolics (TPC), content of flavonoids (TFC) and antioxidant activity measured through Total Antioxidant Capacity (TAC) and Cuprric Reducing Antioxidant Capacity (CUPRAC) assays. Pea grown in both systems had the highest content of photosynthetic pigments Chl *a* and *b* (S-505.31±5.69 and C-500.23±1.37 µg/g of FM), TPC (S-2.08±0.01 and C-1.37±0.01 mg/g of galic acid equivalents (GAE) of FM), and antioxidant activity (expressed as mg/g ascorbic acid equuivalents (AAE) in FM) in both assays: TAC - 1.94±0.05 (S) and 2.21±0.09 (C) and CUPRAC - 8.46±0.62 (S) and 5.27±0.33 (C). Black mustard grown in high-purity cellulose substrate was richest in TFC (2.40±0.21 mg/g of rutin equivalents (RE) of FM), whereas contents of β-carotene and lycopen were highest in radish grown in soil (79.89±10.63 µg/g of FM) and pea grown in high-purity cellulose substrate (311.55±1.01 µg/g of FM), respectively. Results indicated differences in the content of the studied parameters in microgreens grown in different systems.

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PFC PP 05

Can the medicinal plant *Symphytum officinale L.* be a rich source of macroelements?

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Symphytum officinale L from the mountain Golija, Republic of Serbia, chemically untreated, was selected for investigation. Concentrations of five macroelements (Ca, Mg, K, Na, P), were determined by ICP-OES method, after samples mineralization. Macroelement concentrations were determined in all parts of the plant separately (leaf, flower, stem, root).

Figure 1. Symphytum officinale L.

Research has shown that the leaf part of comfrey is the richest in Ca and K, while the flower was richest in Mg and P. The root is almost the richest in K and Na content, while it is the poorest in Ca, Mg and P concentrations. The concentrations of macroelements in the comfrey stem were higher than in the root. Compared to the stem, the root contains only more phosphorus.

According to the available literature data, there has been no similar research on Golija so far, which gives the topic importance, and the obtained experimental data will contribute to the scientific database.

Acknowledgements

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PFC PP 06

Teas for weight loss-truth or myth? Teas as lipase inhibitors *in vitro*

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Obesity is one of the most serious health issues, affecting millions worldwide and the number of individuals with excessive body weight is rising rapidly. Contributing factors include genetics, physical inactivity and improper diet. Healthcare workers emphasize dietary changes as key components of prevention. Certain food compounds, such as polyphenols, plant-derived secondary biomolecules, are known to help prevent and reduce overweight.

The aim of this study was to analyze the ability of 12 teas, sold as weight loss or detox teas, to inhibit lipase, an enzyme necessary for lipids digestion. Lipase inhibitors reduce the gastrointestinal absorption of fat, and in this study, it was examined if this is one of the possible mechanisms of action of the mentioned teas. The potential of the teas to inhibit lipase was evaluated using a spectrophotometric assay that measures the absorbance of *p*-nitrophenol released from the hydrolysis of 4-nitrophenyl palmitate by lipase. Orlistat, a standard lipase inhibitor, was used as a positive control. Additionally, the content of total phenols, tannins, and flavonoids in teas was determined using spectrophotometric methods [1].

The examined teas contain varying amounts of the investigated polyphenols. Among 12 analysed teas, only four exhibited lipase inhibition. A weak correlation between the inhibitory activity and the flavonoid content was observed.

The results indicate the potential of various teas to inhibit the lipase. These findings may serve as a valuable basis for further research into mechanisms of action through which these teas may contribute to obesity prevention and reduction.

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PFC PP 07

Antiradical activity of Prunus spinosa fruit extract determined by EPR spectroscopy

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Prunus spinosa, commonly known as blackthorn, is a fruit-bearing shrub widely recognized for its rich content of bioactive compounds, including phenolics and flavonoids. These compounds are known for their potential antioxidant properties, which may contribute to the neutralization of harmful free radicals, reducing oxidative stress and associated pathologies. In this study, an aqueous extract of *Prunus spinosa* fruits was prepared, and its antiradical activity was evaluated using electron paramagnetic resonance (EPR) spectroscopy. Two radical scavenging assays were performed: hydroxyl radical (•OH) and 2,2-diphenyl-1-picrylhydrazyl (DPPH) free radical scavenging.

The results indicate that the *Prunus spinosa* extract exhibited significant activity against hydroxyl radicals, with an inhibition percentage of 88.51%, demonstrating its high potential as a hydroxyl radical scavenger. Its activity against DPPH radicals was found to be moderate, with an inhibition of 31.35%. These findings suggest that the extract has a selective and potent capacity to neutralize highly reactive hydroxyl radicals and highlight the potential of the extract for incorporation into functional foods or therapeutic agents to alleviate conditions associated with oxidative stress.

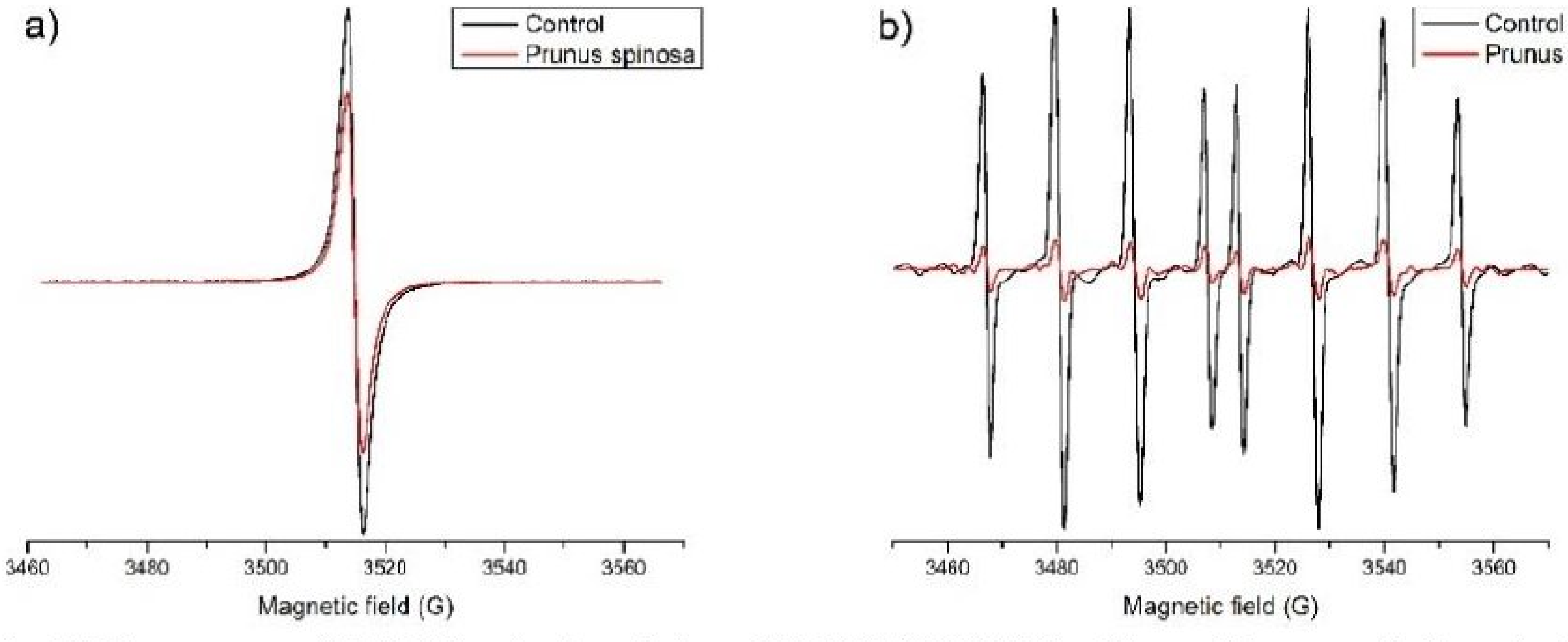

Figure 1. EPR spectra of DPPH solution (a) and DEPMPO/OH adduct (b) recorded at the beginning (black) and 2 minutes after addition of aqueous extract of Prunus spinosa (red)

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PFC PP 08

Radical scavenging potential of medicinal plants used in wart treatment: An EPR study

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Plants traditionally used for their antiviral properties, especially in wart treatment, are gaining attention for their bioactive compounds. This study focuses on sap of three such plants: *Ficus carica*, *Chelidonium majus*, and *Euphorbia cyparissias*. The aim of this research was to evaluate their ability to scavenge free radicals, specifically hydroxyl radicals, superoxide radical anions, and DPPH (2,2-diphenyl-1-picrylhydrazyl), using electron paramagnetic resonance (EPR) spectroscopy [1].

Results (Figure 1) revealed that *Ficus carica* exhibited potent antioxidant activity, removing 98.84% of superoxide radical anions, 96.80% of hydroxyl radicals, and 77.86% of DPPH. *Chelidonium majus* showed the highest efficacy against superoxide radical anions, with scavenging capacity of 99.74%, while it removed 33.03% of hydroxyl radicals and 24.49% of DPPH. *Euphorbia cyparissias* demonstrated strong activity against hydroxyl radicals, removing 97.71%, while it removed 57.58% of superoxide radical anions and 91.77% of DPPH.

These findings suggest that *Ficus carica*, *Chelidonium majus*, and *Euphorbia cyparissias* possess significant radical scavenging properties. The marked differences in their activity towards specific radicals highlight the importance of further investigation into their mechanisms of action, which could contribute to the development of natural antiviral therapies.

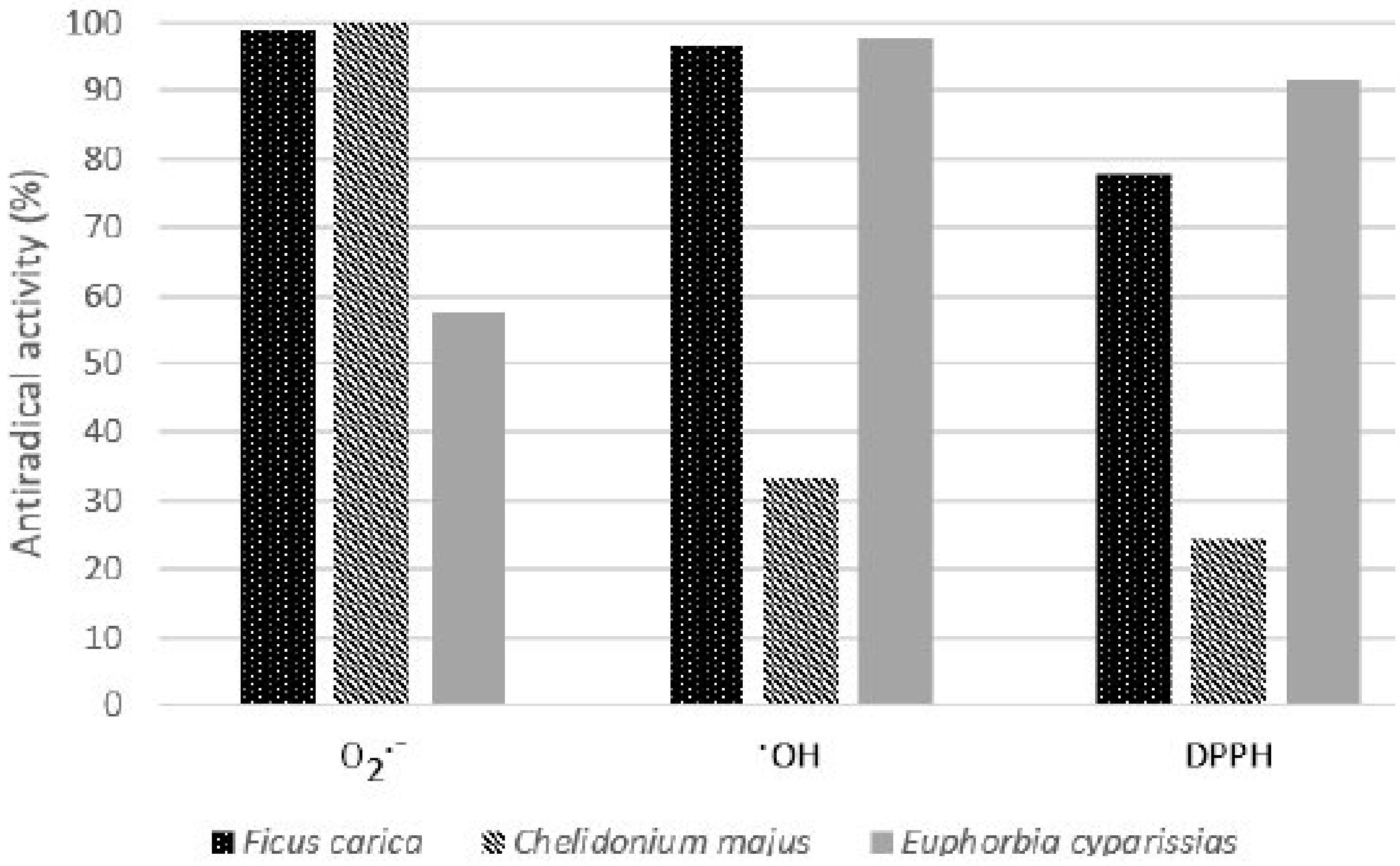

Figure 1. Antiradical activities of selected plant saps

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PFC PP 09

Amino acid composition in selected sorghum genotypes (*Sorghum bicolor* L. Moench)

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Sorghum (*Sorghum bicolor* L. Moench), belonging to the *Poaceae* family, is considered to be a functional food ingredient due to the presence and high content of various bioactive components [1]. Researching and using novel raw materials with bioactive qualities has become imperative due to the widespread trend of developing functional products. Sorghum offers the food industry a wide range of possibilities to satisfy global consumer trends, which are increasingly looking for high-quality products and alternatives to traditional gluten products. Amino acid analyses of 16 food-grade genotypes was performed by ion-exchange chromatography using an automatic amino acid analyzer (Biochrom, Cambridge, UK) following the method described by Spackman et al. [2].

According to the obtained results, samples **S11** and **S16** had the highest overall amino acid content (13.74 and 13.06, respectively, presented in g 100 g^{-1} of the sample). In contrast, samples **S2** (9.64 g 100 g^{-1}), and **S8** (9.66 g 100 g^{-1}) had the lowest quantified amino acid. Sample **S14** had a characteristic amino acid profile with elevated amounts of glutamic acid, proline, methionine, isoleucine, leucine, and phenylalanine but lowered amounts of glycine, lysine, and arginine compared to other samples. Although the amino acid composition of food-grade genotypes can differ based on factors such as cultivar, fertilization, maturation, or climate conditions, understanding this variation is crucial for further processing and customer approval.

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PFC PP 10

Characterization of natural deep eutectic solvents extracts of raspberry with ^{1}H NMR multisuppression experiment

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Red raspberries are attracting more and more attention for their nutritional and bioactive components such as vitamins, minerals, proteins, sugars and polyphenolic compounds. Daily consumption of raspberries reduces the risk of many chronic diseases, such as neurodegenerative conditions, various types of cancer, type 2 diabetes, cardiovascular disease, obesity and hypertension. In recent years, more environmentally friendly techniques have been developed that use eco-friendly (green) solvents, such as natural deep eutectic solvents (NADES) [1]. Nevertheless, solid-phase extraction of plant mixture NADES extracts is an indispensable step in the LCMS analysis [2]. The aim of this study was to investigate the possibility of using ^{1}H NMR for NADES signal suppression and characterise obtained extrats in a single run without additional purification steps. The intense NADES signals in the spectrum, the viscosity and the ionic strength of the obtained extracts were challenges that had to be overcome. The multi-suppression experiment was optimise for use with polar NADES, which contained choline chloride and urea (molar ratio = 1:2) with the addition of deuterium oxide (D_2O). In addition to the successful suppression in the ^{1}H NMR spectrum, 2D ^{1}H-^{1}H *J*-resolved spectra were obtained.

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PFC PP 11

Can ”weight loss” teas inhibit α-amylase?

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Teas designed for weight loss have become increasingly popular as a natural method for losing weight, often advertised as an easy way to enhance metabolism, burn fat, and detoxify the body. The main ingredients of these teas are plants rich in polyphenols. Polyphenols have numerous biological activities, including hypoglycemic, manifest through inhibition of α-amylase and α-glucosidase. The aim of this study was to examine whether these teas have the potential for inhibition of amylase, a carbohydrate-digesting enzyme. Inhibition of this enzyme leads to the excretion of carbohydrates out of the body, before they can be digested, and in that way reduces energy intake [1].

In this research were included 12 different teas, commercially available on the market in Novi Sad and sold as teas for losing weight. Teas were prepared according to the manufacturer's instructions. The teas' ability to inhibit the activity of amylase was determined *in vitro*, by the previously described Caraway iodine/potassium–iodide method, using acarbose as a positive control. The study also assessed total polyphenols, tannins and flavonoids content in teas using spectrophotometric methods [2].

Significant variation was observed in the total polyphenolics, tannins and flavonoids content among the samples. Of the 12 analysed samples, 6 expressed the potential to inhibit the amylase. A weak correlation was observed between enzyme inhibition and total tannin and polyphenolic content. To the best of our knowledge, this is the first research about hypoglycemic potential of weight loss teas in Serbia. Obtained results reveal considerable differences among samples and indicate a need for further research about the health properties and biological activity of these samples.

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PFC PP 12

Application of 2D EPR imaging in studying the redox and oxymetric properties of lettuce and chia seedlings

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Lettuce and chia are known for their antioxidant properties[1], which help neutralize free radicals and reduce oxidative stress. This study investigates the spatial redox status of lettuce and chia seedlings to clarify the biochemical and physiological processes related to plant health and stress response [1].

Seedlings (~8 mm) were incubated in an aqueous solution of trityl radical spin probe, followed by analysis using electron paramagnetic resonance spectroscopy (EPRS) and imaging (EPRI). These techniques revealed the spatial-temporal distribution of redox-active components, such as reactive oxygen species (ROS). However, variations in the EPR signal, caused by antioxidant reduction and reoxidation by ROS, complicated 2D EPR imaging interpretation. To address this, we combined 2D EPR imaging with oximetry, which provided precise spatial resolution of the redox state and oxygen profile in plant tissues. Results indicated a higher ROS concentration in the seedlings' central part, reflecting spin probe reoxidation due to the presence of ROS. Oxygen concentration did not exceed 21%, but the broadening of the signal, similar to elevated oxygen levels, was linked to ROS, such as hydroxyl and peroxyl radicals. Antioxidant-rich regions at the seedling ends neutralized ROS, resulting in signal loss.

These findings underscore the balance between reactive species and antioxidants in plant health and highlight the potential of combined EPR methods for understanding oxygen dynamics during seed germination.

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PFC PP 13

Antioxidant and antidiabetic potential of grape pomace extracts

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Grape pomace, a byproduct of winemaking, is a significant source of bioactive compounds. The extraction of bioactive compounds from grape pomace is quite an interesting field, not only for researchers but also for the pharmaceutical, food, and cosmetic industries [1]. The main objective of this study was to obtain green extracts of grape pomace with the highest antioxidant and antidiabetic activity. Freeze-dried pomace from the indigenous Merlot grape variety from the Fruška Gora region was used. Extraction was performed using natural deep eutectic solvents (NADES): choline chloride-glycerol (1:1), choline chloride-1,2-propanediol (1:1), choline chloride-citric acid (1:1) and choline chloride-ascorbic acid (2:1), along with two conventional solvents: 50% ethanol and 50% ethanol acidified with 1% hydrochloric acid. To determine the antioxidant activity of extracts, DPPH (2,2-diphenyl-1-picrylhydrazyl) radical scavenging activity was measured. Additionally, the phenolic content was estimated using Folin-Ciocalteu assay, and the total anthocyanin content was investigated using the pH differential method. The antidiabetic potential of the extracts was determined by measuring their *in vitro* α-glucosidase inhibitory activity. The highest concentration of total anthocyanins was extracted using the combination of choline chloride and 1,2-propanediol. The extract derived from the NADES composed of choline chloride and ascorbic acid exhibited the highest antioxidant activity, the highest phenolic content, and the highest *in vitro* inhibitory effect on α-glucosidase activity compared to other extracts. All extracts showed good anti-diabetic potential, presenting a novel approach to the treatment of diabetes.

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PFC PP 14

Hydroxyl radical scavenging activity of *Dictamnus albus* and *Asplenium ceterach* assessed by EPR spectroscopy

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Oxidative stress plays a crucial role in the development of various diseases, and natural antioxidants are gaining attention for their potential therapeutic applications. In this study, we investigated the hydroxyl radical ($^{\bullet}$OH) scavenging activities of *Dictamnus albus* and *Asplenium ceterach*, two plants known for their traditional medicinal use and adaptation to harsh, dry environments. Hydroxyl radicals were generated via the Fenton reaction, and their scavenging by plant extracts was assessed using electron paramagnetic resonance (EPR) spectroscopy. The spin trap technique with DEPMPO as spin trap allowed for accurate detection of hydroxyl radicals and the quantification of their reduction by the plant extracts.

The EPR analysis revealed that *Dictamnus albus* was more effective in eliminating hydroxyl radicals, with a scavenging activity of 60.49%. *Asplenium ceterach* demonstrated moderate activity, eliminating 43.71% of the radicals. These findings suggest that *Dictamnus albus* and *Asplenium ceterach* possess significant antioxidant potential, which may contribute to their traditional medicinal use. Future work will focus on isolating and characterizing the active compounds responsible for these effects, as well as evaluating their efficacy in biological systems.

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PFC PP 15

Unveiling household food waste: Survey results from the housholds from Vojvodina region, Serbia

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The prevention and proper management of household food waste is a collective challenge. Food waste is a multifaceted and complex problem that raises social and ethical concerns, but also deeply affects the environment. In this sense, addressing the problem is a priority that requires actions that target our entire food system. Around 88 million tonnes of food waste is generated in the EU every year and the associated costs are estimated at €143 billion. While an estimated 20% of all food produced is lost or wasted, 33 million people cannot afford to eat quality food every other day (according to Eurostat, 2018). FAO reported, that 1.3 billion food wastes are generated worldwide in a year. The purpose of this study was to examine the attitudes and behavior of families in Vojvodina region in Serbia regarding food waste and to estimate the monthly amount and economic value of discarded food waste in households, using a self-filling method. The questionnaire consisted of 19 questions, which were filled in by a total of 193 people. The average age of the applicants were between 18 and 40 years old. According to the results 80,9% of the respondents are concerned about food waste trying to avoid it if possible. 64,8% of respondents are from the countryside, and 35.6% of those are involved in composting. The weekly amount of food waste in households was reported between 250 g-1kg.

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PFC PP 16

Eating habits of students from Vojvodina

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Adolescence is a period of growing independence and self-determination in all areas of life, including nutrition. Changes in eating habits in this period of life are mostly aimed at worsening nutrition, so this period is considered a period of high nutritional risk. Adolescents' typical diet is characterized by excessive consumption of sweets, fatty, salty snacks and sugar-sweetened beverages, as well as inadequate fruit and vegetable consumption [1]. As a result of the imbalance between the aforementioned high-calorie diet and energy consumption, the prevalence of overweight and obesity among adolescents is a global problem today. The aim of the research is to examine the level of knowledge about nutrition and nutrients among adolescents of Generation Z (Zoomers), as well as the possible relationship between eating habits and the development of obesity or malnutrition. I collected data on the frequency of meal consumption, choice of snacks and knowledge of the amount of basic nutrients with the help of a questionnaire. The number of completed surveys is 112, by teenagers in Vojvodina (Serbia), aged 16 to 19. I analyzed the relevant data and finally compared the results obtained in secondary schools, depending on gender and in relation to body mass index, and if the majority of the interviewed adolescents were of normal weight, 77.7%, and 8% overweight, while 13.4% of students belonged to the moderate category.

Summing up the results, dietary habits did not show a significant correlation with BMI index numbers, which can also be explained by the fact that the vast majority of those who completed the questionnaire were in the normal category. Based on the results regarding nutritional knowledge and knowledge of nutrients, I concluded that the students studying in all four secondary schools still need to improve in the field of knowledge of nutrients and nutritional habits.

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PFC PP 17

Synthesis of small libraries of natural products: Identification of the new esters from the essential oil of *Pelargonium asperum* (Geraniaceae)

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The plant species belonging to the genus *Pelargonium* produce essential oils rich in natural products that are highly valued in the perfume industry.[1] As esters are an important group of aroma-active volatiles, the composition of the ester fraction of a commercially available sample of *Pelargonium asperum* essential oil was studied in detail. Chromatographic separation of *P. asperum* essential oil led to the discovery of numerous esters with potential olfactory interest, some of which were undetectable through direct GC-MS analysis of the unfractionated essential oil. A GC-MS analysis of the mentioned fraction revealed, among more than 240 identified constituents, the presence of four compounds that were tentatively identified, based on their mass spectral fragmentation, as isomeric heptyl formate, (iso)pentyl and (iso)hexyl (isohexanoate), and (*Z*)-hex-3-en-1-yl ester of one of the isomeric hexanoic acids. Since the mass fragmentation patterns in the MS spectra for the isomeric esters are very similar, along with the corresponding RI data, we decided to prepare a small combinatorial library of all possible isomeric esters, totaling 75 compounds (including 39 completely new ones). All synthesized esters were spectrally characterized by NMR, IR, and/or MS techniques. GC-MS co-injection of the essential oil sample with synthesized standards confirmed that the analyzed fraction contains 5-methylhexyl formate, 3-methylbutyl 3-methylpentanoate, 4-methylpentyl 3-methylpentanoate, and (*Z*)-hex-3-en-1-yl 3-methylpentanoate. The four identified esters represent new natural products, while 3-methylbutyl 3-methylpentanoate has a rather restricted occurrence in the Plant Kingdom.

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PFC PP 18

Mineral profile of persimmon (*Diospyros kaki* L.) fruit

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Persimmon (*Diospyros kaki* L.) is a plant native to Chine that belongs to the *Ebenaceae* family. The persimmon fruit is an important and peculiar functional food due to its high nutritional value and commercial importance. Many studies have shown that persimmon fruit is a good source of many bioactive compounds, including polyphenols, terpenols, caratenoids, minerals and dietary fiber [1,2]. Some of these compounds have beneficial effect on human health, as they can prevent or control various diseases [2]. Additionally, persimmons are noted for their antioxidant properties, which can help combat oxidative stress and inflammation. This makes them a valuable addition to a balanced diet aimed at promoting overall well-being. This study aims to determine the mineral profile of persimmon fruit based on twenty-two elements using the optical emission spectrometry with inductively coupled plasma (ICP-OES) technique. The analysed elements were: aluminium (Al), arsenic (As), boron (B), barium (Ba), calcium (Ca), cadmium (Cd), cobalt (Co), chromium (Cr), copper (Cu), iron (Fe), potassium (K), lithium (Li), magnesium (Mg), manganese (Mn), sodium (Na), nickel (Ni), phosphorus (P), lead (Pb), sulphur (S), selenium (Se), strontium (Sr), and zinc (Zn). The results show that the concentrations of major elements in analysed sample are as follows: 1469.09 (K), 58.03 (Mg), 52.06 (Ca), 1052.28 (P) and 103.24 (S) expressed as $\mu g\ g^{-1}$. The content of microelements was: 1.00 (Fe), 0.39 (Mn), 0.06 (Se), 0.12 (Sr) and 0.21 (Zn) $\mu g \cdot g^{-1}$, while the concentrations of some toxic elements such as As, Cd, Co, and Pb were below method quantification limits in the studied sample. In conclusion, the study shows that persimmon fruits have a significant concentration of essential macro- and microelements and a lower content of potentially toxic elements, indicating their safety and nutritional value.

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PFC PP 19

Impact of cultivation year on total phenolic content and radical scavenging activity in strawberry genotypes: a comparative analysis of parental and progeny lines

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Strawberries (*Fragaria x ananassa* Duch.) are renowned for their nutritional benefits, high contents of polyphenols, and strong antioxidant properties. In the numerous global strawberry breeding programs, key factors for selection and breeding include fruit quality, flavor, and aroma, which are crucial for commercial appeal. Additionally, the radical scavenging activity (RSA), which assesses the fruit's ability to neutralize radicals, is an indicator of its antioxidant compound levels and overall quality [1,2].

The results indicated a variation in radical scavenging activity across different cultivation years, with progeny lines demonstrating lower RSA. Additionally, the total phenolic content in strawberry extracts was greater in the first breeding year and was found to be higher in the parental line (Fig 1).

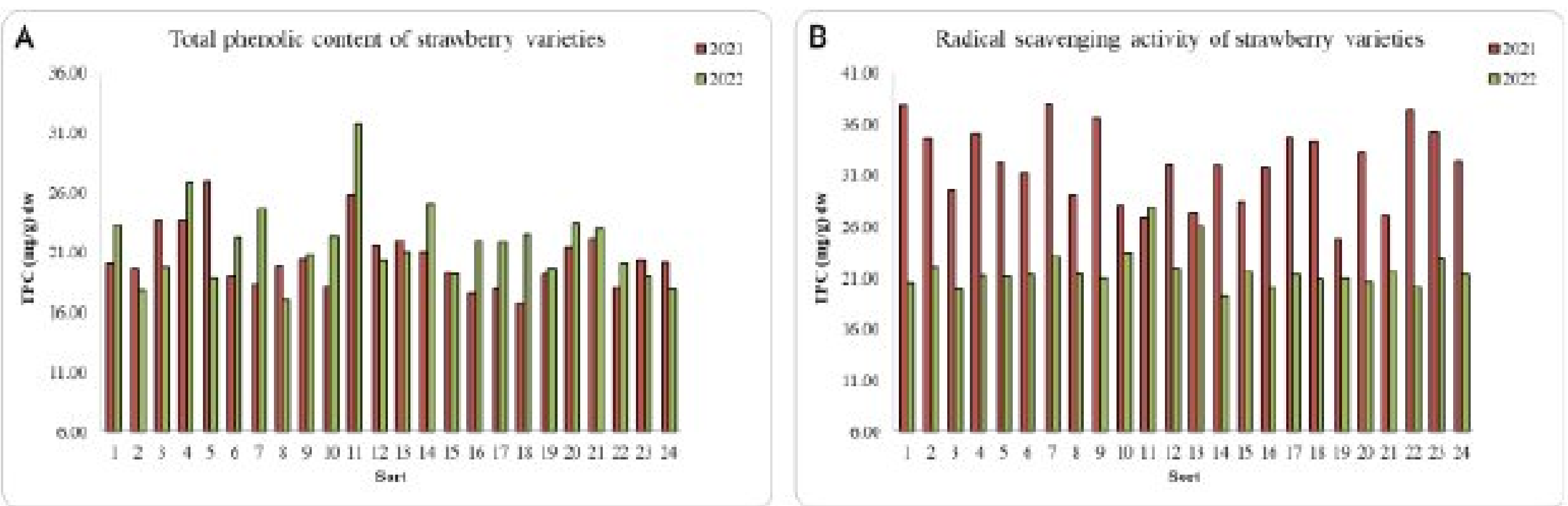

Figure 1. Total phenolic content (TPC) and radical scavenging activity (RSA) of selected strawberry varieties cultivated in 2021 and 2022.

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PFC PP 20

Influence of cultivation year on sugar profiles in strawberry genotypes

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Strawberry (*Fragaria x ananassa* Duch.) is highly valued for its distinctive aroma, vibrant red color, juicy texture, and sweetness. The main "sweet" metabolites in strawberry are glucose, fructose, and sucrose. Because the levels and quality of these sugars are closely tied to the fruit's genotype, breeding initiatives are focused on developing new cultivars that meet changing consumer demands for superior fruit quality. Although genetic factors significantly affect sugar levels, cultivation practices and pre-harvest conditions also play an important role [1,2].

In this study, sugar profile of 24 strawberry genotypes was investigated during two years of cultivation. The harvest from the second year exhibits a more diverse sugar profile, with higher levels of individual sugars. Additionally, the progeny line contains greater amounts of disaccharides and trisaccharides, resulting in a richer sugar profile (Fig 1).

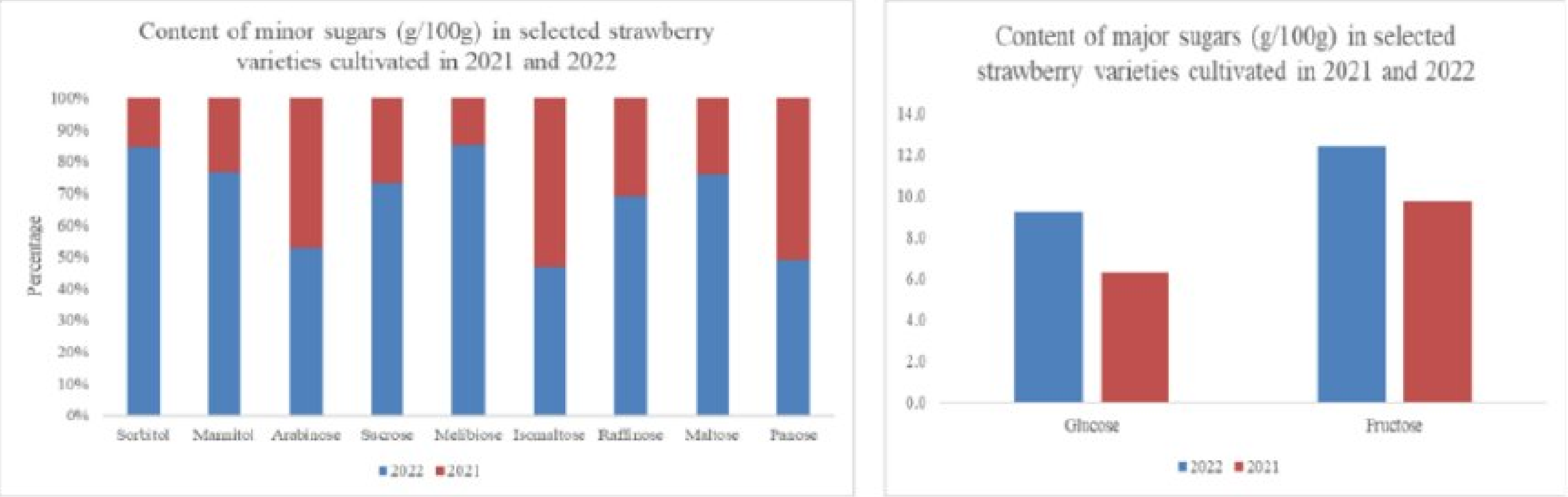

Figure 1. Content of selected sugars (g/100g) quantified in strawberry extracts from harvest of two years

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PFC PP 21

Assessment of physico-chemical parameters in strawberry genotypes: chemometric differentiation of parental and progeny lines

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Strawberry (*Fragaria* × *ananassa* Duch.) is among the most widely consumed berries globally, prized for their delightful taste. It is rich in micronutrients and phytochemical compounds, including anthocyanins, vitamin C, sugars, acids, and phenolic compounds (Fig 1). The concentrations of these phytochemicals significantly impact both the sensory and the nutritional value of the fruit. Sugars are the primary soluble components in ripe strawberry fruits, with glucose, fructose, and sucrose making up nearly 99% of the total sugar content [1,2].

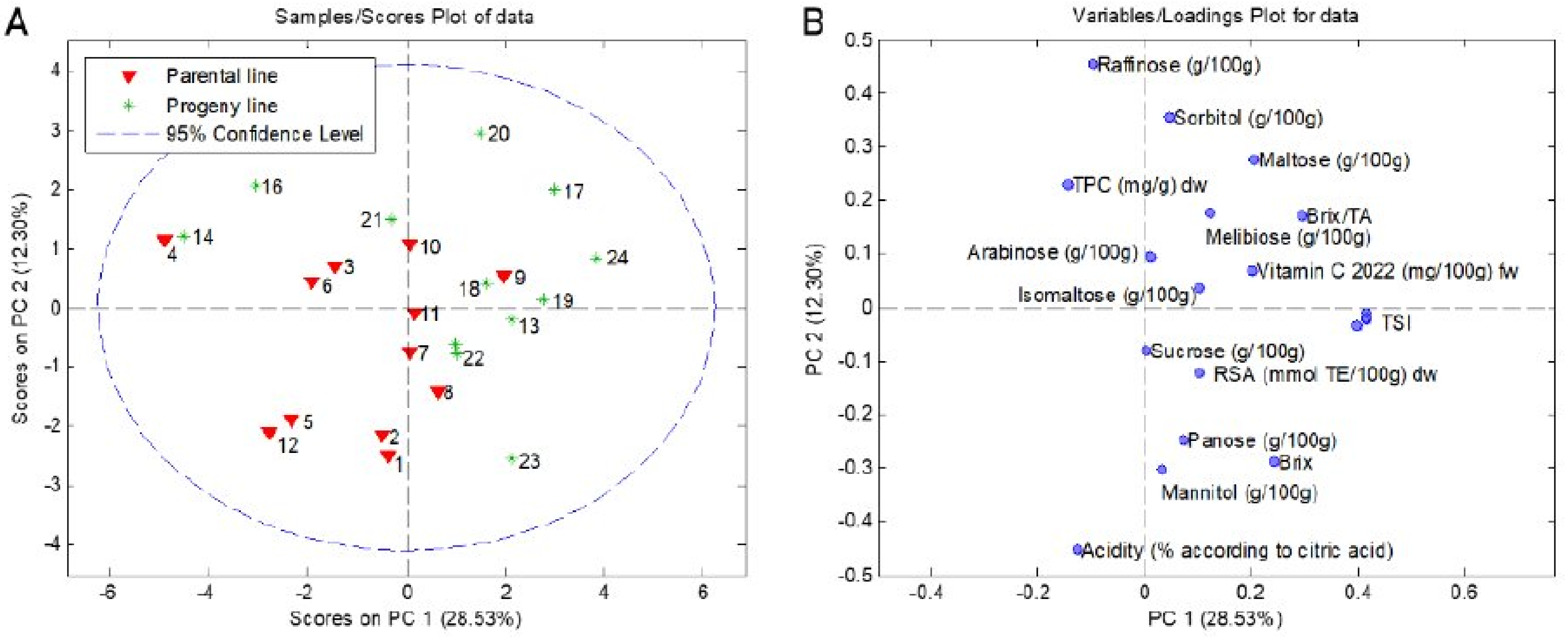

Figure 1. Principal component analysis - The difference between parental and progeny genotypes; score plot (A) – parental samples 1-12, descendant samples 13-24, and loading plot (B) – variables.

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PFC PP 22

Functional and biological properties of pumpkin leaf concentrates for potential application in the food industry

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Some estimates say that global demand for food is increasing at a rate faster than the rate of population growth. A possible solution to the problem of food sustainability could be found in the shift to diets based on plant proteins. It is widely recognized that these proteins have an important role in human nutrition and can potentially supplement/replace proteins from animal origin. In addition, functionality is the important factor of plant proteins that not only complements their established nutritional value but also improves their potential for applications in the food industry. Pumpkin leaves represent waste material after harvest and could be potential source of crude proteins with high nutritional value. Proteins from pumpkin leaves were recovered and separated to produce the green and the white protein concentrates. Functional properties (solubility, water and oil holding capacities) as well as surface hydrophobicity of pumpkin leaf concentrates were evaluated. Additionally, antioxidant activity, as biological property, was determined. The results indicated that the solubility of the green concentrate was three times lower compared to the white one. Green and white protein concentrates isolated from pumpkin leaves, with their advanced functional and biological properties, could be excellent sources for applications in the food sector.

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PFC PP 23

Phenolic profile and hypoglycemic potential of petal extracts of new garden rose genotypes grown in Vojvodina (Serbia)

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Often regarded as the "queen of flowers", roses are one of the most important horticultural plants. Not just used for decoration and production of essential oil, they also have a long tradition of use as food. They are used for making delicious salads, desserts, and beverages. Rose petals are a rich source of vitamins, minerals, and phenolic compounds with diverse beneficial activities on human health [1].

In this study, flowers of 10 new genotypes of *Rosa* × *hybrida* were harvested in June 2023 from the experimental fields of Pheno Geno Roses company near Temerin, Vojvodina. Petals were macerated with 80% MeOH and extracts were chemically characterized by determining total phenolic (TPC), flavonoid (TFC) and monomeric anthocyanin contents (TAC) as well as LC-MS/MS quantitative analysis. Hypoglycemic activity was evaluated by α-amylase and α-glucosidase inhibition assays [2].

The examined extracts are rich in phenolic compounds: TPC ranged from 87 to 179 mg gallic acid eq /g dw, TFC from 6.4 to 70 mg quercetin eq/g dw, and TAC from 0.4 to 12 mg cyanidin 3-*O*-Glc eq/g dw. LC-MS/MS analysis revealed that the dominant phenolics are quercetin and kaempferol glycosides. Extracts showed low inhibitory potential against α-amylase, while strongly inhibiting α-glucosidase.

These results demonstrate that new genotypes of garden roses are rich sources of polyphenols and have strong inhibitory activity against α-glucosidase making them interesting candidates for the development of novel functional food products for combating hyperglycemia, obesity and diabetes.

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PFC PP 24

Assessment of rosehips from new garden rose genotypes grown in Vojvodina as a potential functional food

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Roses, classified in the Rosaceae family and the genus *Rosa*, comprise more than 30,000 cultivars. These plants produce pseudo-fruits known as rosehips, which have a longstanding history of use in both traditional food and medicinal applications. Namely, they have been used for making tasty teas, jams, juices, marmalades and beverages. Additionally, they have been used for treating cold, flu, gastrointestinal and kidney diseases, and diabetes. Numerous studies have shown that rosehips possess antioxidant, anti-inflammatory, and neuroprotective properties [1].

In this study, we examined the rosehips of five new genotypes of Rosa hybrida cultivated in the Vojvodina region of Northern Serbia. The rosehips were macerated with 80% methanol, and the extracts were chemically characterized by measuring total phenolic content (TPC) and total flavonoid content (TFC). Additionally, we performed LC-MS/MS quantitative analysis of 45 selected compounds, while neuroprotective activity was assessed using acetylcholinesterase inhibition assays[1].

The examined extracts are rich in phenolic compounds, with TPC in the range from 35.8 to 61.2 mg GAE/g d.w., and TFC between 0.8 and 2.1 mg QE/g d.w. LC-MS/MS analysis identified catechin, quercetin, kaempferol, quercetin and kaempferol glycosides, gallic and *p*-coumaric acids as the dominant compounds. Furthermore, the extracts demonstrated moderate neuroprotective activity.

The results indicate that rosehips from garden roses exhibit significant quality, comparable to that of common rosehips from *Rosa canina* L. These findings highlight their potential as a functional food with properties that could aid in the prevention of neurodegenerative diseases.

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PFC PP 25

HPTLC fingerprint and bioautographic evaluation of antibacterial activity of *Galium verum* L. monocomponent tea

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In this study, the components of the methanolic extract of *Galium verum* L. monoherbal tea were separated using high-performance thin-layer chromatography (HPTLC). Silica gel was used as the stationary phase, and two mobile phases were applied for separation of extracted metabolites. The first mobile phase, consisting of ethyl acetate/toluene/formic acid/water (16/4/3/2, *v/v/v/v*), was suitable for polar compounds, while the second mobile phase, composed of toluene/ethyl acetate/methanol (55/40/5, *v/v/v*), was used for non-polar compounds. The zones were visualized by exposing the chromatographic plates to UV light at 254 nm and 366 nm, followed by derivatization with natural product/propylene glycol (NP/PEG) and *p*-anisaldehyde/sulfuric acid (ASA) reagent. The characteristic colors of the zones observed under UV light and following derivatization could indicate the presence of flavonols and phenolic acids in the polar mobile phase, whereas in the non-polar system, they indicate the presence of mono- and triterpenes.[1] Both chromatographic systems were subjected to direct bioautography to evaluate the antibacterial activity of the extract against *Staphylococcus aureus* ATCC 6538 and *Klebsiella pneumoniae* ATCC 29665. Bioautogram images were processed using ImageJ software, and the results were expressed as equivalents of streptomycin per milliliter of extract. The calibration curve for streptomycin was determined by plotting peak area against applied concentrations (µg/band). The results demonstrated stronger antibacterial activity of non-polar compounds compared to polar ones, with *S. aureus* showing higher sensitivity than *K. pneumoniae*. This approach provided valuable insights into the antibacterial potential of *G. verum* and highlighted the classes of compounds with the most promising activity.

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PFC PP 26

Deep eutectic solvent for eco-friendly extraction of phenolic compounds from endemic plant *Stachys iva* Griseb. – optimization by Box-Behnken design

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Stachys iva Griseb., an endemic plant from Macedonia, is recognized for its significant medicinal properties, including anti-inflammatory, antioxidant, antidiabetic, and analgesic effects. There is growing interest in medicinal plants, which has led to the development of novel green deep eutectic solvents (DES) as a tool for improving polyphenol recovery from various plant materials.

In this study, deep eutectic solvent (DES) combined with ultrasound-assisted extraction (UAE) was used to extract phenolic compounds from the aerial parts of the Macedonian endemic plant *Stachys iva* Griseb. The DES consisted of choline chloride and urea in a 1:1 molar ratio. Optimal extraction conditions were determined using a Box-Behnken design, with three factors at three levels: extraction time (10, 25, and 40 minutes), water content (20%, 30%, and 40% w/w), and solid-to-liquid ratio (0.1:5, 0.1:10, and 0.1:15 g/mL). For comparison, methanol was used under the same extraction conditions. As a response value, total phenolic content (TFC) was measured spectrophotometrically using the Folin-Ciocalteu reagent.

The obtained data were fitted to a quadratic polynomial model, and second-order regression models were developed, showing a good fit with the observed data. Extraction time was identified as the most significant factor. The influence of first-order linear effects on total phenolic content (TFC) decreased in the order of time > water content > solid-to-liquid ratio. The interaction between extraction time and solid-to-liquid ratio, as a second-order quadratic effect, also had a significant impact on TFC. The optimal extraction conditions were determined to be 40 minutes of extraction time, 20% water content, and a solid-to-liquid ratio of 0.1:5 g/mL. Validation showed that small variations between the experimental responses and predicted values confirmed the validity of the Box-Behnken design model's optimal conditions.

Acknowledgments

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PFC PP 27

Efficient detection of invertase adulteration in honey using ion chromatography

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Invertase (*β*–fructofuranosidase) is an enzyme naturally present in honey, however, this isoform of the enzyme catalyzes the hydrolysis of the glycosidic bond only in the sucrose molecule. The addition of a foreign invertase leads to the hydrolysis of glycosidic bonds of some other oligosaccharides such as raffinose [1]. This characteristics of the added invertase was utilized to optimize a method that monitors the consumption of raffinose and the formation of melibiose during the hydrolysis of the raffinose [1,2].

Specific amount of invertase and raffinose was added to honey samples, and a series of experiments were conducted in which various experimental conditions were varied. Optimal conditions for invertase activity were determined based on the amount of melibiose produced after incubation. The results showed that invertase exhibits the highest activity at a pH of 5.8 and when the honey solution is heated at 55 °C for 18 hours. The proposed method was then applied on adulterated and authentic honey samples; a significant difference in the amount of melibiose produced was observed (Fig. 1). In authentic honey, melibiose content did not exceed 0.040 g, whereas the melibiose content in adulterated honey reached up to 0.635 g (per 100 g of honey).

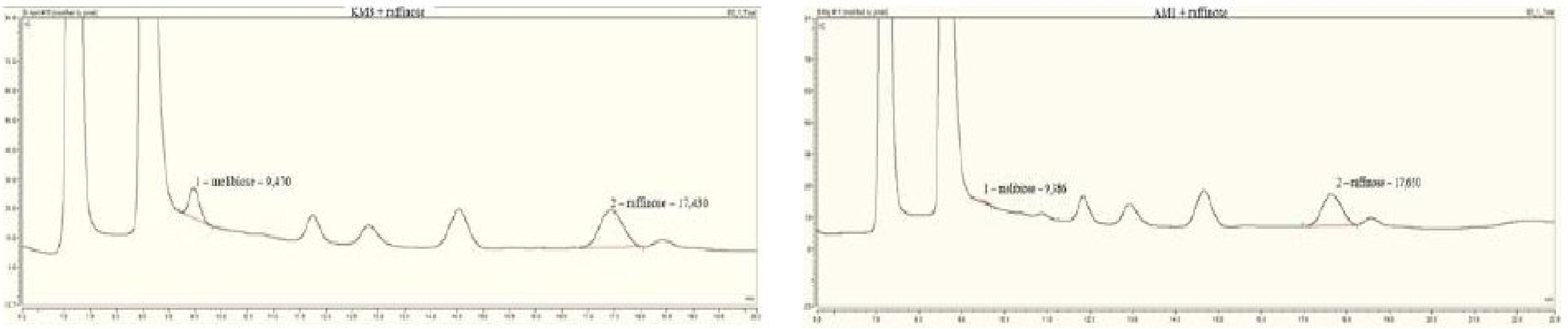

Figure 1. Chromatograms of adulterated and authentic honey samples after raffinose addition

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PFC PP 28

Application of a gas-diffusion flow injection system with activated platinum electrode for the bromate determination in real samples

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An amperometric sensor with a platinum electrode was applied to the bromate determination in real samples. The electrode was submitted to anodic activation by holding the electrode on a positive potential of +1.2 V for 100 s which increased the overall sensitivity [1]. A simple flow injection system with a gas-diffusion unit was optimised and used for deliveringall solutions to the flow-through amperometric cell [2]. The system is based on the reduction of bromate to bromine in acidic solutions, in the presence of bromide (Eq 1). A gas-diffusion cell was used to selectively transfer bromine through a porous membrane from the donor to the acceptor flow, which brings it to the amperometric cell where the reduction of bromine takes place. Under the optimal FIA conditions (+0.7 V *vs.* Ag/AgCl, 400 µl injection volume, 500 µl for reaction coil, flow rate 0.5 ml/min, 50 mmol/L KBr as reagent and 2 mol/L H_2SO_4 as carrier) linear response of the amperometric detector in the concentration range from 0 to 100 µmol/L was obtained. The corresponding equation was $I = -2.49\cdot10^{-8}\cdot c + 1.57\cdot10^{-7}$, and calculated limit of detection (3σ/s) was 2.8 µmol/L of bromate. The FIA system was successfully applied on determination of bromate in different commercially available water samples.

$$10Br^- + 5BrO_3^- + 6H^+ \rightarrow 3Br_2 + 3H_2O \qquad \text{(Eq 1)}$$

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PFC PP 29

Alkan-2-ones and alken-2-ones in *Laurus nobilis* L. essential oil

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Laurus nobilis L. is an aromatic plant that has been used for centuries due to its valuable properties. The essential oil of this plant is notable for its rich content of bioactive compounds, which exhibit antibacterial, antifungal, and antioxidant effects. These attributes make *Laurus nobilis* not only an ornamental plant but also a valuable resource across various fields, including agriculture, medicine, and the food industry. In agriculture, its essential oil can be utilized as a natural pesticide or fungicide, offering an environmentally friendly alternative to chemical treatments. In medicine, its antibacterial and antifungal properties hold potential for developing new drugs or as adjuncts to existing therapies. In the food industry, the oil serves as a natural preservative or flavoring agent, extending the freshness of products and enhancing their taste. A detailed analysis of one fraction of the essential oil, obtained through dry-flash chromatography and characterized by a cheese-like aroma, was conducted using gas chromatography-mass spectrometry (GC-MS). This analysis revealed the presence of saturated alkan-2-ones, both normal and branched-chain (*iso*-), within the C_9-C_{13} range. Additionally, unsaturated alken-2-ones with a normal chain structure were identified, with the position of the double bond precisely determined by characteristic ions in the mass spectrum of the DMDS-derivatized sample. The identified compounds include 5-undecen-2-one, 4-undecen-2-one, 3-undecen-2-one, (*Z*)-6-tridecen-2-one, (*E*)-6-tridecen-2-one, (*Z*)-6-pentadecen-2-one, and (*E*)-6-pentadecen-2-one. Both of these components, alkan-2-ones and alken-2-ones have been identified for the first time in the essential oil of *Laurus nobilis*. Until now, these compounds were only recorded in the essential oil of *Ruta angustifolia* and among the metabolic products of certain bacteria. This discovery not only enriches our understanding of the chemical composition of *Laurus nobilis* essential oil but also indicates the existence of undiscovered volatile compounds with potentially significant applications.

PFC PP 30

Evaluation of *Pleurotus ostreatus* (Jacq. ex Fr.) P. Kumm. edible mushroom as a novel source of natural antioxidants

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Pleurotus species, particularly *Pleurotus ostreatus*, are popular for their edibility, ease of artificial cultivation, and are the second most widely cultivated mushroom species worldwide. *P. ostreatus* is especially renowned for its culinary value, significant dietary components, and diverse biological activities [1].

The aim of this study was to assess the relationship between total phenolic content (TPC) and antioxidant activity of crude hydroethanolic (70% EtOH) and chloroform ($CHCl_3$) extracts of dried *Pleurotus ostreatus* samples obtained from the local market in Novi Sad, Serbia [2]. TPC values for $CHCl_3$ and EtOH extracts were 1.13 ± 0.16 mg GAE/g dry weight (d.w.) and 15.15 ± 0.20 mg GAE/g d.w., respectively. Antioxidant activity was evaluated using three standard assays, with radical scavenging potential measured via DPPH and ABTS assays. The IC_{50} values for $CHCl_3$ and EtOH extracts in the DPPH assay were 227.57 ± 3.09 µg/mL and 89.28 ± 2.49 µg/mL, respectively, while for the ABTS assay, they were 354.10 ± 4.80 µg/mL and 109.69 ± 5.48 µg/mL. The reducing power, as measured by the FRAP assay, was 32.10 ± 1.65 mg AAE/g d.w. for $CHCl_3$ and 56.99 ± 2.35 mg AAE/g d.w. for EtOH extracts. These results indicate that the polar EtOH extract exhibited significantly higher antioxidant activity and phenolic content. A strong correlation was observed between TPC and antioxidant activities in the ABTS ($r^2 = 0.84$) and FRAP assays ($r^2 = 0.99$) for the EtOH extracts. These findings suggest that *P. ostreatus* is a promising source of phenolics and potent antioxidants, particularly in polar extracts.

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PFC PP 31

Influence of pH value on the mineral composition of medical mushrooms

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This research aims to compare the pH values and mineral composition of three types of medicinal beech mushrooms: Fomes fomentarius (FF), Ganoderma lucidum (GL) and Trametes versicolor (TV). The samples were collected from the natural habitat and analyzed to determine the content of macroelements and microelements, as well as potentially toxic elements [1]. Aluminum (Al), barium (Ba), calcium (Ca), cadmium (Cd), chromium (Cr), copper (Cu), iron (Fe), mercury (Hg), potassium (K), magnesium (Mg), manganese (Mn), sodium (Na), phosphorus (P), lead (Pb), sulfur (S), selenium (Se), strontium (Sr) and zinc (Zn) were determined.

The analysis showed significant differences in the mineral composition and pH values among the examined mushroom species. Fomes fomentarius had high concentrations of calcium (4408±301 mg/kg) and aluminum (33.37±9.67 mg/kg), while iron was present to a lesser extent (42.03±6.93 mg/kg). Ganoderma lucidum had the highest content of iron (154.3±36.2 mg/kg) and sodium (60.28±9.15 mg/kg), but at the same time showed lower calcium values (2345±87.2 mg/kg) compared to the fungus Fomes fomentarius. Trametes versicolor stood out for the highest content of barium (62.03±6.13 mg/kg) and magnesium (2660±185 mg/kg), as well as elevated iron levels (122.3±98.4 mg/kg).

The pH values of the selected types of medicinal mushrooms ranged from 4.0 to 5.5, which indicates the slight acidity of the samples. Fomes fomentarius had the highest acidity among the analyzed species, which may affect its metabolism and biological activities. Given the different minerals present in each species, these results suggest that mineral composition and pH may have a significant impact on the nutritional and health characteristics of these mushrooms. These results contribute to a better understanding of the chemical profiles of medicinal mushrooms and can serve as a basis for future research on their application in phytotherapy and nutrition [2]. Additional research should focus on the biological activity and potential health benefits associated with established mineral profiles and pH values.

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PFC PP 32

Effect of ripening process in an uncontrolled atmosphere on the nutritional elements in medlar fruits

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Medlar (*Mespilus germanica* L.) is a plant species that belongs to the Rosaceae family. The plant flowers from May to June, whereas the seeds ripen in November when the fruit is harvested. The fruits are edible throughout the winter, as they can be stored in ordinary storage for two to three months, or in a cold storage for much longer. Medlar is a nutritionally valuable fruit, due to its complex chemical composition [1]. In this work nutritionally essential elements Ca, Cu, Fe, K, Mg, Mn, Mo, P and Zn were determined in unripe and ripe medlar fruits obtained from a local producer. Fruits were harvested as hard fruits and than left in a home cellar to ripe and soften (an uncontrolled atmosphere, at a temperature of 10 °C for 34 days). The content of 9 elements in medlar fruits was quantified by means of inductively coupled plasma with optical emission spectrometry (ICP-AES) after microwave enhanced digestion of the fruits [2].

The results of the study reveal that the concentrations of elements in unripe (UM) and ripe (RM) medlar fruits were in the ranges beween 3.34±0.05/0.64±0.01 mg/kg (Mn) and 28960±67/5508±77 mg/kg (K), respectively. Concentration of Mo was below the limit of detection (LOD) in both unripe and ripe fruits. The values of quantified elements in the medlar fruits were in the following order: K>P>Ca>Mg>Fe>Zn>Cu>Mn (for UM) and K>Ca>P>Mg>Fe>Zn>Cu>Mn (for RM). The decrease in the concentration of the studied elements was observed during the ripening of fruts in a storage, which can be attributed to the physiological processes that occur in fruit and storage conditions. Still, fresh fruits were good source of most of nutritional elements; the intake of 300 g of ripe fruits could supply significant ammounts of K (82.6%), Cu (35.4%) and Ca (15.6 %) on daily basis.

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PFC PP 33

Extraction of propolis polyphenols with natural deep eutectic solvents

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In recent years, the scientific community's interest has been directed towards developing and applying green solvents that can be used to obtain high-quality and safe extracts. Due to their positive pharmacological properties, propolis extracts are used in the pharmaceutical, food and cosmetic industries. The main objective of the research is to determine and compare the effect of different natural deep eutectic solvents (NADES) on propolis extracts and to select the best NADES that will extract the largest amount of bioactive compounds. The experiment was conducted with 40 different NADESs. The total polyphenol content of the obtained extracts was determined spectrophotometrically, and their antioxidant activity was estimated using the DPPH (2,2-diphenyl-1-picrylhydrazyl) test. Based on the obtained results, it can be concluded that NADES solvents that showed high extraction efficiency are N14 (lactic acid-fructose in a molar ratio of 5:1) with the highest content of total phenols and N15 (L-proline-lactic acid in a molar ratio of 1:2) as the solvent that showed the highest antioxidant activity determined by the DPPH test. The total polyphenol content in extract N14 was 104.77 mg GAE/g DW, while the estimated antioxidant activity of extract N15 was 73.58 mg TE/g DW. Based on the obtained results, further research will be directed towards optimizing key parameters such as extraction time and temperature, and the molar ratio of raw material to solvent, to achieve the highest content of bioactive compounds with potential applications in the pharmaceutical, food, and cosmetic industries.

Acknowledgments

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PFC PP 34

Potential and application of Natural Deep Eutectic Solvents (NADES) as co-solvents in the extraction of bioactive compounds from sage (*Salvia officinalis L.*)

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Medicinal plants represent a significant source of natural bioactive compounds that can be used as alternatives to synthetic drugs. Despite their great potential, these resources are underutilized, mainly due to the lack of technologies that would enable their efficient and economical use. Sage (*Salvia officinalis L.*) belongs to the group of medicinal plants recognized for their antidiabetic activity, contributing to its utilization in traditional medicine. Aiming to obtain sage extracts with high biological activity, specifically targeting antioxidant and antidiabetic, this research is focused on examining the possibility of using and improving the performance of subcritical water extraction by adding co-solvents.

The extraction process was carried out at a temperature of 130°C under the pressure of 110 bar for 20 minutes with and without co-solvents. Four different natural deep eutectic solvents were used as co-solvents: Fructose and glycerol (N1), choline chloride and glycerol (N2), L-proline and lactic acid (N3), L-proline and glycerol (N4). The obtained extracts were analyzed for their total phenol and flavonoid content. The biological characterization of the extracts included *in vitro* determination of antioxidant (by DPPH assay) and enzyme-inhibitory activity (based on their ability to inhibit the enzymes α-amylase and α-glucosidase). The results indicated high levels of total phenols (181.01 - 285.89 mg GAE/g) and flavonoids (63.81 - 143.14 mg RE/g), with co-solvents positively influencing their content in the extracts.The antioxidant capacity was in range IC_{50}=0.0105 - 0.0231 mg/ml. Regarding the antidiabetic activity it was shown that inhibitory concentration for α-amylase varied in the range of 4.25-6.02 mmol AE/g, while in the case of α-glucosidase ranged from 7.21 to 10.03 mmol AE/g. The efficiency of NADES mixtures decreases in the following order: N4>N1>N3 >N2. These results suggest that the chemical composition of NADES plays a key role in optimizing extraction, enabling efficient dissolution, stabilization, and preservation of bioactive compounds.The presented results show that NADES mixtures significantly improve the extraction of bioactive compounds from plant materials and indicate their potential application for obtaining extracts with enhanced biological activities.

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Solution Chemistry and Chemical Equilibrium (SCCE)

SCCE PP 01

The distribution of aqueous species and saturation index calculations in the mineral waters of Mataruška Spa

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Mineral waters represent a special group of groundwater, often characterized by elevated mineralization, increased content of microcomponents, and dissolved gases, which distinguishes them from low-mineralized groundwater. These waters often exhibit a complex hydrochemical composition, and a better understanding of the formation of their chemical composition can be studied through aqueous solution chemistry. The area selected for research is Mataruška Spa, located in central Serbia [1]. The study utilized nine chemical analyses of mineral water samples with the aim of determining the distribution of aqueous species and calculating the saturation indices of specific minerals. To address this issue, modern modeling methods were applied using the geochemical modeling software PHREEQC [2]. This program enabled the conversion of total element concentrations obtained from chemical analyses into the activities of the individual aqueous species in the given mineral waters. Additionally, according to the laws of chemical equilibrium, the program allows for the calculation of saturation indices for the minerals with which these waters come into contact. This approach enables the evaluation of the conditions under which the chemical composition of these waters is formed. Based on this approach, it can be concluded that the waters belong to the group of sodium-, magnesium-, bicarbonate-type waters with elevated fluoride and silicon content. The waters are classified as neutral to slightly alkaline, with a temperature of up to 50°C. The formation of these thermal mineral waters is associated with the dissolution of igneous rocks (primarily silicate minerals), as indicated by the saturation index results for these minerals.

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SCCE PP 02

Reactive extraction of lactic acid using different extractants

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Lactic acid (LA) is increasingly used in industry, primarily due to the production of biodegradable polymers. This is the reason to look for new, cheaper, and greener methods of producing and purifying LA. Reactive extraction is gaining attention as a promising approach due to its efficiency, simplicity, and lower production costs.[1]

This study investigated the efficiency of LA extraction using three extractants (trioctylamine (TOA), tributyl phosphate (TBP) and adogen 464, Fig. 1) in toluene as the organic phase. In addition to toluene, experiments were conducted with sunflower oil. Using potentiometric titration, the amount of LA was quantified in both phases at different concentrations of acid and extractant.

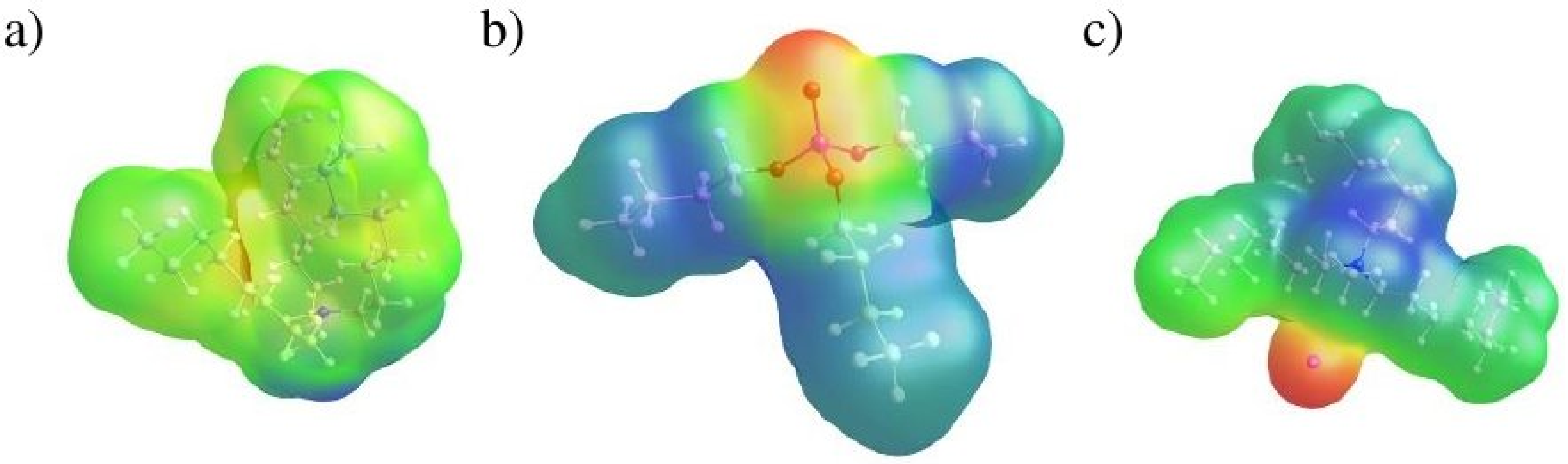

Figure 1. Electrostatic potential maps of a) TOA, b) TBP and c) adogen 464

The extraction efficiency decreased in the following order of extractants: TOA, TBP and adogen. Supramolecular extraction complexes with a stoichiometric acid: extractant ratio of 2:1 were observed with TOA and, to a lesser extent, with adogen. The use of TOA in sunflower oil instead of toluene did not result in a significant decrease in extraction efficiency.

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Supramolecular Chemistry and Functional Materials (SCFM)

SCFM PP 01

Sorptive extraction of aniline from aqueous solution using reusable molecularly imprinted polymer

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Aniline, a representative of primary aromatic amines, is a key intermediate in the chemical industry particularly in the synthesis of dyes and pigments extensively utilized in the textile sector [1]. The choice of the appropriate desorption agent as well as the ease of regeneration, and reusability of the sorbent, are key parameters for enhancing the efficiency, feasibility, environmental friendliness, and cost-effectiveness of the sorption process [2]. In this study, the sorptive extraction of aniline from aqueous solutions was investigated using a molecularly imprinted polymer, MIP-peha. The influence of pH value on the sorption capacity was examined, as well as the possibility of regeneration and reusability of the analyzed MIP. Varying the pH value in the range from 2 to 10 it was observed that the value of the maximum sorption capacity (2.05 mg/g) reaches at pH value of 6. The possibility of desorption of aniline from MIP-peha was tested using three organic solvents - ethanol, methanol and acetonitrile and the results show that the highest desorption capacity of about 0.83 mg/g is achieved with acetonitrile as a desorption agent, while the lowest desorption capacity is observed using ethanol (0.13 mg/g). The reusability of MIP-peha was evaluated by performing several sorption/desorption cycles using acetonitrile. After four cycles of sorption/desorption, a loss of 8 % sorption capacity was observed in relation to the initial one, which confirmed that MIP-peha can be used in at least four cycles of sorption/desorption.

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SCFM PP 02

Correspondence between photocatalytic and photoluminescent properties of novel nanophosphors

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In this study, the photocatalytic and photoluminescence properties of newly synthesized nanostructural phosphors were observed. Up-converting $SrGd_2O_4$ co-doped with different concentration of Yb^{3+} ions (2, 4, 6 at%) and constant concentration of Ho^{3+} ions (1 at%), and down-converting $SrGd_2O_4$ doped with Dy^{3+} ions (1, 3, 5 and 7 at%) were prepared *via* combustion method. X-ray diffraction investigation revealed a pure single phase with an orthorhombic lattice corresponding to the $SrGd_2O_4$ spinel structure. Scanning Electron Microscopy discovered irregularly shaped agglomerated particles that were different in size. UV/Vis Diffuse Reflectance Spectroscopy enabled obtaining energy bandgap values, which were found to be 4.3 eV, for each sample. Investigation of luminescent properties verified the existence of characteristic emission peaks related to Ho^{3+} or Dy^{3+} ions. Photocatalytic efficiency was monitored *via* the degradation of Methylene Blue for up-convertors and Rhodamine B for down-convertors. The obtained results indicate a successful dye decomposition rate after only 4 h. Moreover, results suggest that samples with the highest luminescence intensity exhibited better photocatalytic efficiency, which meant substantial potential for as-synthesized nanopowders to be used as multifunctional materials.

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SCFM PP 03

Analysis of the structure and chemical composition of the laser-modified Ti/Cu/Ti system

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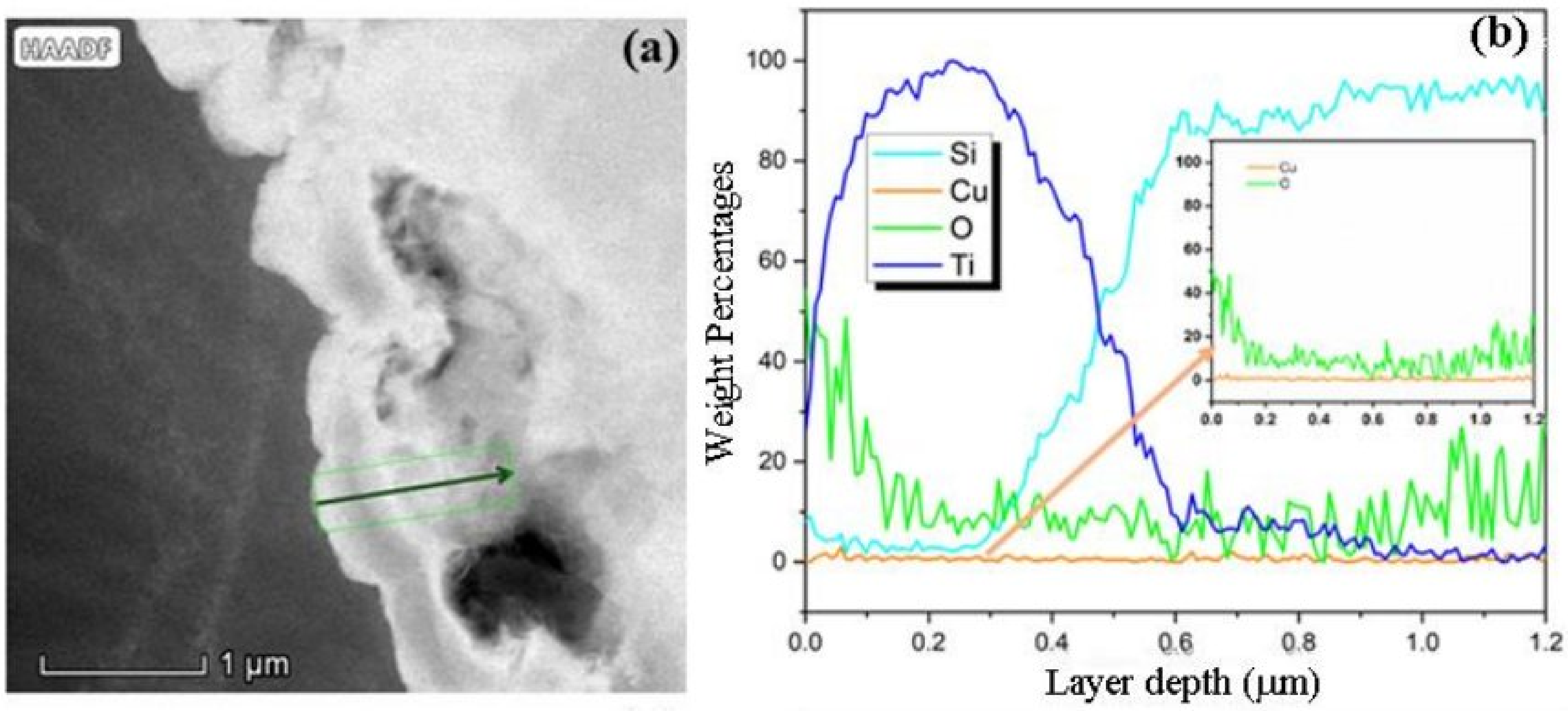
The elemental composition of the modified Ti/Cu/Ti system was investigated by scanning transmission electron microscopy, together with EDX analysis, which confirmed the previously presented results of TEM and HR-TEM analysis. The figure bellow presents a STEM/HAADF photomicrograph of a laser-modified Ti/Cu/Ti layer, take in the dark field, and the same figure under (b) shows the relative concentration profiles of the elements corresponding to the sample area marked with a green line in the figure under (a). The profiles of the individual elements (titanium-blue, copper-orange, oxygen-green and silicon-turquoise color) clearly show that due to the effect of the laser radiation, atom diffusion and mixing of the deposited layers of titanium and the sub-surface layer of copper, occurred within the Ti/Cu/Ti layer, as well as at the interface with the Si substrate. As a result of the enhanced diffusion [1,2], copper is not localized in the sub-surface area of the sample, but is evenly distributed throughout the depth of the layer with a concentration of about 2 weight percent (see the inset in the figure under b).



STEM-HAADF image of Ti/Cu/Ti laser-patterned thin film with the 400 nm thick layer with corresponding EDX maps.

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SCFM PP 04

Impact of the laser irradiation parameters on the surface characteristics of coarse- and ultra-fine-grained β-Ti alloy

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The purpose of this study was to investigate the effect of laser irradiation in different gas atmospheres on the surface properties of coarse-grained (CG) and ultra-fine-grained (UFG) β-Ti alloys with emphasis on surface roughness, chemistry and ablation. Field-emission scanning electron microscopy was used to obtain information on the surface morphology of the irradiated area, energy dispersive spectroscopy was utilized to analyze the chemical composition in the central irradiated area, while profilometric analysis was conducted to attain information on the surface topography of the irradiated area. Laser-generated surface structures in the form of conically-shaped craters, ripples, and droplets, as well as periodic and capillary waves on the morphologically and chemically altered CG and UFG alloy surface, were developed as a result of the hydrodynamic and oxidation processes occurring during the laser beam and alloy interaction. Also, during the process of laser surface modification, the laser-induced plasma was created in front of the irradiated alloy surface. Results attained during the present study showed that the alloy surface properties were noticeably impacted by the alterations of laser irradiation intensity and applied gas atmosphere. Namely, under the ultra-short pulsed irradiation conditions the presence of more pronounced surface structures, increased damage degree along the target depth, appearance of more distinct ejected, melted, and solidified material, as well as noticeable material evaporation were evident over the whole irradiated area. Moreover, the application of higher laser output energy led to an increase in the surface damage features dimensions, and an enhancement of the surface roughness and volume of the ablated material which, in turn, caused more intensive surface oxidation. Finally, the conducted research showed that the presence of refined UFG microstructure significantly contributed to the enhanced impact of the laser irradiation process on the occurrence of surface alterations that are favorable for the applicability of the investigated β-Ti alloy in orthopedic and dental implantology.

Acknowledgments

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SCFM PP 05

The ion selectivity of the cryptand: prediction of ion selectivity by quantum chemical calculations XVII[$]

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Virgil L. Goedken and Shie-MingPeng developed cryptand. They investigated it with the help of computational chemistry (B3LYP/LANL2DZp) and its interaction with metal ions was examined.[1] It was investigated in order to gain insight into the influence of the flexibility of the chelate N-C-C-N group on the overall selectivity towards the metal ion. According to our research the most suitable cation for the cryptand is Li^+, because Na^+ is too large, and this was proven using DFT calculations. We were able to confirm that it is the most effective method for hosting the guest cations is for the cryptand to twist itself, and the flexibility of the chelating N-C-C-N group serves as the most effective structural motive for the Goedken-Peng cryptand to interact with the guest cation. [2]

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SCFM PP 06

Ru-doped TiO_2: Novel photocatalyst for Reactive Orange 16 dye degradation

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Contamination of wastewater and hence water in general has become a major concern especially because of the immense use of highly toxic synthetic dyes. Stable, environmentally friendly, and low-cost titanium dioxide has already been widely applied in photocatalysis, which is an advanced water purification treatment. However, TiO_2 is poorly active in the visible light region but this issue can be overcome by doping with transition metal ions [1]. Hence, this work aimed at preparing Ru-doped TiO_2 photocatalyst for dye degradation which will be highly active under simulated solar light.

To synthesize Ru-doped TiO_2, the suspension containing TiO_2 (anatase) and RuO_2 in mole ratio 5:1 was hydrothermally treated at 180 °C for 48 h. The pH value of the suspension was adjusted to 13 by adding the potassium hydroxide solution (c=0.4 mol dm^{-3}). The obtained powder was dried at 25 °C for 24 h and characterized by XRD and TG/DTA while its photocatalytic activity was examined towards the degradation of Reactive Orange 16 dye.

XRD results showed that the prepared sample consisted of the single-phased anatase (PDF #64-0863). Calculated unit cell parameters and volume (a=3.8028(2) Å, c=9.5046(7) Å, V=137.45(1) Å^3) were higher than expected for the undoped anatase meaning that Ru^{4+}-ions were likely incorporated into TiO_2 lattice. Namely, the octahedrally coordinated Ru^{4+} is larger (r=0.620 Å) than the octahedrally coordinated Ti^{4+} (r=0.605 Å) so the lattice had to be expanded to accommodate a larger cation. The crystallite size of the obtained Ru-doped TiO_2 was sufficiently small, i.e. around 25 nm, which is important for photocatalytic application. Photocatalytic activity tests confirmed that the Ru-doped TiO_2 could be used as a photocatalyst since 61 % of the dye was degraded after 180 min under simulated solar light.

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SCFM PP 07

Preparation of curcumin-loaded polysaccharide-based films for food freshness monitoring

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The development of novel bifunctional food packaging for monitoring and maintaining food freshness is of great importance for food safety [1,2]. In this research, films based on biocompatible and biodegradable polysaccharides chitosan and alginate/κ-carrageenan were prepared by self-assembly of two oppositely charged polysaccharides. The preparation process and the composition of these films have been optimized. To obtain the pH-responsive formulations that can be used for detection of food spoilage, curcumin, a natural compound, was incorporated into the films as a sensing component. In order to enhance encapsulation of hydrophobic curcumin within the films, curcumin was also loaded in the form of β-cyclodextrin/curcumin inclusion complex. The obtained results indicated better mechanical properties of films and higher encapsulation efficiency of curcumin when it was used in the form of β-cyclodextrin/curcumin complex. Additionally, these composite films demonstrate potential for the application as coatings or packaging material for various types of food, thanks to the excellent antioxidant and antimicrobial properties of curcumin, that can extend the shelf life of food products. Finally, the proposed films were applied to monitor the freshness of different types of meat. The results indicated high sensitivity of films and their rapid response to pH changes. Based on the all obtained results, it can be concluded that the prepared polysaccharide-based films with encapsulated curcumin have excellent potential for food freshness monitoring, as well as food preservation, providing a novel approach to the design and development of multifunctional food packaging films.

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SCFM PP 08

Production and characterization of polylactic acid-based biocomposites

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Some food industry by-products have high fiber content, such as waste from the brewing industry. Most of these products end up in landfills, where they are subject to rotting, which creates greenhouse gases. Brewery spent grains (BSG) can be used as raw materials for composite with polylactic acid (PLA). Biocomposites based on PLA and natural fibers are a growing area of research. These composites combine PLA's biodegradability and environmentally friendly properties with natural fibers' strength and lightweight characteristics [1, 2]. The demand for natural composite materials is increasing since they can be used in food packaging.

Figure 1. Biocomposites based on PLA, with 10% BSG of different particle size.

This research is dedicated to producing biocomposites using PLA as a matrix, and BSG as reinforcement materials. The biocomposites were formed through compression molding, with a different content (10 to 50%) and particle size (150-600 μm) of reinforcing material (Fig. 1). BSG contained 40% insoluble fiber, of which 18% was cellulose. The physico-chemical, thermal, and mechanical properties of the obtained biocomposites were compared with those of non-reinforced, pure PLA. The study also evaluated the potential of these biobased and biodegradable composites for food packaging based on their properties.

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SCFM PP 09

A novel lignin-based nanomaterial from silicon-doped dehydrogenated polymer of coniferyl alcohol

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In this study, we proposed a novel approach to synthesize nanomaterial utilizing dehydrogenated polymer (DHP) derived from coniferyl alcohol (CA) with silicon doping. The synthesis of DHP involves enzymatic dehydrogenation of CA in a phosphate buffer using horseradish peroxidase (HRP) and hydrogen peroxide. This is followed by the hydrothermal synthesis of nanoparticles in the presence of ethylenediamine, which acts as a cross-linking agent and introduces amine groups in the final nanoparticle structure. Previous research has demonstrated that the introduction of silicon in the process of enzymatic polymerization significantly reduces the formation of large fractions of DHP and introduces Si-OH groups in the DHP structure [1]. We utilize silicon-doped DHP to improve the resulting nanoparticles' size, physicochemical properties, and performance. Our findings show that silicon significantly influences the structure and reduces the size of nanoparticles, as evidenced by a comparison of nanoparticles with and without incorporated silicon. The physicochemical properties and morphology of the synthesized nanoparticles are characterized using analytical techniques such as dynamic light scattering (DLS) and atomic force microscopy (AFM). As lignin-derived materials, these nanoparticles have the potential to act as antimicrobial agents. Considering that DHP demonstrated antibacterial activity [2], nanomaterials based on this polymer offers a promising path for the development of advanced materials for the pharmaceutical industry. Moreover, silicon-doped nanomaterials, mimicking lignin with improved characteristics due to silicon incorporation, hold significant promise for diverse applications such as drug carriers for targeted drug delivery or fabrication of biocides for agricultural production.

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SCFM PP 10

Controlled drug delivery using methacrylate-based hydrogels: Copolymerization as a strategy to mitigate the burst effect

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Hydrogels are effective matrices for drug delivery due to their porous structure and high-water retention, which mimic human tissue and enable controlled drug release [1]. Their customizable properties allow for precise delivery kinetics and versatility in various administration routes, including oral and transdermal. The burst effect, an initial rapid release of a significant portion of the drug, can occur upon contact with the surrounding medium, but it can be minimized through strategies like optimizing polymer composition and using multi-layered systems [2].

This study focuses on the copolymerization of methacrylate-based monomers, oligo(ethylene glycol) methacrylate (OEGMA) and oligo(propylene glycol) methacrylate (OPGMA), and its impact on the swelling behavior of hydrogel. We utilized sodium diclofenac as the model drug to evaluate the performance of these hydrogels as drug carriers. The goal is to optimize the burst effect to enhance therapeutic efficacy in drug delivery.

The results indicate that copolymerization of OEGMA with the hydrophobic OPGMA monomer in equal shares creates a hydrogel with reduced water uptake and swelling capacity, thereby slowing drug diffusion for more controlled release. Also, the resulting copolymeric hydrogel exhibits a volume phase transition temperature at the upper limit of physiological temperatures, positioning it as a promising candidate for controlled drug release in cancer treatments, including magnetic or photothermal therapy.

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SCFM PP 11

Methyl orange degradation with photocatalytic suspension: efficiency across concentrations

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The synthesis, characterization, and application of newly designed photocatalytic suspensions on facade paint surfaces (without the presence of titanium dioxide TiO_2) were performed. The design of the photocatalytic suspensions was carried out in two steps: 1. Synthesis of a concentrated suspension based on anionic clays (method of doping TiO_2) under controlled pH conditions - TiO2_ZnAl_LDH doped with 1 wt.% $(NH_4)_2WO_4$. ; 2. Dilution and stabilization of the concentrated suspension with the addition of appropriate dispersants.

After obtaining stable suspensions, they were thoroughly characterized, and the selected system was further applied to facade paints, after which the photocatalytic activity was tested on different concentrations of model pollutant Methyl Orange. At marked spots on the wall, a photocatalytically active suspension based on anionic clays was applied. After the suspension dried, solutions with concentrations of 0.5%, 1, 3, 5, 10, 20, and 50% by mass of the model pollutant Methyl Orange were applied over the suspension. Each concentration of the solution was applied to the corresponding marked spot on the wall designated for that concentration. A LED lamp was used as the visible light radiation source. The efficiency of degradation of different concentrations of the Methyl Orange solution was monitored using in-situ FTIR analysis and colorimetric measurements. The iradiation lasted for 240 hours, and measurements were taken before and after the 240 h period. The measurement results showed that degradation by the photocatalytic suspension was effective for all concentrations.

This study opens opportunities for further exploration and potential applications of developed suspensions in sustainable technologies for inner wall protection and preservation.

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SCFM PP 12

Molecular imprinting of polymers with lactoferrin

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Lactoferrin (LF) is a protein naturally present in milk whey; it plays a significant role in the modulation of the immune response and participates in the body's defense against reactive oxygen species and oxidative stress. Studies have shown that determining LF concentration in different body fluids is essential for the accurate diagnosis of various diseases, such as acute urinary tract infections [1]. This work is based on the synthesis of different molecularly imprinted polymers (MIPs) with LF in order to develop new matrices for the determination of LF in body fluids. Three MIPs and their nonimprinted analogs (NIPs) for LF were synthesized, using different molar equivalents of methacrylic acid (MAA) to the template as functional monomers. Acrylamide was used as an auxiliary monomer in all polymers. The polymers were characterized by infrared spectroscopy and examination of the binding efficiency of templates for different polymers. The selectivity of the obtained polymers for papain, riboflavin-binding protein, transferrin, and bovine serum albumin was also examined.

To investigate the influence of the amount of MAA, MIP II and MIP III and their unlabeled pairs were synthesized and the results showed no protein binding. The MIP I binds a higher percentage of LF than other MIPs in the range of initial solution concentrations tested. There was no MIP I saturation at the highest concentration of LF solution (3.0 mg/mL), and binding capacity could not be obtained. The MIP I imprinting effect increases to a concentration of 1.5 mg/mL, then slightly decreases, and the obtained imprinting factor for MIP I was 7.27. The selectivity tests confirm that the MIP I has been imprinted and specific sites have been formed due to papain weaker binding to MIP I than LF. On the other hand, MIP I has shown no selectivity towards transferrin, which has almost the same molecular weight.

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SCFM PP 13

Preparation of sorbents with a potential application in solid-phase extraction of octyl salicylate

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To minimize the effects of UV radiation, the use of sunscreens in cosmetic preparations has been increasing. 2-Ethylhexyl salicylate (octyl salicylate) is a colorless oily liquid, used as an ingredient in sunscreens and cosmetics to absorb UV rays from the sun. Many studies have confirmed the presence of UV filters in human biological samples and marine organisms. The main challenge is to optimize new methods to detect UV filters in real samples, trying to follow their distribution in the environment and marine organisms. [2] Molecularly imprinted polymers (MIPs) are synthetic materials designed to recognize and bind specific molecules. Molecular imprinting is a process in which the target molecule acts as a template around which interacting and cross-linking monomers are arranged and copolymerized to form a cast-like shell. Depending on the types of chemical bonds that maintain the template–monomer complexes, there are three distinct molecular imprinting approaches for preparing MIPs: covalent, non-covalent, and semi-covalent molecular imprinting.[1] The aim of this study is the synthesis of polymers by a semi-covalent and non-covalent approach for ethylhexyl salicylate and the optimization of the conditions under which ethylhexyl salicylate binds the best to polymers. For a semi-covalent approach, one pair of polymers was synthesized, one molecularly imprinted polymer, and one non-imprinted polymer for octyl salicylate. The functional monomer was methacrylic acid and cross-linker was divinylbenzene. The ester bond between the template and functional monomer was hydrolyzed with a methanol solution of sodium hydroxide. For the non-covalent approach, two polymer pairs were synthesized for the same template. In the first pair of polymers, the functional monomer was octyl salicylate methacrylate and the cross-linker was divinylbenzene, and for the second pair the same functional monomer, octyl salicylate methacrylate, but the cross-linker was ethylene glycol dimethacrylate. The binding of octyl salicylate to the polymers was obtained by high-performance liquid chromatography (HPLC).

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SCFM PP 14

Methacrylate esters of riboflavin as novel functional monomers for molecular imprinting of polymers with riboflavin binding protein

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Molecular imprinting is a powerful technology that enables the incorporation of molecular affinity sites into polymeric matrices, allowing for the selective recognition of a wide range of templates, including large biomacromolecules like proteins. When applied to proteins, classical imprinting techniques face challenges. Proteins' fragility can lead to irreversible conformational changes during polymerization, and their large size complicates separation and rebinding to cross-linked polymer matrices. Cross-reactivity and non-specific adsorption are also major issues [1]. In this study, a riboflavin derivative was utilized as a functional monomer to investigate the effect of an affinity ligand on the efficiency of imprinting and binding of the resulting polymers. Six molecularly imprinted polymers (MIPs) for riboflavin-binding protein from chicken egg white were synthesized, using riboflavin derivatives as functional monomers. These derivatives differed in the number of covalently attached methacrylic acid units. For the synthesis of the first set of polymers, acrylamide (AA) was used as a co-monomer, while 2-(hydroxyethyl)-methacrylate (HEMA) was used for the second set. In the final set of polymers, a modified approach was employed, incorporating both a riboflavin derivative as a functional monomer and *N,N*-(diethylaminoethyl)-methacrylate (DMAEM).

The binding results indicate that the formation of a stable pre-polymerization complex is crucial for producing successfully imprinted polymers. Polymers containing riboflavin derivatives were more efficiently imprinted by the protein (imprinting factor 2.35) compared to polymers without derivatives (imprinting factor 1.49). The positive influence of affinity ligand presence in the polymer structure was much more pronounced in imprinted polymers, demonstrating the significant effect of molecular imprinting. Additionally, the binding results showed that the imprinting effect increased with higher concentrations of initial solutions

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SCFM PP 15

Solid phase extraction of Padimate O using sorbents based on molecularly imprinted polymers

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Molecularly imprinted polymers (MIPs) are synthetic materials designed for selective recognition and binding of the target molecule (template). They are prepared through a polymerization process in which a template is used to form a polymer structure around it. Due to their ability to selectively recognize and bind target molecules, they are widely applied in separation and quantification techniques. Their wide range of use also stems from the fact that they can be synthesized for a number of different templates, one of them being UV filters, which are a non-negotiable basis in sunscreens [2]. Despite their primary protective role, they can be damaging to the environment (mainly aquatic ecosystem), as well as potentially damaging to human skin cells. Padimate O, which is a UV filter found in commercial sunscreens has been proven to penetrate through the skin and cause oxidative stress by generating reactive species [1]. In this research, a potential method of extracting Padimate O from its complex matrix and quantifying it has been developed on spiked sunscreen samples using a sorbent based on molecularly imprinted polymers in solid phase extraction (SPE). Two MIPs used in this study were synthesized using 2-acrylamido-2-methylpropane sulfonic acid (AMPS) as a functional monomer, as well as divinylbenzene (DVB) and ethylene glycol dimethacrylate (EDMA) as cross-linkers, respectively. The recovery of Padimate O from the solid phase extraction reached up to 100%, followed by quantification using HPLC.

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SCFM PP 16

Controlled release of furosemide in physiologically relevant media by molecularly imprinted polymers

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Furosemide is a diuretic drug used in many medical conditions where water is retained in the organism. Depending on the condition, one to four pills of furosemide are taken daily. Molecularly imprinted polymers (MIPs) are functional materials nowadays used in various fields of chemistry, biochemistry, pharmacy, etc. MIPs are obtained by polymerization of functional monomer and cross-linker in the presence of template molecule which forms selective binding sites in the polymer. These polymers can be used for the controlled release of drugs [1,2] Several polymer pairs of imprinted polymers and non-imprinted analogs (NIPs) were synthesized, using 4-vinylpyridine and dimethylaminoethyl methacrylate as functional monomers, and divinylbenzene and ethylene glycol dimethacrylate as cross-linkers. The template was washed out of the obtained polymers, and then, in the rebinding experiment, a known amount of furosemide was bound to the polymers. The controlled release was monitored in fasted state simulation of intestinal fluid and fed state simulation of intestinal fluid during several hours. The release of furosemide is monitored by HPLC with UV detection.

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SCFM PP 17

Synthesis of silica-based matrices modified with Rhodamine B derivate for the sorption of α-1-acid glycoprotein

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For precise diagnostics, many low-abundance biomarkers have been isolated and determined in relevant biological samples [1]. One of these biomarkers is α-1-acid glycoprotein (AGP) found in human blood serum. AGP is a glycoprotein with a molecular mass of 41-43 kDa, pI value of 2.8-3.8, and is one of the positive acute-phase proteins [2]. The goal of this research is the synthesis and characterization of modified silica-based matrices for sorption of AGP, with potential application in the purification of AGP from blood serum. In this research, the interactions of synthetic ligands with α-1-acid glycoprotein immobilized on a chiral HPLC column were examined. The strongest binding was shown by the ethylenediamine derivative of Rhodamine B (EDA-RB), which was used to synthesize affinity matrices based on silica with different pore sizes. The obtained modifications were characterized by Fourier transform infrared spectroscopy (FT-IR). Fluorescence spectroscopy was used to determine the number of binding sites and the binding constants of EDA-RB to α-1-acid glycoprotein (AGP) and human serum albumin (HSA) at different pH values. The batch binding method was used to investigate the binding of AGP standards, HSA standards, and a mixture of AGP and HSA standards to the synthesized sorbents at different pH values. The desorption of bound molecules from the synthesized sorbents was also examined. Detection during sorption and desorption was performed using reversed-phase high-performance liquid chromatography with a diode array detector (RP-HPLC-DAD).

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SCFM PP 18

Microwave-assisted synthesis as a sustainable alternative: comparing two methods for poly(N-isopropylacrylamide) polymerization

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Poly(N-isopropylacrylamide) (PNIPAM) is a well-known stimuli-responsive polymer that exhibits sensitivity to temperature and pH, with a lower critical solution temperature (LCST) of approximately 32 °C in aqueous solutions. In this study, PNIPAM was synthesized using two distinct approaches: a conventional method and a novel microwave-assisted technique. For the conventional synthesis, we varied the amount of initiator (0.1, 0.3. and 0.5%) and the reaction temperature (60 and 70 °C) to investigate their effects. In microwave synthesis, we further explored the influence of initiator concentration (0.5, and 1%) and reaction time (4 and 6 min). Fourier transform infrared spectroscopy (FTIR) was used to confirm the successful synthesis, while thermal properties and phase transitions were analyzed using Differential Scanning Calorimetry (DSC). Comparison of FTIR spectra revealed that microwave-assisted synthesis can be effectively employed for PNIPAM production. Additionally, DSC results demonstrated that the microwave-assisted synthesis significantly impacts the thermal behavior and phase transition temperatures of the resulting PNIPAM, by increasing LCST. This study highlights the potential of microwave-assisted synthesis as an environmentally friendly, waste-free, and time-efficient alternative to conventional methods for the production of PNIPAM.

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Acknowledgments

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SCFM PP 19

Examination of the effect of functional monomer mole fraction on the imprinting of polymers with procaine

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The aim of this work is the synthesis of molecularly imprinted polymers (MIPs) for procaine, using different ratios of monomers and crosslinkers, to examine the impact on the success of polymer imprinting. Procaine is an effective local anesthetic that blocks nerve impulses, especially in dentistry and minor surgical procedures. Although procaine is considered a substance of low toxicity, there is a real chance of overdose, and symptoms include nausea and respiratory problems. In contrast, in rare situations, overdose can lead to anaphylactic shock and death [1]. Therefore, there is a need for the synthesis of MIPs for procaine that would enable both a simple and reliable diagnosis of its concentration in body fluids and tissues using electrochemical detection methods, as well as a system that allows a prolonged effect of the substance, relying on the ability of some types of MIPs for controlled releasing the template over a more extended period.

Ten polymers were synthesized; five were molecularly imprinted, and five were non-imprinted (NIPs). The binding of procaine to the obtained polymers was examined, and adsorption isotherms were constructed. Based on the data obtained from the isotherms, binding constants and capacities for the obtained polymers were determined. The selectivity of the synthesized polymers towards procaine was also examined with two structurally similar amines, propranolol and carvedilol.

The most favourable template to monomer to crosslinker ratio was 1:3:20. It was concluded that the ratio of monomer and crosslinker, as in the case of MIP2 (MAA 3:20 EDMA), results in the formation of a significantly higher number of high-affinity binding sites (73.26 μmol/g polymer) with still significantly high-affinity constants (1.37×104 mol/L) with a not so significant loss of low-affinity binding sites (113.59 μmol/g polymer). Comparing the binding of two competitors, carvedilol and propranolol, to MIPs and NIPs with the binding of procaine to the corresponding polymers confirmed the successful imprinting of polymers with procaine.

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SCFM PP 20

HPLC-monitored controlled release of donepezil by molecularly imprinted polymers under various physiological conditions

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Donepezil is an acetylcholinesterase inhibitor and is as such used as a medication for alleviation of certain symptoms of dementia and Alzheimer's disease. Molecularly imprinted polymers (MIPs) are synthetic materials capable of mimicking the selective binding of target molecules (e.g. enzymes and antibodies). MIPs are a special form of controlled drug release in which the molecule of interest - the template - can be released under certain physiological conditions. MIPs imprinted with donepezil using methacrylic acid as a functional monomer, and divinylbenzene and ethylene glycol dimethacrylate as cross-linkers, in acetonitrile as porogen were previously obtained [1]. The controlled release of donepezil from three different MIPs was monitored via HPLC. The controlled release was observed in three different aqueous systems that emulate different bodily fluids: fasted-state simulated intestinal fluid (FaSSIF), fed-state simulated intestinal fluid (FeSSIF), and simulated gastric fluid. All used MIPs have shown satisfactory controlled release in all three bodily fluids, ranging from 7 mg (FaSSIF, after 6 hours) to 47 mg (simulated gastric fluid, after 3 hours) of released donepezil per gram of MIP.

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SCFM PP 21

Investigation of UV and moisture induced degradation of $FAPbI_3$ perovskite: impact of polyionic additives on stability and phase transition

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Formamidinium lead tri-iodide, $FAPbI_3$, a perovskite material, has garnered significant attention for its potential as a solar light absorber and its ability to convert energy into current in photovoltaic applications. However, its long-term stability, particularly under environmental stressors such as ultraviolet (UV) radiation and moisture, remains a critical challenge. [1] This study investigates the degradation mechanisms of pristine $FAPbI_3$ and evaluates the influence of two polyionic additives PolyTFSI Li and PolyTFSI Imidazolium on its degradation behavior under UV and water vapor exposure. [2] Chemical and structural changes occurring during degradation were monitored through X-ray photoelectron spectroscopy (XPS) and X-ray diffraction (XRD). Scanning electron microscopy (SEM) was employed to observe morphological alterations, while UV-VIS spectroscopy monitored the degradation kinetics, which compromises the material's suitability for use in solar cells. Pristine $FAPbI_3$ degraded after 45 minutes, while $FAPbI_3$ with PolyTFSI Li and PolyTFSI Imidazolium degraded after 75 and 110 minutes, respectively, under 65% relative humidity at room temperature. UV-VIS spectroscopy indicated the formation of the delta-phase perovskite, confirmed by XPS and XRD. Significant morphological changes were observed via SEM. Pristine $FAPbI_3$ completely degraded after 6 hours of UV exposure. In contrast, $FAPbI_3$ with PolyTFSI Imidazolium and PolyTFSI Li showed improved stability. Pristine $FAPbI_3$ exhibited crystal detachment from the surface layer, along with deformation and irregular structural features. PolyTFSI Imidazolium-treated $FAPbI_3$ exhibited minimal visual changes, with no noticeable color or morphological alterations, as confirmed by SEM. This research aims to provide insights into the stabilization of $FAPbI_3$ and its potential improvement for sustainable solar cell technologies.

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SCFM PP 22

The impact of organic polymers on the mechanical properties of geopolymers based on fly ash and slag

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The combustion of coal in thermal power plants throughout Serbia results in the production of large amounts of industrial waste, predominantly in the form of fly ash and slag. While this waste has the potential for various applications, the majority of this is still deposited in landfills. This study aims to evaluate the feasibility of utilizing fly ash and slag as raw materials for the production of geopolymers, which are synthesized at low temperatures to reduce carbon emissions. The investigation focuses on the influence of organic macromolecules, such as polyvinyl alcohol (PVA), chitosan, and starch, on the mechanical properties of geopolymers created from a fly ash and slag blend (containing 100% or 70% of fly ash). Characterization of the starting materials was performed using Fourier-transform infrared spectroscopy (FTIR), X-ray fluorescence spectroscopy (XRF), and X-ray powder diffraction (XRPD). The results indicate that both the composition of the starting materials and the addition of additives play a crucial role in determining the compressive strength of the geopolymers, which ranged from 6 MPa to 13 MPa. Notably, the addition of 2.5% polyvinyl alcohol (PVA) led to the most significant improvement in mechanical strength, while chitosan also contributed to an increase in strength. In contrast, the inclusion of starch had a negative impact, reducing the compressive strength. These findings underscore the importance of carefully selecting additives to optimize the mechanical performance of geopolymers.

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