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Book of Abstracts

4th November 2023

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Acknowledgement

Acknowledgement to the University of Novi Sad - Faculty of Sciences for the use of the space of the faculty during the 9th Conference of Young Chemists' of Serbia.

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10:20	*Popular Scientific Lecture* **Luka Mihajlović** (Analysis doo)
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18:00	*Closing ceremony* • **Best Oral Presentation Award** • **Best Poster Presentation Award**
18:15	*End of the Conference*

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

VENUE:

- Lectures and oral presentations will be taken place at the “Mihajlo Pupin“ amphitheater on the ground floor at the Department of Matematics and Informatics and the Department of Physics, Faculty of Science, University of Novi Sad (address: Trg Dositeja Obradovića 4, Novi Sad).
- The Poster sessions will take place in the hallway in front of the “Mihajlo Pupin“ amphitheater.

Plenary Lecture

PP OP 01

Determining the structure of natural products using NMR spectroscopy - is it enough or not?

Gordana B. Krstić

University of Belgrade - Faculty of Chemistry, Belgrade, Serbia

Isolation of secondary metabolites of plant, animal or any other material is an extremely challenging task and requires great knowledge and skills of the experimenter in order to isolate the metabolite in quantities sufficient to fully describe its structure. Once a metabolite is isolated, the next step in the further process is to determine its structure. The first choice of techniques for determining its structure are NMR techniques. Recording 1D and 2D NMR spectra is the first step in that process. Based on the data obtained from the recorded spectra, the structure is solved and the confirmation of the obtained molecular formula is done by recording high-resolution mass spectra. This is the most common way of solving the structure of isolated metabolites, however, questions arise whether this way of solving the structure of compounds is sufficient and whether we can make a mistake even if we get confirmation that the molecular formula is correct. Answers to these questions and suggestions for the correct solution of the structure will be discussed using an example from practice.[1]

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Acknowledgments

This research was done as part of postdoctoral studies at the Faculty of Pharmacy, University of Szeged (Hungary). I would like to take this opportunity to thank my supervisor Prof. Dr. Judit Hohmann for allowing me to be part of her research team and to learn a lot from them. Also, I would like to thank the Ministry of Science, Technological Development and Innovation of the Republic of Serbia, which financially supported my postdoctoral study through a scholarship for postdoctoral studies.

Invited Lectures

PPP OP 01

From waste streams to biotherapeutics: making a connection using bacteria

Jelena O. Lazic, Jasmina B. Nikodinovic-Runic
University of Belgrade - Institute of Molecular Genetics and Genetic Engineering, Belgrade, Serbia

Microorganisms, our planet's original inhabitants discovered with the invention of the first microscope in the 17th century, have consistently facilitated our daily life. However, our modern life generates enormous amounts of wastes, such as plastic, food, and chemicals from the pharmaceutical industry. Bacterial natural products hold an important position in this industry, as drug leads in synthetic chemistry and biology, essential for the discovery of effective agents against a variety of human diseases. If the existing waste is used as a nutrient source for microbial production of valuable biomolecules, that concept is called "waste to value" or "upcycling".

This concept was explored using bacterial biopigment prodigiosin (PG, Fig. 1) as part of the BioECOLogics project. This proof of concept demonstrates how the bacteria *Serratia marcescens* ATCC 27117 can use a waste stream from the food industry as a carbon source to grow and produce its bioactive secondary metabolite PG. The unique structure of this molecule was changed through green chemical [1] and biopolymer formulation [2] approaches, as well as metal complexation. Finally, these sustainable biotherapeutics were validated *in vitro* (antimicrobial, anticancer) and *in vivo* (nematode *Caenorhabditis elegans* and zebrafish *Danio rerio*).

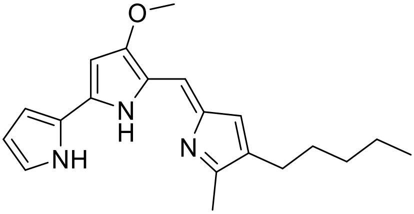

Figure 1. Structure of bacterial biopigment prodigiosin (PG).

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Acknowledgments

This work was financially suported by the Science Fund of the Republic of Serbia, IDEAS (BioECOLogics, 7730810) and the Ministry of Science, Technological Development and Innovation of Serbia (451-03-47/2023-01/200042).

PPP OP 02

Towards future food supplement ingredients: chemical modification of natural antioxidants

Valentina Metličar[1], Krištof Kranjc[2], Alen Albreht[1]
[1] *National Institute of Chemistry, Department of Analytical Chemistry, Laboratory for Food Chemistry, Ljubljana, Slovenia*
[2] *University of Ljubljana - Faculty of Chemistry and Chemical Technology, Ljubljana, Slovenia*

Xanthophylls are natural compounds that have many beneficial effects on our health. As a consequence, they are employed in various industrial applications, but the majority of them suffer from one major drawback – chemical instability, especially in the presence of either oxidants, acids, and metals or when exposed to light or increased temperatures. Moreover, xanthophylls are often extracted from plants by non-sustainable means, leaving behind a significant carbon footprint.

Here, we present a green technology for the production of xanthophyll esters as a means to increase their chemical stability and enable their use as improved food supplement ingredients. These esters (55 in total) were synthesized using β-pinene as a bio-derived solvent at ambient temperature and pressure with excellent selectivity (median 97%) and finally isolated in high yields (median 81%) and with high purities (median 97%). The production of tailored xanthophyll esters can also be achieved via a solvent-free reaction, further contributing to environmental sustainability. The use of food waste and invasive alien plant species, such as Japanese knotweed, not only helps to preserve biodiversity but these materials also represent a renewable and practically unlimited source of natural pigments.

Finally, 13 structurally and electronically distinct model lutein diesters were subjected to a forced degradation study and the relationships between their structure and their degradation rate were systematically determined. Not all diesters showed an increase in stability, but three branched products proved particularly important, as they were as much as 1.5 – 21 times more stable compared to free lutein. We also show that the matrix of the Japanese knotweed plays a crucial role in pigment degradation kinetics. Thus, the proposed valorization strategy is certainly feasible, but the esterification approach should be tailored to the intended use of a particular lutein diester.

Acknowledgments

This work was supported by the Slovenian Research Agency [research program and research project grant numbers P1-0005 and J4-3092].

PPP OP 03

Polyphenols as modulators of prostaglandin E_2 and thromboxane A_2 production

Tatjana M. Majkić[1], Ivana N. Beara[1]
[1] *University of Novi Sad - Faculty of Sciences, Novi Sad, Serbia*

Prostaglandin E_2 (PGE_2) and thromboxane A_2 (TXA_2) are products of the cyclooxygenase (COX) pathway of the arachidonic acid metabolism. They have an important function in homeostasis of the cardiovascular, gastrointestinal, reproductive and renal systems. On the other hand, when overexpressed, they are involved in the inflammation and pathogenesis of many diseases: cardiovascular disorders, atherosclerosis, thrombosis, hypertension and preeclampsia, development and progression of cancer.[1] Having in mind the importance of regulation of PGE_2 and TXA_2 production in inflammation and due to the low activity or contraindications of currently approved anti-inflammatory drugs, an intensive research on new therapeutics is ongoing, and natural compounds are considered as one of the possible, safe anti-inflammatory agents.

The potential of polyphenols, as well as *Plantago* extracts and Merlot wine (a rich sources of polyphenols) to modulate the production of PGE_2 and TXA_2 was studied in an *in vitro* model system - monocytes or macrophages (U937 cell line), where inflammation was induced by lipopolysaccharide (LPS). Experiments were conducted using three variations of this model system: unstimulated monocytes, LPS-stimulated monocytes and LPS-stimulated macrophages. Quantification of produced PGE_2 and TXA_2 was done by LC-MS/MS technique. RT-qPCR was used to determine effect of examined samples on expression of mRNA related to the enzymes involved in the synthesis of PGE_2 and TXA_2: phospholipase A_2, COX-1/2, three prostaglandin E synthases and thromboxane A_2 synthase.

Obtained results indicate that modulation of cyclooxygenase pathway of arachidonic acid metabolism could be one of the mechanisms of anti-inflammatory action of *Plantago* species, wine and polyphenols in general. Further studies on potential synergistic effect of polyphenols are suggested, in order to discover more potent inhibitors of PGE_2 and TXA_2 production and to understand their combined mode of action.

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Acknowledgments

The authors gratefully acknowledge the financial support of the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grant No. 451-03-47/2023-01/200125).

Oral presentations

CS OP 01

Teaching chirality on dynamic systems

Branislav Z. Kokić[1], Vladimir D. Ajdačić[1], Igor M. Opsenica[2], Mario V. Zlatović[2]
[1] Innovation Centre of Faculty of Chemistry Ltd., Belgrade, Serbia
[2]University of Belgrade - Faculty of Chemistry, Belgrade, Serbia

Chirality is among the most important concepts in organic chemistry and, accordingly, has to be taught with care. Although the traditional approaches towards teaching chirality-related phenomena are intuitive and reliable, they heavily rely on geometry and symmetry operations. We propose an alternative pedagogical pathway for chirality introduction at college-level organic chemistry courses that can complement usual teaching strategies. It is based on chemical equilibrium, kinetics, and molecular motion, phenomena that are familiar to undergraduate students, and it guides students to perceive molecules in their natural dynamic state, rather than static 3D visualization of drawings on paper. As an integral part of our approach, atropisomerism and transient chirality are explained in-depth .

Acknowledgements

Financial support from the Ministry of Science, Technological Development and Innovation of Republic of Serbia Contract numbers: 451-03-47/2023-01/200168, 451-03-47/2023-01/200288.

CB OP 01

Design, synthesis and biological evaluation of carbamates as cholinesterases inhibitors in the treatment of Alzheimer`s disease

Ana Matošević, Anita Bosak
Institute for Medical Research and Occupational Health, Zagreb, Croatia

Alzheimer's disease (AD) is the most common and widespread neurodegenerative disease characterized by memory and judgment ability loss and personality changes. Today, it affects more than 50 million people worldwide and this number continuously grows as a result of the aging of the world's population. Although the multifactorial nature of this disease points to the existence of a number of possible targets, the existing treatment of AD is symptomatic and based mainly on increasing the concentration of the neurotransmitter acetylcholine (ACh) by inhibiting the action of the enzymes responsible for its hydrolysis, primarily acetylcholinesterase (AChE), as well as butyrylcholinesterase (BChE).[1] Considering the role of BChE in the regulation of brain ACh levels in late AD, the focus in this study was placed on the selective inhibition of BChE as a promising new approach in the treatment of middle and advanced AD.

We synthesized 25 carbamates and determined their inhibitory potential toward both of the cholinesterases, inhibition selectivity, ability to cross the blood–brain barrier by passive transport, cytotoxic profile and ability to chelate biometals[1]. According to our results, we point to three carbamates as promising compounds for the development of more effective drugs for the treatment of advanced stages of AD.[1]

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Acknowledgments

This work was supported by the Croatian Science Foundation Grant No. IP-2020-02-9343.

DCS OP 01

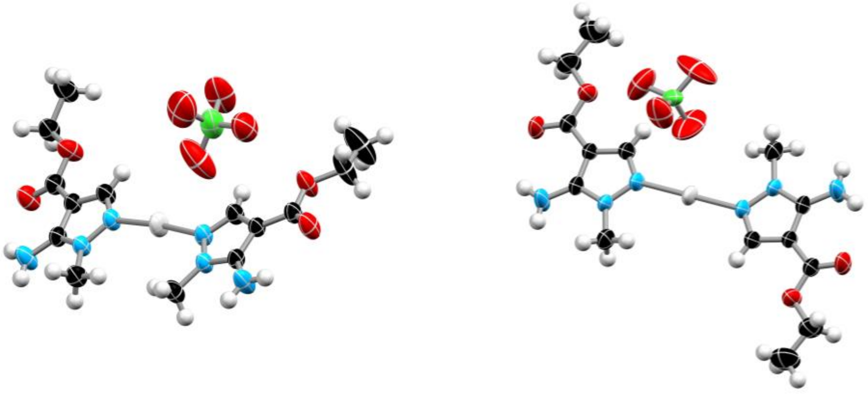
Syntheses and structures of Ag(I) complexes with pyrazole-type ligand

Nikola D. Radnović[1], Nađa Štetin[1], Berta Barta Holló[1], Marko V. Rodić[1].
[1] *University of Novi Sad - Faculty of Sciences, Novi Sad, Serbia*

The reaction of warm methanolic solution of ethyl 5-amino-1-methyl-1*H*-pyrazole-4-carboxylate, L, with $AgClO_4$ yielded the complex $[AgL_2]ClO_4$ (**1**). The same reaction in presence of 4-formylbenzonitrile produces an isomer $[AgL_2]ClO_4$ (**2**).

The molecular structure of **1** and **2** (Fig. 1) consists of an Ag^+ ion, two L, and a perchlorate ion. The silver atom is situated in linear environment, composed of two ligands that are coordinated in a monodentate manner through the nitrogen atom in both complexes. The rotation of the ligand, influenced by 4-formylbenzonitrile as a modulator, caused different crystal structures. The crucial structural difference lies in the environment of the silver atom. In compound **1**, the silver atom is surrounded by one perchlorate anion, whereas in compound **2**, it is surrounded by two anions. Besides electrostatic attraction of complex cations and perchlorate anions, there is also the N–H···O hydrogen bonding that stabilizes crystal structures.

Selected crystallographic data and refinement details: **1** $C_{14}H_{22}AgClN_6O_8$, $P2_1/n$, a = 9.9519(3) Å, b = 20.2175(9) Å, c = 10.4909(4) Å, β = 102.439(4)°, V = 2061.25(14) Å^3, Z = 4, R = 3.8 %, for 329 parameters and 5184 independent reflections; **2** $C_{14}H_{22}AgClN_6O_8$, $C2/c$, a = 19.2463(3) Å, b = 7.3840(3) Å, c = 15.4865(7) Å, β = 93.945(4)°, V = 2195.64(16) Å^3, Z = 4, R = 4.3 %, for 140 parameters and 2718 independent reflections.



(a) (b)

*Figure 1. Molecular structures of complex **1** (a) and **2** (b).*

EA OP 01

Photodegradation of organic UV filters in water using UV/chlorine and UV/H_2O_2

Marija Z. Kuč[1], Tajana M. Simetić[1], Jelena J. Molnar Jazić[1]
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Specific organic micropollutants from the list of priority substances of the European Union Water Framework Directive and pollutants of new generation, the so-called pollutants of emergent concern, present a great risk to the quality of both surface water and groundwater. Among these substances, ultraviolet (UV) filters are getting increasing attention, due to the wide use in sunscreens and other personal care products, in order to protect consumers from harmful effects of UV light. As a result of high stability of UV filters, the conventional treatment processes (e.g. filtration, coagulation, flocculation,) and even some of oxidation processes (such as ozonation) have limited ability to remove UV filters from water. This study investigates the efficacy of various water treatments including UV photolysis, UV/chlorine and UV/H_2O_2 processes for the 3-(4-methylbenzylidene) camphor (4-MBC) and ethylhexyl methoxycinnamate (EHMC) removal from water. The obtained results indicate that the degradation of both organic UV filters was significantly more effective when using UV/H_2O_2 and UV/chlorine processes than UV photolysis alone. The reason for this is the formation of non-selective hydroxyl radicals ($HO^•$) and selective reactive chlorine species (RCS), such as chlorine atom radicals ($Cl^•$) and oxychloride radicals ($ClO^•$), during the advanced oxidation processes. By applying UV/H_2O_2 and UV/chlorine processes, using 0.03 mM of oxidants and UV fluence of 200 mJ/cm^2, a degree of 4-MBC and EHMC degradation in water was higher than 90%. For the same degree of degradation in surface water, it was necessary to apply a higher H_2O_2 and sodium hypochlorite dose (0.3 mM) and UV fluence (1400 mJ/cm^2), indicating the effect of water matrices on the degradation efficacy during the free radical-driven oxidation processes.

Acknowledgments

The authors gratefully acknowledge the financial support of the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grant No. 451-03-47/2023-01/200125)

EA OP 02

Physico-chemical and structural characterization of the pharmacologically active ionic liquid tetracainium-ibuprofenate

Sara V. Pepić[1], Jovana J. Panić[1], Milan B. Vraneš[1], Željana M. Stanković[1]
[1]*University of Novi Sad - Faculty of Sciences, Novi Sad, Serbia*

Ionic liquids are defined as salts with melting point lower than 100°C. The aim of this paper was the synthesis of tetracainium-ibuprofenate ionic liquid using pharmacologically active substances, the local anesthetic-tetracaine and the anti-inflammatory drug ibuprofen. Additionally, density, viscosity and electrical conductivity were examined at different temperatures, as well as thermal stability and structural properties of obtained compound. Confirmation of the structure of synthesized ionic liquid was done by infrared (IR),^{1}H and ^{13}C nuclear magnetic resonance spectroscopy (NMR). The Newtonian behaviour of tetracainium-ibuprofenate was confirmed from viscosity measurement results, while the interactions of this compound were analyzed based of the measured density values, electrical conductivity, and calculated values of thermal expansion coefficients and activation energy of viscous flow. Based on the obtained results, it was concluded that the ionic stability technology was synthesized from its already existing tetracainium-hydrochloride formulation, which is mostly used in the form of drops for eye anaesthesia. Therefore, ibuprofen-based technologies may be promising candidates for the development of effective formulations of this drug.

PCC OP 01

The crystal structure of 3-(1-pyrazolyl)-L-alanine and its Ag(I) polymeric complex

Milica G. Bogdanović[1], Mirjana M. Radanović[1], Marko V. Rodić[1]
[1] *University of Novi Sad - Faculty of Sciences, Novi Sad, Serbia*

Pyrazole-based chelating ligands form diverse coordination complexes with different metal ions, offering varied coordination structures. The ease of synthesizing pyrazoles with various substituents is particularly intriguing, enabling precise control over electronic and steric properties in metal complexes [1]. In this study, we investigate the crystal structures of the ligand 3-(1-pyrazolyl)-L-alanine (L) and its complex $\{[AgL](ClO_4)\cdot H_2O\}_n$.

The ligand L crystallizes in the monoclinic space group $P2_1$ with unit cell parameters: $a = 5.2546(2)$, $b = 28.5437(10)$, $c = 5.2563(2)$ Å, $\beta = 114.953(5)°$, $V = 714.78(5)$ Å^3, $Z = 4$. The structure was refined to $R_1 = 3.90\%$ for 5334 independent reflections and 202 parameters. The asymmetric unit of L consists of two symmetrically independent zwitter-ionic molecules connected by N–H···O hydrogen bonds between ammonium and carboxylate groups of each molecule. Complex $\{[AgL](ClO_4)\cdot H_2O\}_n$ is a di-periodic coordination polymer which crystallizes in orthorhombic space group $P2_12_12_1$ and unit cell parameters: $a = 5.1677(2)$, $b = 13.8929(5)$, $c = 15.6346(6)$ Å, $V = 1122.48(7)$ Å^3, $Z = 4$. The structure was refined to $R_1 = 2.18\%$ for 2739 unique reflections and 170 parameters. The asymmetric unit consists of one Ag(I) atom, one ligand molecule, one perchlorate anion and one water molecule. The metal atom is situated in a deformed Y-geometry made up of one pyrazole *N* atom from one ligand, and two *O* atoms from carboxylate groups of other two ligands. In this complex, L is coordinated in O_2N tridentate mode, through the nitrogen atom of the pyrazole ring and two carboxylic oxygen atoms, binding to three Ag(I) atoms (Fig. 1). This mode of coordination leads to the formation of cationic $\{[AgL]^+\}_n$ layers parallel the crystallographic plane *ab*.

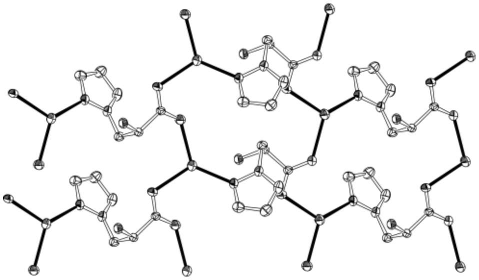

Figure 1. Fragment of cationic $\{[AgL]^+\}_n$ layer in the complex.

References

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PCC OP 02

Benzene coordination strengthens cation-π interactions: A DFT study

Katarina A. Ćeranić[1], Dušan P. Malenov[2], Snežana D. Zarić[2]
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[2] *University of Belgrade – Faculty of Chemistry, Belgrade, Serbia*

Noncovalent interactions between ions and aromatic rings play important roles in many biological and chemical systems. It was shown that cation-π and anion-π interactions can be strengthened if aromatic rings are coordinated to metals in sandwich and half-sandwich compounds.[1,2] In this work, cation-π interactions between Li^+, Na^+, K^+, Mg^{2+}, Ca^{2+}, NH_4^+ ions and coordinated benzene in sandwich compounds bis(benzene)chromium (Fig. 1), bis(benzene)molybdenum and bis(benzene)tungsten were studied using quantum chemical methods. DFT calculations at B3LYP(-D3)/def2-TZVP level showed that cation-π interactions of coordinated benzene have shorter distances between cation and aromatic ring and show more favourable interaction and binding energies than cation-π interactions of uncoordinated benzene. The strengthening of cation-π interactions of coordinated benzene is particularly pronounced for Mg^{2+} and Ca^{2+} ions. The interaction energies decrease in the following order: $Mg^{2+} > Ca^{2+} > Li^+ > Na^+ > NH_4^+ \approx K^+$, while interaction energies are very similar for all studied sandwich compounds.

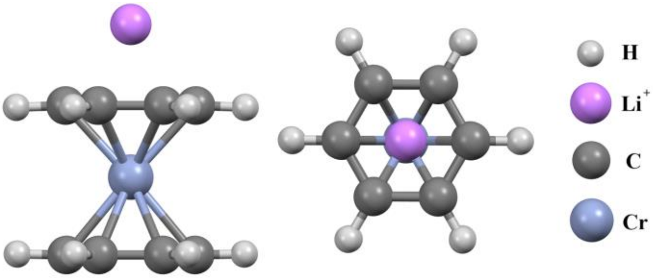

Figure 1. Cation-π interaction between Li⁺ ion and bis(benzene)chromium.

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PFC OP 01

Validation and optimization of ion chromatography based method for citric acid determination in *Robinia pseudoacacia* honey

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Honey is very complex natural substance consisted of sugars, water, and other compounds in smaller quantities such as proteins (enzymes), organic acids, vitamins, minerals, phenolics, and a large variety of volatile compounds. Discriminating the honeys according to botanical and/or geographical origin may be possible according to their characteristic constituents including organic acids profile. These acids are related to the colour and flavour of honey and its chemical properties such as acidity, pH and electrical conductivity. Honey is deceptively acidic, as the high sugar content tends to mask the acidity in the taste. Citric acid among other acids, is present in honey in moderate amount but it's presence could be potentially used as marker for authenticity control [1].

Fraudulent addition of compounds in honey sets a necesity to establish the natural level of the specific substances, and subsequently determine when this level is exceeded, indicating adulteration. Citric acid can be added to decrease pH in adulterated honey where normal pH levels have been exceeded. Also increased citrate concentration in honeys could be a result of addition of invert syrup to honey. Therefore there is a need for a method to determine citrate content in honey quickly and efficiently[1]. In current work a method for determination of organic acids profile in honey using ion chromatography with conductometric detection (IC-CD) without prior separation of compounds and chemical derivatization was developed. This approach for citric acid determination is characterized by LOD and LOQ values of 0.05 and 0.20 mg/L, respectively. Low RSD $S_{y/x}$ value and r^2 level of 0.9999 indicates a good regression model. Trueness of method was confirmed by good recoveries (108%, 104% and 95% for spiked levels 75%, 100% and 125%, respectively), while precision was confirmed by HorRat value (0.30) less than 2 [2].

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PFC OP 02

Comparative assessment of preeminent sugars and organic acids in fruits of several apple cultivars

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Soluble sugars and organic acids have a strong impact on the overall sensory quality of fruits. Organic acids also facilitate in stabilization of anthocyanins, and they extend the shelf-life of fresh fruits and their processed products. The production of new apple-based products with health beneficial properties is leading to agronomical and chemical re-evaluation of old apple cultivars.

In this study the mesocarp samples of five conventional, five resistant and fifteen autochthonous apple cultivars from a single growing season were deliberated. Assessment was based on contents of four sugars, one sugar alcohol and five organic acids that were determined by the usage of HPAEC-PAD and HPAEC-CD systems. Fructose was detected as dominant sugar in all cases (50.4 – 77.9 mg/kg FW) and malic acid as dominant acid (1.1 – 4.5 mg/kg FW). Regarding the average values, xylose and sorbitol were in higher amount in autochthonous cultivars compared to others. In resistant cultivars shikimate and malate were found in lower concentrations compared to other cultivar types. Among the obtained data, highest correlation values were found between citrate and isocitrate, and also between citrate and malate (0.905 and 0.839, respectively).

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PFC OP 03

Arthrospira platensis and *Porphyra sp.* – prospective serum-substitute in HEK293T cell culture

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Both *Arthrospira platensis* (Spirulina) and *Porphyra sp.* (Nori) are algae known for their richness in vitamins, minerals, antioxidants, proteins, such as phycobiliproteins (PBPs). Thanks to their exceptional nutritional properties they have potential to be considered as a high-quality substitute for fetal bovine serum (FBS) in cellular cultivation, which has numerous drawbacks since it can be involved in contamination development and its composition is still unclear. In this study we investigated the influence of Spirulina and Nori extracts on HEK293T cell line growth and viability in serum-reduced conditions. In DMEM/F12 medium supplemented with 0–10% FBS, the concentration-dependent effects of PBPs on cell proliferation were investigated. Cell viability and cytotoxicity were evaluated by MTT assay. During 3-day observation prior to MTT assay and MTT assay itself showed that HEK293T exhibited improvement in viability at lower PBP concentrations, while presence of higher concentrations resulted in inhibition of growth and change in morphology as a consequence of their cytotoxicity at higher concentrations. These findings suggest that PBPs have a positive outcome on cell growth at relevant doses. In general, in this study were obtained results proving the potential advantages of PBPs at lower doses on cell proliferation in serum-reduced conditions, but also HEK293T cells ability to adapt in non-standard cultivation set-up.

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SCCE OP 01

Hydration properties of the antidiabetic drug metformin in the presence of selected artificial sweeteners

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Metformin (Fig. 1a) is the primary drug used to treat type 2 diabetes (*diabetes mellitus)*. Its widespread use is owed to its ideal combination of effectiveness, price and safety. However, its bitter taste causes serious problems with patient compliance. Combining it with a sweet substance can improve its taste [1]. Artificial sweeteners, due to their very high sweetness, low caloric value and theoretical nonparticipation in metabolic processes, are ideal candidates to improve the taste of metformin. It has been shown that the hydration properties of a substance affect its taste and are of crucial importance for further research [2].

In order to better understand the interactions between metformin and select artificial sweeteners within a water medium, measurements of density, sound velocity and viscosity, for solutions of metformin in water and 0.1 $mol\cdot kg^{-1}$ aqueous solutions of sodium saccharin (Fig. 1b) and acesulfame potassium (Fig. 1c) were performed in a temperature range from 278.15 K to 318.15 K and concentration range from 0.02 to 0.12 $mol\cdot kg^{-1}$. From experimental data, the values of the apparent molar volume (V_{ϕ},), the apparent molar volume at infinite dilution (V_{ϕ}^{0}), the *Hepler* coefficient, the apparent molar limiting expansion (E_{ϕ}^{0}), the values of the *Masson* slope (S_{v}), the viscosity coefficient B of the Jones-Dole were calculated. From the calculated values of specific molar volumes, the influence of the tested artificial sweeteners on metformin˙s organoleptic properties was evaluated. The values gained are further discussed in terms of solute-solute and solute-solvent interactions.

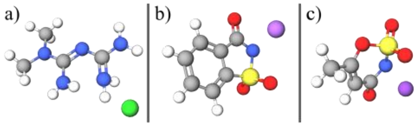

Figure 1. 3D structure models of: a) metformin HCl; b) Na saccharin and c) acesulfame-K

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SCFM OP 01

A novel gamma rays dosimeter based on organic dye and PVA: microwave synthesis and spectroscopic studies

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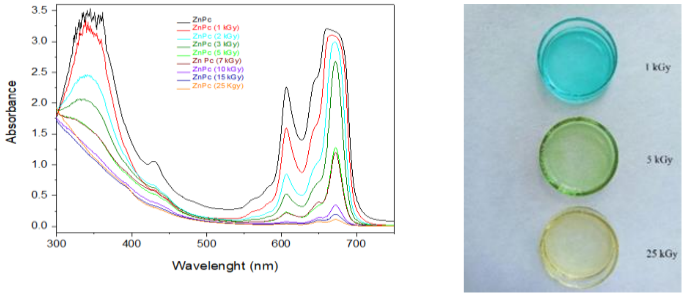
With the quick progression of radiation and irradiation technology such as medical diagnostics, food irradiation, and sterilization, the field of radiation protection has become of great importance. In that context, great fineness sensors are desired to detect the dose of nuclear radiation such as γ-rays [1]. In the present research, we have developed novel chemical-based radiochromic film dosimeters based on zinc phthalocyanine and polyvinyl alcohol (ZnPc/PVA) for the high ionizing radiation, gamma ray. The radiation-induced color bleaching of microwave-synthesized organic dyes [2] increases gradually with increasing absorbed dose in the dose range of 1-25 kGy (Figure 1). Also, the lower absorbance intensity could be observed in changing the color of samples from blue to pale yellow, depending on the dose of gamma radiation. The prepared dosimeters were irradiated with gamma rays from a ^{60}Co source. Furthermore, X-ray diffraction (XRD) measurements and Fourier transform infrared spectroscopy (FT-IR) showed excellent stability for the ZnPc molecule produced by microwave synthesis at the highest applied dose of 25 kGy.



A) B)

Figure 1. A) Absorption spectra of gamma-irradiated ZnPc in DMSO under dose at 1-25kGy, and B) selected ZnPc/PVA films.

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Poster presentations

Chemistry and Society

CS PP 01

The effect of an instructional strategy based on digital hybrid illustrations on students' achievement in the chemistry topic Hydrocarbons

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The study examines the effectiveness of instructional strategy based on the interactive learning tasks that integrated digital hybrid illustrations on students' achievement in the teaching theme “Hydrocarbons”. This study is a continuation of previous work[1], with an experimental-control group research design used within a larger research sample. A total of 323 Serbian elementary school students (14 -15 years old) from four schools located in Novi Sad participated in this study. Prior to the study, the students were assigned to one experimental group (N = 149) and one control group (N = 174), based on the results of the initial chemistry knowledge test. In the first stage of the study, the students from both groups followed the same teaching and learning activities about hydrocarbons. In the second stage of the study, the control group continued with the traditional teaching and learning practices, while the experimental group followed the review and practice activities with interactive learning tasks that integrated digital hybrid illustrations on cell phones via the Moodle platform. The digital hybrid illustrations were originally designed by combining realistic drawings and/or photographs with conventional elements that are characteristic of chemistry (symbols, formulas, equations, and models). After the treatment, both experimental and control groups were subjected to the knowledge test on hydrocarbons. The obtained results from the testing indicated that the applied instructional strategy used in the experimental group helped students achieve higher scores expressed in percentages (M (E_group) = 41.95% and M (C_group) = 34.06%), as a statistically significant difference between the groups was found.

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CS PP 02

The law of conservation of mass in action. Workshop approach in teaching

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The development of more effective and scientifically adjusted strategies for teaching chemistry laws is one of the goals of the chemistry education community. Chemical laws represent a vital matter and require the introduction of tangible elements to enable students to build mental models for conceptual understanding. Primary school students find it difficult to apply chemistry laws in solving problems. The majority of students will know how to reproduce the law, but the issue arises when they are asked to explain it. More precisely, they would know how the law of conservation of mass goes, but not to balance out some chemical reaction. Integrating contemporary teaching tools into the teaching of chemical laws may reduce the complexity and enable better understanding. This work shows a workshop aimed at explaining the law of conservation of mass. At the same time, it presents unique teaching material for primary school teachers, combining workshop approach and game in teaching. A workshop is defined as a classroom environment where students are actively engaged in learning and developing essential skills by working in self-managed teams on activities that involve guided discovery, critical thinking, and solving problems and include reflection on learning and assessment of performance. To additionally engage students, the designed workshop pulled through elements of an educational game (challenge, result, and success). The conducted study involved 98 8th grade primary school (both female and male) students. The effects of the designed workshop on students' knowledge were examined with a specially designed instrument. The data gathered after the practical class revealed that the students successfully comprehended the basic concepts of the law of conservation of mass. The designed practical class can be an example of good teaching practice but can also be included as additional material in traditional teaching.[1]

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Chemistry meets Biology

CB PP 01

Novel 17α-(pyridine-2-yl) derivatives of estrane: synthesis, antiproliferative activity, and *in silico* testing

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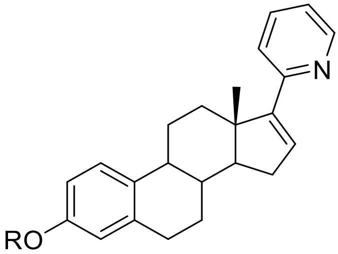
Steroidal derivatives with a heterocyclic ring, side chain with a heteroatom, or one or more core carbons substituted with a heteroatom showed increased biological activity with fewer side effects and/or with new pharmacological properties. Steroidal heterocyclic derivatives can be powerful agents in the prevention and treatment of a great number of types of hormone-dependent cancers. With this in mind, we have synthesized three novel 17-(pyridin-2-yl)estra-1,3,5(10),16-tetraen compounds 1-3 (Figure 1). These compounds have shown good in silico ADME properties obtained using web online tool SwissADME. In order to determine the proteins (receptors or enzymes) for which the synthesized compounds will potentially bind, and thus their biological activities, ligand-based virtual screening was performed with the SwissTargetPrediction online tool. The antiproliferative activity of all synthesized compounds was tested against six tumor cell lines (MCF-7, MDA-MB-231, PC3, HeLa, HT-29, and A549) and one healthy cell line (MRC-5) using the standard MTT assay.



1 R=H
2 R=Me
3 R=Bn

Fig. 1. Structures of synthesized compounds

Acknowledgments The authors acknowledge the financial support of Provincial Secretariat for Higher Education and Scientific Research of the Autonomous Province of Vojvodina [Project: New steroid derivatives - potential chemotherapeutics, No. 142-451-3133/2022-01].

CB PP 02

Comparative analysis of virtual tools for *in silico* ADME calculations

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In silico research in medicinal chemistry enables faster drug discovery and reduces the costs of expensive preclinical and clinical testing. *In silico* ADME (abbr. absorption, distribution, metabolism, excretion) analysis reduces the number of potential compounds that need to be synthesized in order to achieve the appropriate biochemical or physicochemical profile.[1] For the purpose of this research, the following virtual tools were compared: ChemDraw, SwissADME, Molinspiration and admetSAR. The ideal parameters observed during the modeling of new drugs, which were set by research group of Lipinski, [2]Muegge, Veber, Ghose and Egan, were calculated by the previously mentioned programs. The efficiency of selected *in silico* tools was compared by analyzing the physicochemical properties of four selected Dhomolactones of the androstane series that showed significant antitumor activity. By comparing the number of data that can be obtained, the possibility of parallel analysis of multiple compounds, speed, and graphical representations that those provide, it was concluded that SwissADME is the most convenient for usage. Moreover, the data provided by all four *in silico* tools indicate a ideal ADME profile for all tested steroid compounds, which with good antiproliferative activity makes them candidates for further biological testing.

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CB PP 03

Efficiency of nanofiltration membrane in the removal of pesticides from water

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Excessive use of pesticides in the agricultural domain has led to their often detection in aquatic environments[1]. Due to the negative impact of pesticides on the environment and human health, their efficient removal from water is required. The aim of this study was to determine the efficiency of a polyamide nanofiltration membrane in the removal of three pesticides. Dead end filtration equipment was used for the nanofiltration process and the pressure was set at 3 bar. The molecular weight cut off (MWCO) of the polyamide nanofiltration membrane is 400 Da. Selected pesticides were carbofuran, acetamipride and propiconazole, with molecular weights of 221,25 Da, 222,674 Da and 342,22 Da, respectively. The pesticide with the highest molecular weight, propiconazole, was not detected in the permeate and, therefore, had the highest removal efficiency. However, lower rejections were observed for pesticides with lower molecular weights. Due to the high MWCO of the nanofiltration membrane in comparison to the molecular weight of carbofuran and acetamipride, rejection rates for these pesticides were around 85% and 70%, respectively.

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CB PP 04

Effect of the laser surface scanning on the surface properties and biocompatibility of the titanium alloy produced by high-pressure torsion

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Laser surface modification has a significant potential to be used as an additional implant material processing method to obtain hard-tissue implants with favourable surface properties and improved biointegration for long-term biomedical applications. Therefore, this study aimed to determine the laser surface scanning influence on the surface chemistry, morphology, and roughness of the high-pressure torsion (HPT)-processed Ti-45Nb (mass%) alloy and its biocompatible properties. Results showed that the laser beam and alloy interaction led to the appearance of diverse morphological and chemical changes on the alloy surface. Depending on the laser pulse energy, a series of processes, such as melting, solidification, ablation, and plasma formation, were generated and accompanied by the appearance of surface damage features, *i.e.* microcracks and micro-patterns, observed by scanning electron microscopy (SEM). In addition, profilometric analysis showed that the appearance of laser-induced micro-structures influenced an increase in the damaged area surface roughness. Moreover, the alloy surface chemical composition was monitored by energy dispersive spectroscopy (EDS), and a significant increase in the irradiated area oxygen content was observed. *In vitro* assessment of the alloy cytotoxicity showed that there were no cytotoxic effects under the given examination conditions. Furthermore, the cell morphology analysis showed that cell attachment, spreading, and proliferation were notably enhanced on the modified alloy surface in comparison with the alloy prior to laser scanning. These findings demonstrate that laser surface scanning can be effectively used to improve the surface properties of the metallic implant material which, in turn, leads to its better biointegration abilities.

Acknowledgments

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CB PP 05

Synthesis and DNA binding properties of some new tryptamine Schiff's bases

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The synthesis of Schiff's bases by reaction of tryptamine and seven different aldehydes has been performed in absolute ethanol. The required Schiff bases were obtained in good yields. Schiff bases are known as compounds with a 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 DNA binding properties of seven novel tryptamine-derived Schiff bases. UV-Vis spectroscopic method was used for the determination of the binding mode between exanimated substances and DNA. In order to obtain the binding strength of compounds to DNA molecules we've calculated intrinsic binding constants K_b (M^{-1}) for tested compounds from the Wolfe–Shimmer equation [2]. All synthesized compounds showed high values for Kb (10^4 M^{-1}) which indicates the strong binding of examined compounds to DNA.

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CB PP 06

Polyethyleneimine(PEI)-graphene composites applied in biosensors to detect Alzheimer's disease

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Carbon screen-printed electrodes modified with polyethyleneimine-graphene composites were used as biosensor platforms to detect Amyloid-βeta (Aβ) antibodies related to Alzheimer's disease. The performance of the electrochemical biosensor depends on the ability of the material to immobilize the biomolecule of interest and also to transduce the biochemical events to electrical signals [1]. The objective of this work is to test the performance of four polyethyleneimine-graphene derivatives composites to detect Aβ-40 antibodies at concentrations varying from 1 ng mL^{-1} to 5000 ng mL^{-1}. Graphene derivatives made by chemical oxidation (GO and Reduced-GO) and electrochemical exfoliation of graphite (EEG and Reduced-EEG) were used to produce the composites. The graphene derivatives were dispersed in PEI solution (2 mg mL^{-1}) followed by the proportion of 0.6% (w/w) and named PEI-GO, PEI-RGO, PEI-EEG, and PEI-REEG. Cyclic voltammetry was performed at potentials varying from -0.6 to 0.6 V to examine the detection of Aβ40 antibodies. It was possible to observe that capacitance increases with increasing concentration of anti-Aβ-40. The biosensors involving PEI-rGO and PEI-EEG composites presented the most adequate calibration curve among the tested composites.

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CB PP 07

Synthesis of nanoparticles using RuBisCO protein derived from pumpkin leaves for controlled release of vitamin B12

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Pumpkin leaves which are considered biomass waste are rich in plant proteins who have an enormous potential and application in the food industry in comparison to proteins of animal origin [1]. One of them is the most abundant protein in nature, ribulose-1,5-biphosphate carboxylase/oxygenase (RuBisCO). This protein contains various functional groups enabling numerous interactions with a substantial number of compounds which make RuBisCO a noteworthy carrier of hydrophilic and hydrophobic biologically active food components. The goal of this research paper is to illustrate and prove the hypothesis that the RuBisCO fraction can potentially be used as a carrier of vitamin B12. The first protein sample was obtained using the thermal-acidic method while the second one was obtained using the thermal precipitation method and by adding ammonium-sulfate (40% w/v). Both of the isolated samples were freeze-dried and structurally analyzed using FTIR. The big and small subunit size (55 and 15 kDa) was determined using gel electrophoresis. The protein content was determined using the Lowry method. Nanoparticles were produced using a cold gelation method, where Ca^{2+} ions were used as crosslinking agents [2]. This process was optimized by varying the concentration of $CaCl_2$ solution in the range between 3 and 5 mM. All particles were characterized in terms of mean size, surface charge and their distribution. Particles that show the best ratio of distribution and particle size were chosen for making encapsulates. The influence of variation in vitamin B12 concentration was examined by preparing 10, 20 and 40 μg/ml concentrated solutions. Encapsulates were also characterized in terms of mean particle size, their distribution, surface charge, and morphologically using TEM analysis. The release of vitamin B12 was successfully reproduced in simulated gastrointestinal conditions, which demonstrates the potential application of RuBisCO as media for the encapsulation of important nutrients.

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CB PP 08

DNA/BSA interactions of zinc(II) complex with prodigiosin, a bacterial pigment from *Serratia marcescens*

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Microorganisms, such as *Serratia marcescens* and *Streptomyces*, represent a source for various compounds endowed with significant biological activities. For instance, these bacteria produce a red biopigment prodigiosin (PG), which has shown remarkable antibacterial and antitumor activities.[1] Considering this and the fact that metal complexes with biologically active ligands could overcome the shortcomings of the clinically used organic-based drugs, we have synthesized the zinc(II) complex with this bacterial pigment (ZnPG). The structure of ZnPG was determined previously by single-crystal X-ray diffraction.[2] In the present study, we investigated the interactions of ZnPG with calf thymus DNA (ct-DNA) and bovine serum albumin (BSA) by fluorescence emission spectroscopy to clarify its binding affinities toward the investigated biologically relevant molecules.

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CB PP 09

Characterization of exo- and endopolysaccharides isolated from two strains of *S. commune* Fr. 1815

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The ability of filamentous fungi to synthesize various metabolites with great socio-economic importance makes them crucial for biotechnological processes. An example is the cosmopolitan species *Schizophyllum commune*, which synthesizes various metabolites, among which polysaccharide (PSH) schizophyllan is the most important. Moreover, submerged cultivation enables the isolation of exopolysaccharides (EXP) from extracellular medium and endopolysaccharides (ENP) from mycelium, which exhibit different properties depending on the structure[1].

Accordingly, the aim of this study was to examine the difference between the structure and conformation of EXP and ENP in two *S. commune* strains, originating from Serbia (SRB) and Italy (IT). The submerged cultivation lasted for 14 days, while samples were analyzed using FTIR spectrum, Scanning Electronic Microscopy (SEM), Congo red and Bradford test.

The FTIR spectra of analyzed EXP and ENP were very similar and showed the presence of impurities, i.e., aromatic compounds and proteins. SEM analysis revealed a smooth surface with a mesh structure containing irregular ruptures in both strains. The results of the Congo red test of PSHs from ITA strain showed that triple helical conformation has been lost, since the value of λ max increased to 485 nm at 0.4 mg/mL concentration of NaOH solution, after which there was a decrease and flattening of the absorbance curve regardless of the increase in NaOH conc. The opposite situation was observed with the analyzed PSHs of the SRB strain, whereas these PSHs are heteropolysaccharides that exist as free chains. In addition, higher porosity was observed in the SRB strain and the results of the Bradford test proved the presence of the protein, indicating that PSHs from SRB are indeed heteropolysaccharides.

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CB PP 10

The effect of Zn on schizophyllan production under submerged cultivation of two *S. commune* Fr. 1815 strains

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Schizophyllan (SP) represents an extracellular polysaccharide composed of glucose monomers with a β-1,3-linked backbone and single β-1,6-linked glucose side chains at every third residue. SP is produced by *Schizophyllum commune*, a white-rot filamentous fungi that uses an array of carbohydrates (CH) and soluble starches in the fermentation process [1].

The aim of this study was to examine the effect of Zn bioaccumulation on production of SP in two *S. commune* strains, originated from Serbia (SRB) and Italy (IT). The submerged cultivation of control (C-without Zn) and test samples (S- with addition of 2.8g/L Zn) lasted for 28 days while every 3 days the total CH content was measured using the PSA method, and the filtrate (F) was analyzed using FTIR spectrum. In both strains, a steady trend was maintained in S and C for 12 days, when CHs conc. increased sharply, followed by a slight downward trend until the end of cultivation in IT strain. This indicates that the IT strain entered the *log* phase faster, opposite to SRB where glucose conc. and yield of F was maintained until the end. The highest glucose conc was observed halfway through the cultivation period (14 days), with higher abundance in SRB, compared to IT strain. Moreover, in the SRB strain a positive effect of Zn bioaccumulation was observed after 12 and 21 days. The obtained results are in accordance with the FTIR spectra, where the most dominant content of CH components (α and β glucans) was observed after 14 days.

In summary, in the SRB strain Zn enrichment enabled prolongation of the *log* phase, in contrast to the IT strain, where Zn had no significant effect on the production of SP. This indicates that in addition to external factors, strain specificity plays a major role in the production of SP.

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CB PP 11

The effect of spermidine dietary supplementation on antioxidative protection in honey bee (*Apis mellifera* L.)

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Oxidative stress is caused by a mismatch between the systemic production of reactive oxygen species (ROS) and the organism's ability to eliminate them and the damage they cause. ROS can induce oxidative stress by damaging essential macromolecules, however, this can be prevented by the organism's ability to neutralize existing ROS using antioxidants such as superoxide dismutase (SOD) and catalase (CAT) which act directly on ROS to prevent oxidative damage [1]. Polyamines are polycations found in all living organisms that have various roles in cells. Spermidine is the most studied polyamine and previous research shows that adding spermidine to food or water can reduce oxidative damage and increase hydrogen peroxide resistance [2]. In this study, we examined how exogenously added spermidine affects the activity and gene expression of two antioxidants, SOD and CAT, in honey bee abdomen and head. Three experimental groups were formed: control (C), and two treatment groups $S_{0.1}$ and S_1 named after the used spermidine concentrations (0.1 mM and 1 mM, respectively). The results showed that in the abdomen CAT activity was significantly decreased in the $S_{0.1}$ group, while it was increased in the S_1 group. In the head, there was a significant increase in SOD and CAT activity in both groups. In addition, in the abdomen, *Sod2* and *Cat* gene expression were significantly upregulated, while there were no changes in gene expression in the head. These results are consistent with previous research, however, further examination is needed to understand the metabolic pathway underlying spermidine activity.

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CB PP 12

Investigating the impact of ionic liquid cosolvents on Rh(III) complexes' interactions with 5'-GMP and CT-DNA.

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Although only a limited number of transition metal complexes, such as cisplatin, are presently utilized in cancer treatment and diagnosis because of the toxic effects, poor solubility, and resistance development, there is excellent potential in complexes containing metals such as rhodium, osmium and ruthenium. [1] Rhodium complexes, once considered unattractive for anticancer research, have become one of the most promising potential anticancer agents due to their inertness. This allows for complex designs targeting specific molecules such as DNA or proteins, making them adaptable and effective in fighting cancer. One major issue with using these complexes for therapy is their limited solubility. Thankfully, there is a potential solution: cosolvents like ionic liquids (IL). These solvents are made entirely of ions and have lower melting points, making them less harmful than traditional organic solvents and better for the environment. Plus, since they are based on ions, they can be adjusted to be non-toxic and safe for use in the human body. [2]

The impact of biocompatible ILs as cosolvents was studied on the interaction of the rhodium(III) complexes with the 5-GMP and the DNA molecule. Interactions were studied using UV-Vis, fluorescent spectroscopy, and viscosity measurements. Obtained results show that the examined ILs exhibit good potential as cosolvents for the examined Rh(III) complexes and indicate a possibility of symbiotic effect.

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CB PP 13

Quantum-chemical, structural, and radical scavenging potency investigation of isoproterenol

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Isoproterenol (ISO) is a non-selective β adrenoceptor agonist and analog of neurotransmitters, norepinephrine and epinephrine. It belongs to the group of catecholamines with an aliphatic chain containing isopropyl moiety attached to the secondary amino group. When bound to the receptors, it mimics the effects of neurotransmitters. In this contribution, the crystalographic structure [1] was optimized by several functionals (B3LYP, CAM-B3LYP, B3PW91, M06-2X, and M05-2X) in conjunction with 6-311++G(d,p) basis set. Upon comparison of experimental and theoretical bond lengths and angles, the M06-2X/6-311++G(d,p) level of theory was selected as appropriate for the optimization. The calculated vibrational wavenumbers were compared to the experimental ones, and it was concluded that the most intense bands were well reproduced. The highest discrepancy was observed for the groups that could form intermolecular hydrogen bonds (OH and secondary amino). The differences between observed and calculated wavenumbers were explained by the physical state of the sample and the formation of interactions. The most intense electronic transition was located at 279 nm in the theoretical spectrum. This value was almost identical to the experimental one at 280 nm, proving that the optimized structure represented well the experimentally examined structure in solution. This transition was assigned as HOMO→LUMO. The radical scavenging potency of ISO was assessed by the spectrophotometric DPPH test. The reduction of radicals was concentration-dependent. The IC_{50} value was determined to be 13 µM, comparable to dopamine, norepinephrine, and epinephrine [2]. This result proved that the ending groups of the aliphatic chain do not contribute to the radical scavenging potency and that the catechol moiety was responsible for the delocalization upon reduction of radicals. Further studies are recommended to investigate the effect of ending groups on antioxidant activity and protein binding affinity.

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CB PP 14

Investigation of pH dependent Fe^{3+} - levofloxacin interactions in water by fluorescence spectroscopy

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Interactions of antibiotics with biometals can affect their antimicrobial activity by changing their bioavailability, redox properties, and stability toward hydrolysis. [1,2] The pH of biological fluids can significantly affect interactions between biometals and ionizable drugs. In this study, we investigated the interactions of Fe^{3+} with levofloxacin in water at different pH using fluorescence spectroscopy. The coordination of Fe^{3+} with levofloxacin is pH dependent due to the ionization of levofloxacin and solubility of $Fe^{3+}_{(aq)}$ ions. The formation of levofloxacin-Fe^{3+} complex was detected in the pH range 4–5 as a decrease in fluorescence intensity of levofloxacin. The Stern-Volmer diagrams of levofloxacin in the presence of different concentrations of Fe^{3+} ion at pH 4 and pH 5 correspond to the static fluorescence quenching confirming the coordination of levofloxacin with high-spin Fe^{3+}. At $pH < 4$ and $pH > 5$ the addition of $FeCl_3$ as a source of Fe^{3+} ions results in an increase in fluorescence intensity which can be attributed to the change of the ionic strength of solution and electrostatic interactions between different ionic species instead of coordination of Fe^{3+} ions with levofloxacin. The coordination of Fe^{3+} with levofloxacin at $pH < 4$ is prevented by protonation of its carboxyl and piperazinyl groups ($pKa_1 = 6.02$, $pKa_2 = 8.15$). At $pH > 5$, despite the presence of zwitterionic and anionic forms of levofloxacin available for coordination, there is no complex formation due to the precipitation of insoluble ferric hydroxide.

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CB PP 15

Antioxidant Potential of Liposome-Encapsulated Grape Skin Extracts from Serbian Indigenous Varieties: EPR Analysis Insights

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Since ancient times, grapes have been recognized as potent healing, prophylactic, and rejuvenating fruits. During the winemaking process, pressed marcs (stem, seed, and skin) are discarded as waste, causing pollution of the soil and surface waters. The untapped industrial potential of this waste lies in the fact that it is rich in numerous polyphenolics and other valuable compounds that have yet to be fully utilized. One of the potential applications of grape skins contributing to the circular economy is the encapsulation of their extracts into liposomes. These nanocarriers could then be used to treat various skin conditions caused by free radicals and oxidative stress.

Herein, using electron paramagnetic resonance (EPR) spectroscopy, the antiradical activity of the hydroethanolic extracts of grape skins from two common Serbian wine grape varieties (Prokupac and Morava) was studied toward hydroxyl and 1,1-diphenyl-2-picrylhydrazine (DPPH) radicals. The grape skin samples were collected upon pressing the grapes. They were dried in the dehydrator and pulverized. The extraction of biologically active compounds was performed in 50% EtOH for 3 hours at 40 °C. The obtained extracts were included in liposomes made of DPPC using thin film hydration and extrusion methods. Extracts were subjected to antiradical activity assessment by means of previously developed methods, showing significant antiradical activity towards $^{\bullet}$OH and $^{\bullet}$DPPH radicals, even upon incorporation into the liposomes. Prokupac extracts showed somewhat higher antiradical potential compared to Morava extracts, which was expected, knowing that red grape varieties (Prokupac) have a higher content of polyphenolics compared to white varieties (Morava). Our results indicate that grape skins should be repurposed by means of producing bioactive liposomes, which have great potential as food supplements and in the cosmetic industry. This aligns with the United Nations Agenda 2030 for sustainable development and the principles of a circular economy. These findings could also contribute to the global promotion of Serbian indigenous grape varieties.

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CB PP 16

Synthesis and biological potential of (+)-cleistanolate

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Natural (−)-cleistanolate (Figure 1.) was isolated from the methanol extract of the leaves of *Cleistochlamys kirkii* in 2017. [1] The first total synthesis of natural product and preliminary cytotoxicity is published in 2022. [2] Herein, we present the modified synthesis of (+)-cleistanolate (Figure 1.) and its cytotoxicity. The influence of functional groups as well as stereochemistry on antiproliferative activity will be discussed in detail.

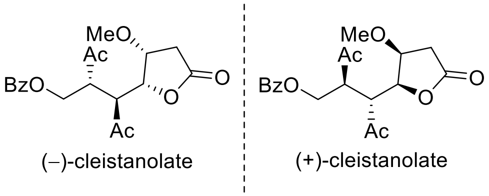

Figure 1. Structures of (−)- and (+)-cleistanolate.

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CB PP 17

Influence of Zr ion on inhibitory potency of Keggin type POMs toward acetylcholinesterase

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Alzheimer's disease (AD) is a progressive neurodegenerative disorder that is characterized by low levels of acetylcholine ACh, β-amyloid aggregation, tau-protein hyperphosphorylation, and oxidative stress. Nowadays, the application of acetylcholinesterase (AChE) inhibitors seems to be the most helpful way to restore the ACh level. [1] Polyoxometalates (POMs) represent an important class of inorganic coordination compounds that have shown significant biological activity. [2] In this study, we investigated the influence of the introduction of metal ions into the structure of POM on its inhibitory activity toward AChE. Keggin-type POM1 ($Na_9[A\text{-}\alpha\text{-}PW_9O_{34}]16H_2O$), and its cluster with Zr ion POM2 ($(Et_2NH_2)_{10}[Zr(PW_{11}O_{39})_2]7H_2O$) were chosen. POM1 is a tri-lacunary Keggin with a -9 net charge, while POM2 has a -10 net charge. Additionally, POM2's Keggin units are bridged with one Zr ion. POM1 has an IC_{50} value of 1×10^{-5}M, while POM with Zr ion shows higher inhibitory activity with an IC_{50} value in the nanomolar concentration range, 5×10^{-8}M. The inhibitory potency of the selected compounds toward this enzyme could be related to POM's high negative charge. Nucleophilic oxygen-enriched surfaces can interact with various positively charged parts of the enzyme, pointing out electrostatic interactions. On the other hand, better POM2 inhibitory potency could be associated with Zr ion presence. Based on the obtained results, it can be concluded that the charge of the selected POMs plays an important role in enzyme inhibition. The interaction between POM and enzyme is electrostatic in nature. The Zr ion introduction in the POM structure increases its inhibitory potency toward the AChE enzyme. Therefore, the performed enzyme assay indicated that selected POMs could represent the basis for the synthesis of new potential drugs against AD.

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CB PP 18

Synthesis and antiproliferative activity new analogues of (+)-protulactone A

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(+)-Protulactone A (**I**) is a natural lactone polyketide that was isolated from a marine fungus *Aspergillus sp. SF-5044*, which showed *in vitro* antiproliferative activity toward several human tumour cell lines (*Figure 1*). [1,2] In this work we present the synthesis of new analogs **1** and **2** that have a phenyl group instead of a methyl group in the C-7 position (*Figure 1*). Also, these compounds lack an acetoxy group at the C-7 position. The *in vitro* antiproliferative activities of synthesized analogues will be briefly discussed. This could provide information about the influence of isosteric replacement CH_3→Ph at C-7 on the cytotoxic activities of these types of molecules.

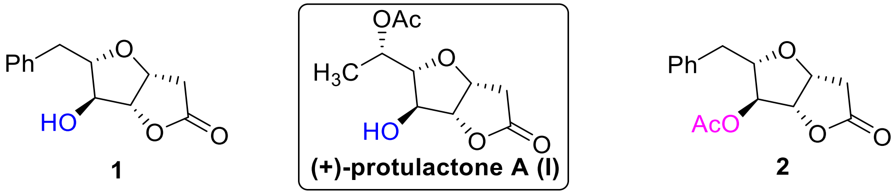

*Figure 1. Structures of (+)-protulactone A (**I**) and its simplified analogues **1** and **2**.*

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CB PP 19

Identification of the new candidate NLRP3 inhibitor using combined computational approach

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The NOD-like receptor pyrin domain-containing protein 3 (NLRP3), an important intracellular sensor in the innate immune system, detects a plethora of exogenous and endogenous stimuli, leading to inflammasome formation and caspase-1 activation. More recently, it emerged as an attractive drug target due to abnormal NLRP3 inflammasome activation implicated in many acute and chronic diseases (including diabetes, atherosclerosis, metabolic syndrome, cardiovascular, and neurodegenerative diseases) [1]. Several direct NLRP3 inhibitors that block its ATPase activity by keeping it in closed conformation have been reported [1,2]. Some of them have entered clinical trials, but still, none of them is FDA approved.

A powerful strategy in identifying potential NLRP3 inhibitors can be *in silico* drug repurposing of compounds with already known safety profiles. In this study, we performed a virtual screening protocol that considers both long- and short-range interactions between molecules. First, the Informational spectrum method developed for small molecules was applied for searching the Drugbank database. Selected candidates were filtered by successive cross-correlation spectra analysis. Finally, after molecular docking, we identified the most promising candidate and proposed it for further experimental testing.

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CB PP 20

Application of chromatography in the assessment derivates' lipophilicity

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Isatins are an important class of heterocyclic compounds with a wide range of applications in organic synthesis, medicine and pharmacology [1]. Bearing in mind that the first step in assessing the existence of biological activity of a new compound involves determining its lipophilicity, for newly synthesized isatin derivatives, this important physico-chemical parameter was determined by software and experimentally [2]. By applying reversed-phase thin-layer chromatography, RPTLC C18/UV254s, in the mixtures of water-ethanol and water-dioxan important parameters were obtained. It was found that the chromatographic behavior of isatin is determined to a greater extent by the nature of the substituent present on the benzene ring than by the applied organic modifier. The chromatographically obtained parameters (R_M^0, m and C_0) were correlated with the software-derived values of the standard measure of lipophilicity ($\log P$), as well as with the selected ecotoxicity parameter by applying linear regression analysis. The obtained mathematical models indicate the reliable application of the chromatographic parameters, R_M^0, m and C_0 in the assessment of the studied isatine derivatives' lipophilicity and ecotoxicity.

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CB PP 21

Antibiofilm potential of the monoterpenes carvacrol and geraniol against oral pathogens

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Caries, a highly prevalent infectious disease, affects over 90% of the global population.[1] The biofilm, formed by bacteria in the mouth, plays a critical role in the demineralization of tooth enamel, which can lead to the development of caries.[2] The initiation of dental biofilm formation, involving the colonization of oral pathogens, is primarily attributed to *Streptococcus* genus bacteria. Our research aimed to assess the antibiofilm potential of monoterpenes, specifically carvacrol and geraniol, against relevant tooth caries-associated isolates, including *Streptococcus mutans, Streptococcus sanguinis, Streptococcus mitis,* and *Streptococcus gordonii*. These two monoterpenes are known for their robust antimicrobial attributes, especially carvacrol which has been explored for its efficacy against selected oral pathogens. [2]

Our study evaluated the capacity of these agents to disrupt the pre-formed biofilm and prevent its formation. Initially, monospecies biofilms were cultivated using each target bacterium and subsequently subjected to treatment with the tested monoterpenes. In another set of experiments, biofilms were cultured in the presence of the monoterpenes, with the aim of assessing their potential to prevent the formation of biofilms. The viability of these biofilms was quantified by measuring total biomass using crystal violet assay, following the method outlined by Stepanović et al. (2000).

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Acknowledgment

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CB PP 22

QSAR analysis of anticancer activity of *O*-alkylated androstane 3-oximes towards acute leukemia cells

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The new series of *O*-alkylated androstane 3-oxime derivatives has been synthesized and their cytotoxic activity towards acute leukemia cell line (CEM) was evaluated [1]. In the present study, the quantitative structure-activity relationship (QSAR) analysis of the aforementioned compounds was carried out based on the multiple linear regression (MLR) approach. The obtained MLR-QSAR model correlates the solvent accessible surface area of all hydrophobic atoms (ASAH) and length perpendicular to the max area (LPmaxA) descriptors with $–\log IC_{50}$ values of cytotoxic activity. The obtained model has very good predictive performance as it was confirmed by cross-validation and by the comparison of the experimental and predicted data (Fig. 1). The calculated statistical parameters (R^2=0.8254, R^2_{adj}=0.8021, R^2_{CV}=0.7676) confirm the statistical quality of the model and qualify it for the practical application in prediction of the cytotoxic activity of new androstane *O*-alkylated androstane 3-oximes.

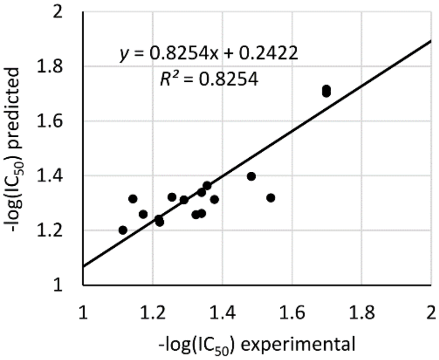

Figure 1. The relationship between the experimental and predicted data

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CB PP 23

Synthesis, antiproliferative activity, ADME-Tox and SAR analysis of novel (–) goniofufurone analogue

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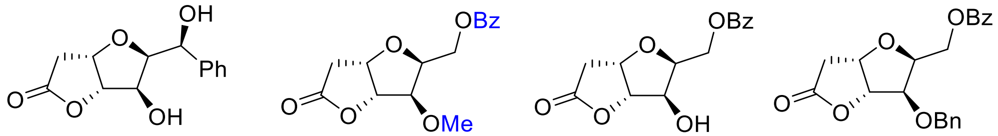
(–)-Goniofufurone (**1**) is an opposite enantiomer of natural product (+)-goniofufurone and both compounds show good cytotoxic activity in vitro. [1]

Novel benzoilated (–)-goniofufurone analogue **2** (*Figure 1*), bearing a methoxy group at the C-5 position, was prepared from L-xylose. Target **2** was evaluated for its *in vitro* cytotoxicity against a number of tumour cell lines, as well as against normal foetal lung fibroblasts. Structure-activity relationship (SAR) of **1**, **2** and two analogues previously synthesized in our laboratory (**3** and **4**), as well as ADME-Tox-based analysis, will be presented in detail.



(–)-Goniofufurone (**1**) **2** **3** **4**

*Figure 1. Structures of (–)-goniofufurone **1**, novel analogue **2** and previously synthesized analogues **3** and **4**.*

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CB PP 24

Small Molecules, Big Dreams: In Search of Multi-Target Directed Ligands for the Treatment of Alzheimer's Disease

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Alzheimer's disease (AD) is the leading cause of dementia in the world, predominantly affecting the population over 65 years old. Global dementia cases are predicted to triple by 2050 as the world's population grows and life-span increases.[1] For this reason, significant efforts have been made in the scientific community aimed at finding an effective cure for the disease. AD is a multifactorial disease characterized by various hallmarks such as a deficiency of the neurotransmitter acetylcholine caused by a loss of cholinergic neurons, deposition of amyloid-β plaques and hyperphosphorylated neurofibrillary tangles in the brain, and biometal dishomeostasis.[2] In our research, we focus on the *in vitro* investigation of small organic molecules to act as multi-target directed ligands, simultaneously acting as inhibitors of cholinesterases that hydrolyze acetylcholine and β-secretase whose activity is necessary for the formation of amyloid plaques, as well as evaluate their ability to chelate biometals and cross the blood-brain barrier. Here, our work will be presented on the example of 4-aminoquinoline derivatives with an *n*-octylamino spacer.

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CB PP 25

The antimicrobial potential of newly synthesized ionic liquids based on tetrabutylphosphonium ion

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The importance of developing effective antimicrobial agents has become more evident in recent times, and quaternary phosphonium-based ionic liquids have shown great potential in this regard [1]. The main focus is to evaluate the synergistic antimicrobial effects between this cation and different selected anions and to determine whether there is an increase in antimicrobial activity as compared to the pure components. The three ionic liquids used for this study are tetrabutylphosphonium nicotinate, tetrabutylphosphonium hexanoate and tetrabutylphosphonium octanoate (Fig. 1).

The antimicrobial activity against various microorganisms including *Escherichia coli, Pseudomonas aeruginosa, Proteus mirabilis, Klebsiella pneumoniae, Micrococcus luteus, Staphylococcus aureus, Staphylococcus epidermidis, Candida albicans, Candida guillermondii, Penicillium verrucosum, Penicillium chrisogenum, Aspergillus flavus* and *Aspergillus niger* was determined. Based on the obtained results, the structure-property relationships of these compounds, including how the type of anions (aromatic or aliphatic) and their hydrophobicity influence the quaternary phosphonium-based ionic liquid's antimicrobial properties will be highlighted. Selected ionic liquids are effective and in most cases improved antimicrobial agents compared to pure components.

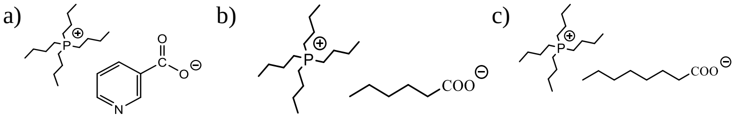

Figure 1. Structures of a) tetrabutylphosphonium nicotinate, b) tetrabutylphosphonium hexanoate and c) tetrabutylphosphonium octanoate

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CB PP 26

Production of pectinolytic complex from *Aspergillus tubingensis* and its application in fruit juice processing

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Pectinases are widely used in the fruit juice industry to clarify, liquefy, and stabilize juices. Primarily, these enzymes are responsible for the degradation of long and complex molecules in the fruit pulp (pectin) [1]. The addition of pectinase reduces the viscosity of the fruit juice and makes the fruit juice easily extractable with a higher yield and clarification [2].

In this study, a pectinolytic complex was produced by solid-state fermentation on agroindustrial wastes (such as sugar beet pulp and wheat bran) from *Aspergillus tubingensis*, a new strain isolated from quince. We applied an Optimal (Custom) Design to achieve maximum enzyme production. Total pectinase activity was determined by the dinitrosalicylic acid (DNS) method. The obtained pectinolytic complex was used to liquefy and clarify fruit juices such as apples, apricots, bananas, oranges and quince. The results show that this pectinolytic complex from *A. tubingensis* can be successfully used in the juice industry.

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CB PP 27

In silico study of chosen lignans of *Anthriscus sylvestris* on the αβ-tubulin

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Anthriscus syvestris is a plant rich in secondary metabolites such as lignans, especially aryltetralines and dibenzylbutirolactones. The importance of lignans lies in their various biological activities, including antitumor activity [1]. *In silico* studies are the first step towards knowledge of the mechanisms of antitumor activity. One of the most commonly used antitumor targets is αβ-tubulin. It is well-known that podophyllotoxin binds to the colchicine-binding site (CBS) of αβ-tubulin. Therefore, it has been assumed that other studied, structurally similar lignans also bind there. The binding of the compound in the CBS prevents the polymerization of microtubules, preventing the cell from producing the mitotic spindle and dividing, leading the cell into apoptosis [2].

In this study, the molecular docking of chosen lignans was done on the heterodimeric αβ-tubulin. In addition to the *in silico* method, the modified *in vitro* cytotoxicity SRB (Sulforhodamine B) assay on three cancer cell lines (HeLa, HT29 MCF-7) and a healthy MCR-5 cell line, has also been performed. The combination of both approaches was used to establish a structure-activity relationship (SAR), which gives us a more detailed explanation of the antitumor activity, which can result in the discovery of new potential and effective ‘lead compounds’ for drug design.

The IC_{50} values for cytotoxicity of the studied lignans ranged from below 0.001 ug/mL (deoxypodophyllotoxin and podophyllotoxin) to above 10 ug/mL. All studied lignans bind to the CBS with a binding affinity from −7.5 kcal/mol to −10.3 kcal/mol. The interactions formed between tubulin amino-acid residues and studied ligands were mainly hydrophobic interactions (π-π, π-alkyl, π-sulfur, carbon-hydrogen bond, van der Waals forces) and electrostatic interactions, with a scarce hydrogen bond.

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CB PP 28

Script to help with docking automation

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We present a novel and modular 3-part wrapper shell script (*run_all.sh*) that automatizes docking protocol (Fig. 1). First, *run_all.sh* calls *process_ligands.sh* that performs the docking with all ligands and receptors present in the working folder, with the output files properly and conveniently named. Next, *run_all.sh* calls *extr_conf.sh* extracts all the conformations (*models*) from the output PDBQT files into separate PDBQT files. Finally, *run_all.sh* calls *merge_log_2.sh* joins all the output TXT files into one properly formatted CSV document ready to be used for sorting and assaying the docking results. The script works in Cygwin and uses AutoDock Vina as a docking tool.[1]

Figure 1. The script overview.

By automating the entire docking procedure, our modular script could enhance data management efficiency during screening, as well as enable the researchers to more efficiently explore novel protein-ligand interactions.

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CB PP 29

The investigation of chitin influence in laser-induced deformation of butterfly wings

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[4] *University of Belgrade - Institute of Chemistry, Technology and Metallurgy, National Institute of the Republic of Serbia, Belgrade, Serbia*

The investigation of laser beam irradiation on different types of butterfly wings has been done previously by using the holographic method [1]. The deformations due to the use of different laser wavelengths were observed [2]. It is well-known that chitin is an abundant component of many complex structures in biological samples, such as butterfly wings. Consequently, as the influence of the chemical structure was taken into account, it was decided to examine the influence of chitin itself in laser-induced deformation in biological samples. Therefore, in this work, the same tests were performed on the film generated from chitin by using different wavelengths of laser. The results obtained strongly suggest that there are no effects of laser beam irradiation on chitin, indicating that chitin itself does not have an influence on the observed deformation of the butterfly wings.

It was decided to make some additional measurements of such wings, which would be important for the further course of research in this direction. Some useful graphs were obtained by X-ray diffraction (XRD) and Fourier-Transform Infrared Spectroscopy (FTIR) measurements of particular butterfly wings. The obtained results contribute to a better knowledge of the structure and morphology and may have applications in the industry of artificial materials, especially polymers [2].

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CB PP 30

Antimicrobial activity of fatty acid-based ionic liquids

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The efficacy of many antibiotics has been decreasing at a concerning rate, due to misuse and overuse during the last century. Therefore, the need for novel antimicrobial agents has become apparent. Quaternary phosphonium-based ionic liquids have shown great potential in this regard [1]. The main focus of this study was to evaluate the effect of medium-chain fatty acids (MCFA) when used as anion components in tetrabutylphosphonium ionic liquids on antimicrobial activity. The two ionic liquids used for this study are tetrabutylphosphonium decanoate and tetrabutylphosphonium dodecanoate (Fig. 1).

The antimicrobial activity against 7 bacterial (*Escherichia coli, Pseudomonas aeruginosa, Proteus mirabilis, Klebsiella pneumoniae, Micrococcus luteus, Staphylococcus aureus, Staphylococcus epidermidis*), 2 yeast (*Candida albicans, Candida* guillermondii) and 4 mold strains (Penicillium *verrucosum, Penicillium chrisogenum, Aspergillus flavus* and *Aspergillus niger*) were determined using *in vitro* broth microdilution method. Based on the obtained results, the relationship between the complexity and structure of the cell walls of included microorganisms and the antimicrobial effect of ionic liquids will be highlighted. Selected ionic liquids are effective and in most cases improved antimicrobial agents compared to pure components.

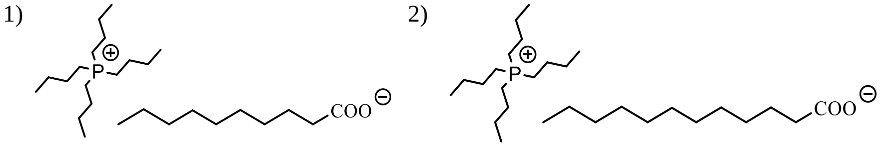

Figure 1. Structures of 1) tetrabutylphosphonium decanoate and 2) tetrabutylphosphonium dodecanoate

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Developments in chemical synthesis

DCS PP 01

Evaluation of the binding affinity of steroid thiazole derivatives for selected steroid receptor isoforms

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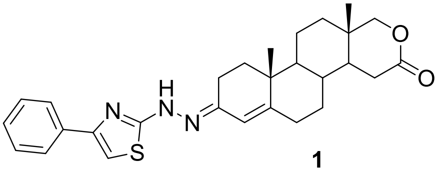
Steroid molecules are pharmacologically potent agents associated with a set of physiological functions. They are important bioactive agents, and their interaction with numerous nuclear receptors is often used in drug design, especially in diseases mediated by impaired expression and function of steroid receptors. In this work thiazole androstane derivatives in 17a-h-omo lactone series were tested in order to evaluate their relative binding affinity for the ligand-binding domain (LBD) of estrogen receptor α (ERα), estrogen receptor β (ERβ) or androgen receptor (AR), using a fluorescent cell assay in yeast. [1,2] Further, *in silico* testing of their physicochemical properties and evaluation of their pharmacokinetics and toxicity (ADMET) were conducted. Compound **2** stood out for its high binding affinity to ERα-LBD, similar to the natural ligand, estrone.



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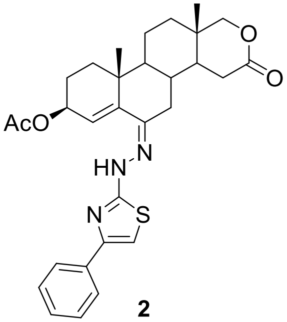

2

Figure 1. Structures of thiazole compounds

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DCS PP 02

Synthesis and characterization of the first Co(II) complex with 2,6-diacetylpyridine-adamantane-1-carbohydrazide Schiff base

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The Schiff bases of 2,6-diacetylpyridine are an interesting topic of research due to the different modes of coordination they adopt. This is also confirmed by the search of the Cambridge Structural Database, which contains structures of over 2500 of these Schiff bases and their complex compounds. Among them, there are 84 Co(II) complexes with Schiff bases of 2,6-diacetylpyridine and some hydrazine bases. This work describes the synthesis and structural characterization of a new Co(II) complex with this type of Schiff base.

In the reaction of a warm acetronitrile suspension of the ligand 2,6-diacetylpyridine-adamantane-1-carbohydrazide – $(Ad)_2dap$, and a warm acetone solution of cobalt(II) chloride, in a molar ratio 1:2, green crystals of a new complex compound of the formula $[Co(Ad)_2dap][CoCl_4]\cdot CH_3CN$ were obtained. The coordination is primarily assumed by the comparison of IR spectrum of the complex with the spectrum of the ligand. The obtained crystals melt at a temperature higher than 250 °C, and the molar conductivity value ($\square_M$=75.86 S cm^2 mol^{-1} – in DMF) indicates that the obtained complex is a 1:1 type electrolyte.

The ligand is coordinated to the central Co(II) atom in its neutral form as N_3O_2 pentadentate, forming four five-membered metallocycles (Fig. 1). Cobalt(II) is placed in a pentagonal bipyramidal environment, where the donor atoms of the chelating ligand (one pyridine nitrogen, two azomethine nitrogens and two carbonyl oxygens) are at the base of this polyhedron, and acetonitrile nitrogen atoms are in axial positions.

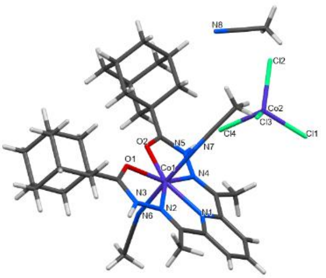

Figure 1. The coordination polyhedron of $[Co(Ad)_2dap][CoCl_4]\cdot CH_3CN$

DCS PP 03

Ru(II)-1-napthylhydrazine complex: synthesis and interaction with human serum albumin

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[2] *University of Applied Sciences Merseburg, Merseburg, Germany*

Ruthenium(II) complexes have shown the ability to interact with biomolecules, particularly nucleic acids, affecting the growth and survival of cancer cells, highlighting their potential as potent anticancer agents [1]. This study focuses on the characterization of a newly synthesized ruthenium(II)-1-napthylhydrazine complex and its binding to human serum albumin (HSA). The complex was synthesized using ruthenium salt, dichloro(*p*-cymene)ruthenium(II) dimer, and 1-naptylhydrazine hydrochloride as a ligand and its structure was confirmed using theoretical analysis. Theoretical structure optimization revealed a pseudo-octahedral structure of the complex, with key interactions including π(C-C)→π*(C-C) interactions within *p*-cymene and napthylhydrazyl rings, as well as interactions between donor atoms or groups and central metal ion. In order to determine the quenching properties and thermodynamic parameters of binding of the complex with HSA, fluorescence spectroscopy was employed. Spectrofluorimetric analysis confirmed interactions with HSA, leading to the quenching of protein fluorescence. The examination of thermodynamic parameters revealed that binding is spontaneous and exothermic, driven by Van der Waals forces and hydrogen bonds [2]. Competitive binding studies with warfarin and ibuprofen demonstrated that the presence of site-specific markers led to the increase in the binding constant. Further experimental and theoretical studies of this complex are advised.

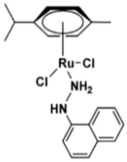

Figure 1. Structure of the newly synthesized Ru(II)-1-naptylhydrazine complex.

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DCS PP 04

Synthesis and structural characterization of gallium(III) complex with (±)-1,3-pentanediamine-*N,N,N’,N’*-tetraacetate

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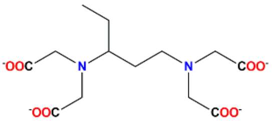
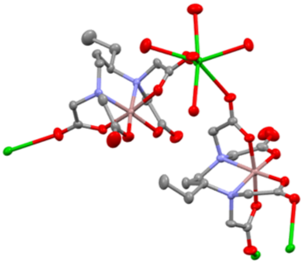
[2]*University of Kragujevac - Institute for Information Technologies Kragujevac, Kragujevac, Serbia*

Diaminopolycarboxylates are well-known chelating agents that can form stable and water soluble complexes with numerous metal ions. [1] This property makes them useful in a wide variety of chemical, medical and environmental applications.[2] Considering this, in the present study, (±)-1,3-pentanediamine-*N,N,N’,N’*-tetraacetate (1,3-pndta) was used as a ligand for the synthesis of a new gallium(III) complex, Ba[Ga(1,3-pndta)]$_2$·3H$_2$O. The characterization of this complex was done by NMR (^{1}H and ^{13}C) and IR spectroscopic methods, while its crystal structure was determined by single-crystal X-ray diffraction analysis. Coordination of 1,3-pndta to Ga(III) ion is achieved through its two nitrogen atoms and four carboxylate oxygen atoms, resulting in a octahedral geometry around the metal ion. The synthesized gallium(III) complex is stable in aqueous solution during 48 h, as revealed by its NMR spectra recorded immediately and 48 h after the dissolution of the complex.



1,3-pndta



Ba[Ga(1,3-pndta)]$_2$·3H$_2$O

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DCS PP 05

Diorganotin(IV) complexes with hydroxamic acids derivatives of some histone deacetylases inhibitors

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Organotin-based complexes exhibit strong antiproliferative activity and reduced toxicity when compared to more extensively studied platinum-based chemotherapeutics. In this study, two novel organotin(IV) complexes were synthesized via the reaction of diphenyltin(IV) dichloride with known physiologically active hydroxamate-based ligands, *N*-hydroxy-4-phenylbutanamide (**HL$_1$**) and *N*-hydroxy-2-propylpentanamide (**HL$_2$**). The anticancer effect of the used ligands is related to the inhibition of histone deacetylase (HDAC), an enzyme crucial for gene expression control [1]. Characterization of obtained complexes was performed by various spectroscopic methods (including IR and ^{1}H, ^{13}C, and ^{119}Sn NMR) and elemental analysis (CHN). The structures were additionally analyzed by quantum-chemical optimizations at B3LYP-D3BJ/6-311++G(d,p)(H,C,N,O)/LanL2DZ(Sn) level of theory. The theoretical IR and NMR spectra of ligands reproduced well the experimental results. The stability of **HL$_1$** and **HL$_2$** isomers was scrutinized using Natural Bond Orbital analysis, emphasizing the importance of intramolecular hydrogen bonds [2]/

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The work was supported by the Ministry of Science, Technological Development and Innovation of Serbia (contract number: 451-03-47/2023-01/200124 and 451-03-47/2023-01/200146). This research is a part of Danijela N. Nikolić's Ph.D. thesis supervised by Prof. Marija S. Genčić.

DCS PP 06

Synthesis and characterization of binuclear azide-bridged hydrazone Cu(II) complex

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The condensation product of 7-acetyl-6-azaindole and Girard's T reagent ((*E*)-2-(2-(1-(1*H*-pyrrolo[2,3-*c*]pyridin-7-yl)ethylidene)hydrazineyl)-*N*,*N*,*N*-trimethyl-2-oxoethan-1-aminium, HL ligand) was used as a ligand in the reaction with $Cu(BF_4)_2{\cdot}6H_2O$ and NaN_3. The reaction led to the formation of a binuclear Cu(II) complex containing two end-to-end (di-$\mu_{1,3}$-N_3) azide bridges, as well as two NNO-donor hydrazone ligands, forming an axially elongated square pyramidal geometry around each Cu(II) center. This end-to-end (di-$\mu_{1,3}$-N_3) azide bridge binding mode has not yet been reported, in Cu(II) complexes containing the NNO-donor hydrazone ligands, which makes the structure of the complex even more interesting for further studies. The complex was characterized by elemental analysis, IR spectroscopy and X-ray crystallography, and it was found that it crystallizes in the triclinic space group P–1 with the asymmetric unit comprising one Cu(II) centre, zwitterionic ligand L, one azide (N_3^-) ligand and BF_4^- counter anion.

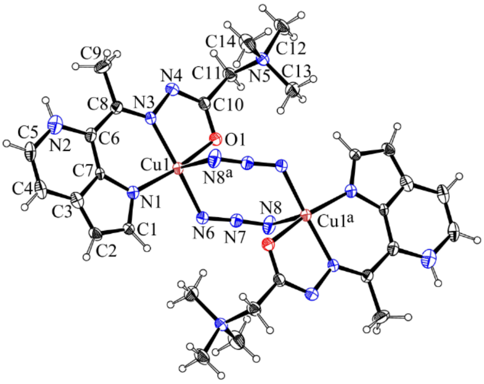

Figure 1. ORTEP presentation of the complex cation $[Cu_2L_2(\mu_{1,3}\text{-}N_3)_2]^{2+}$

Acknowledgments

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DCS PP 07

In vitro antioxidant activity evaluation of selected xanthene derivatives

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Xanthendiones (1,8-dioxooctahydroxanthenes) are a special class of oxygen-incorporating tricyclic compounds bearing as a basic feature a pyran nucleus fused on either side with cyclohex-2-enone rings. They are often found as a structural motif in natural products with a wide range of biological activities, such as: antioxidant, antimicrobial, trypanocidal, antiinflammatory, antiproliferative and anticancer. A convenient and efficient approach toward the synthesis of seven aromatically substituted xanthendiones 1–7 and one structurally-related xanthenone 8 through condensation of dimedone and the appropriate aromatic aldehyde is reported. The relationship between the chemical structure and pharmacological activity was determined empirically using appropriate software packages and *in vitro* using the 2,2'-azinobis-(3-ethylbenzothiazoline-6-sulfonic acid (ABTS) method. The results of the ABTS assay indicate that five compounds possess the ability to scavenge the ABTS•+ radical cation. Based on the comparison of the IC_{50} values, the activity of the compounds was found to be as follows: 6 > 1 > 7 > 2 > 8.

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DCS PP 08

Cyclotrimerization of activated alkynes on solid phase of SiO_2

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Cyclotrimerization of alkynes to generate benzene derivatives is an important reaction in organic chemistry, due to the importance and presence of benzene nuceus in organic systems. Some cyclotrimerization reactions use enaminones, metal or acid catalysis and a solvent. [1,2] We aimed to perform this reaction on solid phase of SiO_2 without solvent. First, we showed that trisubstituted benzene can be obtained in high yield by the reaction of enamino ester **1** with 2 moles of ethyl propiolate at the temperature of 100 °C (Fig. 1).

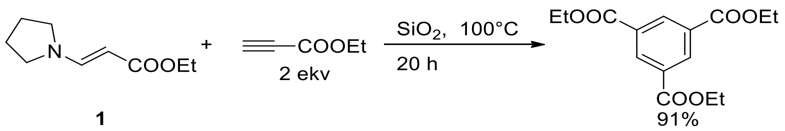

Figure 1: Synthesis of trisubstituted benzene by the reaction of enamino ester with ethyl propiolate.

We then optimized reaction conditions to use catalytic amount of pyrrolidine (Fig. 2). In this preliminary report, the reaction scope was examined by using activated alkynes with ester and keto functional groups and the products were isolated in good to high yields (Fig. 2).

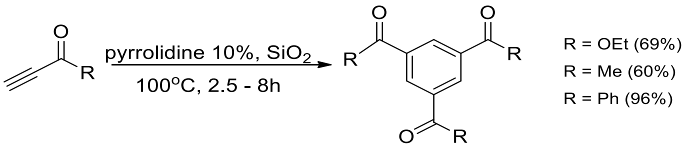

Figure 2: Synthesis of trisubstituted benzenes by cyclotrimerization of activated alkynes.

The performed reactions, having no solvent, metal catalysts and with minimal chemical waste (catalyst only), are in accordance with some of the principles of green organic chemistry.

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DCS PP 09

Synthesis and structural characterization of gold(III) complex with letrozole

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Recently, in our laboratories, new gold(III) complexes of the general formula [$AuCl_3$(azole)], where azole stands for clotrimazole, econazole, tioconazole or voriconazole, have been synthesized, structurally characterized and biologically evaluated [1]. In a continuation of our ongoing research on the biologically active metal complexes of clinically used azoles, in this study we synthesized and structurally characterized gold(III) complex with letrozole, [$AuCl_3$(letrozole)]. The complex was synthesized by reacting K[$AuCl_4$] with an equimolar amount of letrozole in ethanol under reflux for 3 h. The complex was characterized by NMR and IR spectroscopic methods, while its crystal structure was determined by single-crystal X-ray diffraction analysis. The obtained spectroscopic and crystallographic results have shown that letrozole is monodentately coordinated to the Au(III) ion *via* the triazole nitrogen atom, while the remaining coordination sites are occupied by chloride anions leading to a square-planar arrangement.

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DCS PP 10

Synthesis of new androstane carbamate derivatives and their *in silico* ADME/T analysis

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Molecules with the carbamate group have a significant role in medicinal chemistry and chemical synthesis, as this functional group can be found in the structure of many therapeutic agents.[1,2] Because carbamates (urethanes) are defined as hybrids of amide and ester groups, they exhibit exceptional chemical stability.[1] Additionally, they possess the N and O atoms, which allows the forming of hydrogen bonds and other interactions with the target enzymes or receptors. On the other hand, it is widely known that steroid molecules exhibit a variety of biological properties, most notably anticancer activity. Combined with carbamate moiety, steroid compounds could act as steroid receptor antagonists or inhibitors of enzymes responsible for steroidogenesis, which are targets for hormone-sensitive cancers. For that reason, the synthesis of new 3-carbamate steroid derivatives in 17-(pyridin-2-yl)methylandrostane series, as well as their *in silico* pharmacokinetic evaluation, were the aims of this study. All synthesized compounds were found to possess druglike properties according to available online tools (SwissADME and ProTox-II).

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Acknowledgments:

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DCS PP 11

Synthesis and determination of *in vitro* biological activity of novel fulleropyrrolidines containing vanillin subunit

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Due to the presence of a large number of double bonds, fullerene C_{60} shows good antioxidant and moderate anti-inflammatory properties.[1] At the same time, natural product vanillin, thanks to its phenolic subunit expresses the same activities, although in a lesser extent.[2] Willing to obtain novel fulleropyrrolidines with improved biological activity, we explored the synthesis of hybrid structures containing fullerene and vanillin. The Prato reaction of the glycine derivative, vanillin and the fullerene C_{60} provided desired products in satisfactory yields. DPPH radical scavenging activity and *β*–carotene-linoleic acid bleaching assay were used to determine antioxidant activity, while for evaluation of anti-inflammatory activity, ovalbumin (OVA) and bovine serum albumin (BSA) thermal denaturation inhibition assays were used. Obtained fulleropyrrolidines showed significantly better biological activity in comparison with starting compounds.

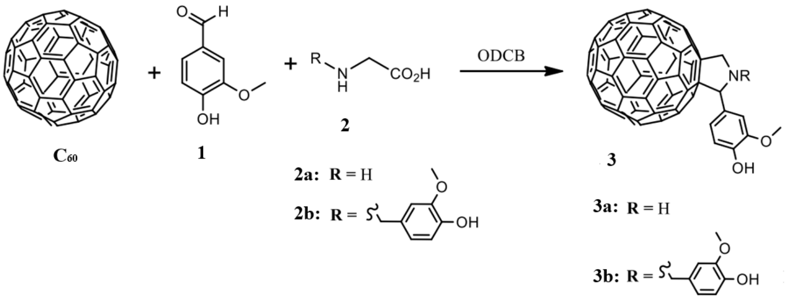

Figure 1. Scheme of synthetic strategy for preparing desired fulleropyrrolidines

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Acknowledgment

This research was supported by the Ministry of Science, Technological Development and Innovation of Republic of Serbia (contracts 451-03-47/2023-01/200168 and 451-03-47/2023-01/200026).

DCS PP 12

Mono- and disubstituted fulleropyrrolidines: synthesis and optimization of reaction conditions

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Fullerene is one of carbon allotropes with extremely low solubility in aqueous solvents and most organic solvents, but high potential of application in various areas, such as medicine, photovoltaics and materials. [1] To overcome this obstacle, fullerene needs to be functionalized. The Prato reaction is decent synthetic method that provides *N*- and *C*-substituted fulleropyrrolidines. We optimized the conditions of the Prato reaction in order to obtain fulleropyrrolidines containing phenol (**3d**) and protected phenol subunits (**3a, 3b**). (Figure 1) The desired products were purified by *dry-flash* chromatography and obtained in satisfactory yields.

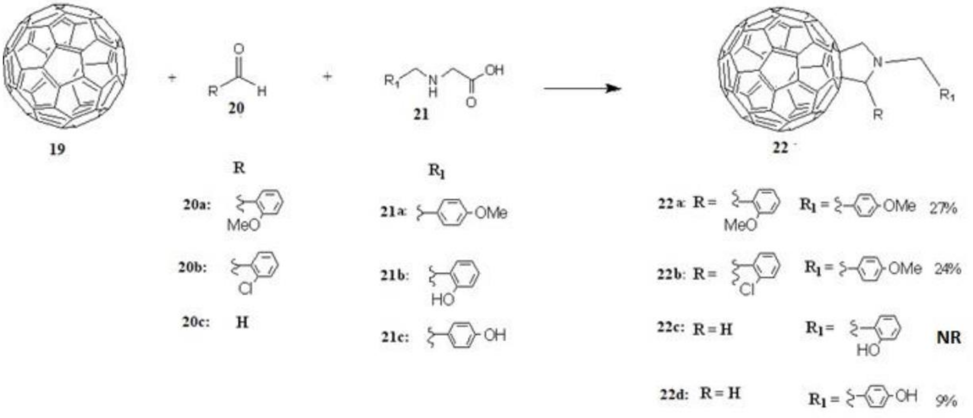

Figure 1. Scheme of synthetic strategy for preparing desired fulleropyrrolidines

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Acknowledgments

This research was supported by the Ministry of Science, Technological Development and Innovation of Republic of Serbia (contracts 451-03-47/2023-01/200168 and 451-03-47/2023-01/200026).

DCS PP 13

Synthesis and determination of *in vitro* biological activity of novel fulleropyrrolidines containing phenol subunit

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Willing to obtain novel fulleropyrrolidines with improved biological activity, we explored the synthesis of hybrid structures containing fullerene and phenol. The Prato reaction of the glycine derivative, aromatic aldehydes with phenol subunit and the fullerene C_{60} provided desired products in satisfactory yields (Figure 1). DPPH radical scavenging activity and *β*–carotene-linoleic acid bleaching assay were used to determinate antioxidant activity, while for evaluation of anti-inflammatory activity, ovalbumin (OVA) and bovine serum albumin (BSA) thermal denaturation inhibition assays were used. Obtained results indicated that performed synthesis gave rise to compounds with dual activity.

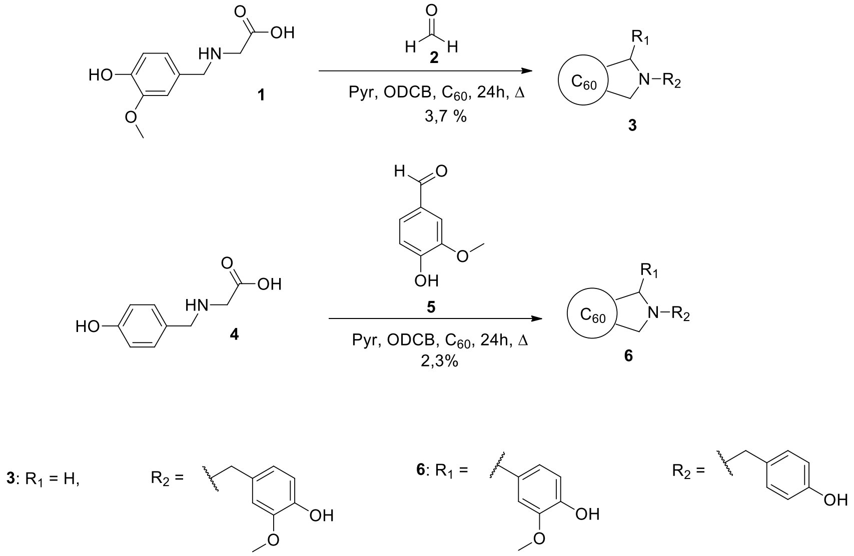

Figure 1. Scheme of synthetic strategy for preparing desired fulleropyrrolidines

Acknowledgments

This research was supported by the Ministry of Science, Technological Development and Innovation of Republic of Serbia (contracts 451-03-47/2023-01/200168 and 451-03-47/2023-01/200026).

DCS PP 14

Synthesis and determination of *in vitro* antioxidant activities of novel fulleropyrrolidines containing aromatic subunit

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Due to the presence of a large number of double bonds, fullerene C_{60} shows good radical scavenging properties.[1] In order to obtain novel fulleropyrrolidine with improved antioxidant activity, we explored the synthesis of a hybrid structure containing fullerene and anisole subunit. The Prato reaction of the *N*-substituted glycine, aromatic aldehyde with anisole subunits and the fullerene C_{60} provided desired products in a satisfactory yield. The obtained compound was added to the series of similar fulleropyrrolidines and subjected to an antioxidant activity test using *β*–carotene-linoleic acid bleaching assay.

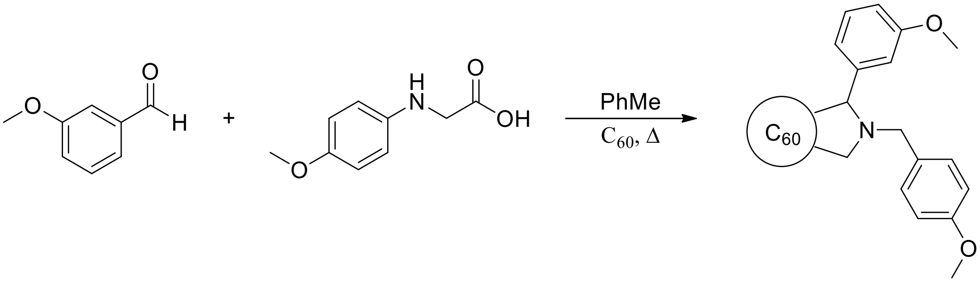

Figure 1. Scheme of synthetic strategy for preparing desired fulleropyrrolidine

References

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DCS PP 15

Tributyltin(IV) compounds with carboxylato *N*-functionalized 2-quinolone ligands: structural characterization and interactions with BSA

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Organotin(IV) derivatives, particularly organotin(IV) carboxylates, have attracted much attention within the last two decades as potential non-platinum chemotherapeutics, showing in many cases even better anticancer activity than the clinically approved drug cisplatin [1]. Although the literature is covered by comprehensive studies about the potential anticancer activity of these compounds, their interactions with biologically active molecules are not significantly studied. In the present study, two novel complexes, (3-(4-methyl-2-oxoquinolinyl-1(2H)-yl)propanoato)tributyltin(IV) (**1**) and (2-(4-methyl-2-oxoquinolin-1(2H)-yl)ethanoato)tributyltin(IV) (**2**), were synthesized and characterized *via* analytical methods. Moreover, the interaction of these compounds with Bovine Serum Albumin (BSA) was evaluated by spectrofluorimetric titration at three temperatures (27, 32, and 37 °C) to determine their binding affinities. Although structurally very similar, these two compounds have shown different BSA binding behavior. The change in enthalpy and entropy of **1** binding to BSA are -262 kJ mol^{-1} and -749 J mol^{-1} K^{-1}, respectively. For the mentioned compound, there is a decrease in the spontaneity of binding with an increase in temperature from -37.3 to -29.8 kJ mol^{-1}. On the other hand, positive change in enthalpy (130 kJ mol^{-1}) and entropy (539 J mol^{-1} K^{-1}) of binding were determined for **2** with the increase in spontaneity of binding with temperature (from -31.2 to -35.6 kJ mol^{-1}). It can be assumed that the entropy factor is crucial for the binding of **2** to BSA. Further molecular docking studies will be performed to explain the difference in binding affinity based on structural differences.

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Environmental awareness

EA PP 01

Alkali-activated wood ash: structural characteristics and adsorption properties

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The aim of this research is to study the possibility of reusing the wood ash to produce the new alkali-activated materials for the removal of cadmium from wastewater. Wood ash was mixed with an alkali activation solution prepared from sodium silicate and 6M sodium hydroxide, volume ratio Na_2SiO_3/NaOH=1.5. The structure properties of wood ash and alkali-activated wood ash (AAWA) were studied by X-ray difraction (XRD), X-ray fluorescence (XRF), diffuse reflectance infrared spectroscopy (DRIFT) and field emission scanning electron microscopy (FESEM). XRD pattern of wood ash showed the main crystal phase of calcite. DRIFT spectroscopy showed that the main vibration band of AAWA corresponds to Si-O-Si/Al-O-Si bands. The SEM images show the morphology changes that occurred after alkali activation of WA sample. Batch adsorption experiments conducted at room temperature showed that the adsorption pattern followed the Langmuir isotherm model and pseudo-second kinetic order, following a high value of correlation coefficient. The maximum removal of cadmium obtained from batch studies were for wood ash and alkali-activated wood ash more than 90%. The results generally showed that alkali-activated wood ash can be considered as a potential adsorbent for the removal of cadmium from aqueous solutions.

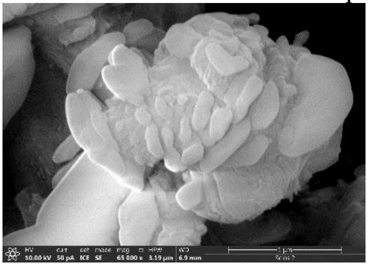

Figure 1. FESEM micrograph of wood ash

Acknowledgments

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EA PP 02

Photocatalytic properties of carbonized nanocomposites based on polyniline and titania nanotubes

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Polyaniline (PANI) is a promising conducting polymer for surface modification and sensitizing of TiO_2 to achieve extended photoresponse to visible light and increased photocatalytic efficiency [1]. Reducing the level of e-/h+ recombination in TiO_2 and photosensitized properties of PANI was the basis for creation of new functional PANI/TiO_2 nanocomposites. Carbonization process additionally contribute improving photoactivity of TiO_2 due to formation of new structures. Namely, after carbonization process of PANI component, graphene-like structures are formed [2]. On the other hand, temperature treatment during carbonization caused appearance of rutile beside anatase crystal structure of TiO_2, so combination of mentioned crystal phases induced better photocatalytic activity. In this study, we report the synthesis of a carbonized PANI/TiO_2 composite with different initial weight ratios of PANI, which was subsequently employed for photocatalytic degradation of methylene blue (MB), Rhodamine B (RB) and Acid Orange 7 (AO7) under white-light irradiation. Molecular and crystal structure, morphology, and photocatalytic response of the synthesized nanocomposite were characterized by Raman spectroscopy, XRD measurements, field-emission scanning electron microscopy, and UV–visible spectroscopy, respectively. Obtained results showed significant enhance of photocatalytic properties of synthesized nanocomposites in comparison to neat titania nanotubes.

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Acknowledgments

The research was funded by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia, through agreements related to realization and financing of scientific research work at the Vinča Institute of Nuclear Sciences -National Institute of the Republic of Serbia (Contract No. 451-03-47/2023-01/200017).

EA PP 03

Modelling and optimization of microwave digestion temperature in the preparation of fly ash samples

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The constant development of industry leads to a daily increase in the need for energy worldwide. Coal burning in thermal power plants in the Republic of Serbia produces a large amount of waste material – fly ash. The annual production of this type of waste material at the global level amounts to 800 billion tons. This waste contains toxic, carcinogenic, and mutagenic elements (Cd, Co, Cr, Ni, Mn, Pb, Zn, As, Hg).

This paper presents a methodology for preparing fly ash samples using a microwave oven. The digestion was performed using a mixture of mineral acids H_2SO_4/HNO_3 with V_2O_5 as a catalyst, while the re-digestion was performed using H_2O_2. Using experimental design four different temperatures (120 °C, 150 °C, 170 °C and 200 °C) were selected for the preparation of samples. Concentrations of heavy metals were measured by the technique of induced coupled plasma with optical emission spectrometry (ICP-OES). The results show that the detected concentrations of heavy metals in a complex matrix such as fly ash are to a large extent dependent on the method of sample preparation. Higher concentrations of metals such as Cd, Co, Cr, Ni, Mn, Pb and Zn, are detected at higher temperatures while volatile elements such as Hg and As are detected in higher concentrations at lower temperatures and digestion should be performed at temperatures up to 120 °C.

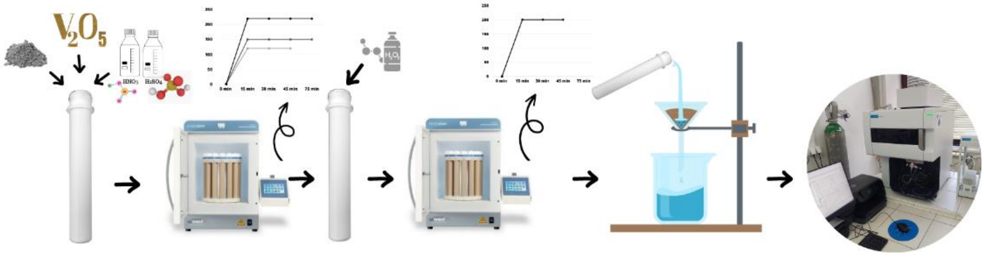

Figure 1. Microwave digestion methodology.

Acknowledgments
This research was supported by the Science Fond of the Republic of Serbia, GRANT No 7743343, Serbian Industrial Waste towards Sustainable Environment: Resource of Strategic Elements and Removal Agent for Pollutants – SIW4SE.

EA PP 04

Thermally induced phase transformation of the zeolite-promising way for immobilization of Ni ions from wastewater

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The increased use of heavy metals has resulted in an increased concentration of metallic substances in the environment. The Ni^{2+} ions from mining, electroplating, and battery manufacturing are the most common pollutants in surface water. Their high concentration can damage aquatic life as well as the health of people who are frequently exposed to them. A promising method for the removal of Ni ions from wastewater and their incorporation into stable crystal structure was described. Ni-exchanged form of LTA zeolite was prepared after 5 successive cation exchanges with 0.1M of $NiSO_4$. After the ion exchange, powder samples were heated at temperatures of 900 to 1300°C in order to obtain a stable crystal structure of Ni-spinel, $NiAl_2O_4$. XRF analysis was used to study ion exchange efficiency. The effect of thermal treatment of Ni-exchanged LTA zeolite on the phase composition was investigated using XRD and FTIR analysis [1,2].

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EA PP 05

Highly microporous sunflower-derived activated carbon for lead and copper removal: Synthesis, characterization, and adsorption mechanism

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Different industrial processes can potentially discharge heavy metals into surface and underground waters. These heavy metals can subsequently accumulate in organisms, posing a significant risk to both the environment and human health. Carbon-based materials such as biochar, carbon nanotubes-based materials, and activated carbon have been extensively researched for their effectiveness in adsorbing heavy metals from aqueous solutions [1]. Today, there is an increased interest in the usage of different low-cost, abundantly available lignocellulosic waste as a precursor for the production of activated carbon material. Activated carbon materials produced from different types of agricultural waste are widely used as adsorbent material for the removal of organic and inorganic pollutants from wastewater. High adsorption capacity is associated with characteristics of the adsorbent such as a large specific surface area, pore structure development, and the presence of different types of functional groups [2]. In this work, activated carbon is produced by the carbonization of sunflower agricultural waste followed by an activation process with potassium hydroxide. Activated carbon samples were characterized by SEM-EDS, BET, FTIR, and XPS. The obtained material has a porous structure with micropores and a large specific surface area, exhibiting a high affinity for the adsorption of lead and copper. Additionally, the main mechanism of lead and copper adsorption by sunflower-derived activated carbon has been successfully predicted.

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EA PP 06

Sustainable removal of 17α-ethinylestradiol from water suspension in the presence of newly synthesized ZnO nanomaterials based on banana peel extract

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Pharmacologically active compounds are organic compounds, which have been present in natural waters as pollutants for decades. 17α-ethinylestradiol (EE2) is an endocrine disruptor, that belongs to the group of syntethic hormones and is used in oral contraceptive pills. Due to the improper disposal of pharmaceutical waste EE2 reaches the aquatic ecosystem causing serious problems [1]. Heterogeneous photocatalysis, one of the advanced oxidation processes, showed a great potential in the degradation of pollutants. It is an eco-friendly technique, since it uses only semiconductors as photocatalysts and renewable solar energy in order to generate reactive oxygen species, which attack and degrade pollutants [2]. The aim of this study was to investigate the efficiency of newly synthesized ZnO nanoparticles, based on the banana peel extract, as photocatalyst for the removal of EE2 from aqueous environment, using simulated solar irradiation (SSI). In this study, the catalyst loading was investigated from 0.5 mg/dm^3 to 2.0 mg/dm^3. After 60 min of irradiation using SSI the system with catalyst loading of 0.5 mg/dm^3 was found to be the most efficient. Also, the experiments were conducted at three different pH values (5, 7 and 10), where the basic conditions proved to be the most efficient. According to the results, it can be concluded that newly synthesized, eco-friendly catalyst showed excellent photocatalytic activity. The highest removal efficiency was achived in the presence of ZnO based on banana extract peel under basic conditions, with catalyst loading of 0.5 mg/dm^3, when 98% of EE2 was removed after 60 min of irradiation using SSI.

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EA PP 07

Occurrence of microplastics in korean mussel (*Mytilus unguiculatus*) collected from local fish markets in South Korea and identification using micro-FTIR spectroscopy

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Microplastics (MPs) have been considered a new type of pollutant in the marine environment and have attracted widespread attention worldwide in recent years. Plastic particles with particle size less than 5 mm are defined as MPs [1].

Mussels were used as an indicator of marine environments contamination in biomonitoring programs [2]. The aim of this study was to determine the abundance of MPs in Korean or hard-shelled mussel, one of the most economically and ecologically important bivalves in South Korea, collected from seafood market intended for human consumption. After extensive removal of biological material by alkaline, enzymatic and oxidative digestion, MPs were characterized by micro-FTIR spectroscopy, which is a proven method for the identification of all types of polymers and enables reliable differentiation between substances of natural and synthetic origin. In total, we found 0.53 MPs per individual which is less than 0.3 MPs per gram of soft tissue. Major types of isolated MPs with their size and shape are shown in Figure 1.

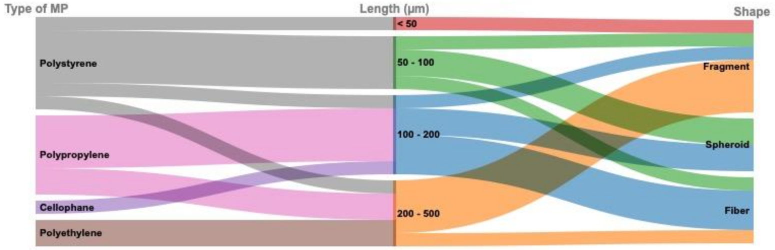

Figure 1. Alluvial diagram of the korean mussel (Mytilus unguiculatus): type od microplastic particles, longest size- length (µm) and shape type of found particles.

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EA PP 08

Potential of ionic liquid-based aqueous two-phase systems in removing pharmaceuticals from wastewaters

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Environmental protection has gained paramount importance, reflecting the growing concern for preserving natural resources and ecosystems. One notable environmental concern is the impact of pharmaceuticals on ecosystems, with non-steroidal anti-inflammatory drugs (NSAIDs) receiving increasing attention due to their harmful effects [1]. This study involved the extraction of four commonly used pharmaceuticals from water: naproxen (NAP), nimesulide (NIM), sodium diclofenac (DIC), and ibuprofen (IBU). The utilization of aqueous two-phase systems with ionic liquids has gained popularity, driven by their eco-friendly characteristics and versatile application. Having this in mind, the extraction performance of tetrabytilphosphonium salycilate (TBPSal) based ABS was investigated in terms of NSAIDs extraction from water. TBPSal is non-toxic and biocompatible [2] IL that has ability to form ABS with potassium carbonate as salting-out agent. Also, the effect of several operational parameters (concentrations of ABS constituents, pH and temperature) on partition behavior of NSAIDs were studied. Liquid-liquid equilibria of ABS and the two-phase region were determined by obtaining the binodal curve using the cloud point titration method. Working compositions for extractions were selected from the biphasic region. The concentrations of NSAID in each phase were quantified using UPLC method. The maximum extraction efficiencies achieved were remarkable, reaching 97% for NAP, 99% for NIM, 99% for DIC, and 96% for IBU. These results underscore the potential of the extraction process using TBPSal/K_2CO_3 ABS. This research sheds light on the highly effective and environmentally friendly approach for removal of NSAID pharmaceuticals, promising substantial benefits for sustainable water remediation strategy.

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EA PP 09

Human health risk assessment based on the element concentrations in landfills' soil

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Landfills represent the simplest and cheapest way of waste management, however, this way of waste disposing significantly contributes to environmental pollution [1]. Among landfills, special attention should be paid to illegal landfills located in agricultural areas. In addition to polluting the surrounding soil, groundwater, and even the air, such landfills lead to the pollution of the surrounding crops and thus contribute to a greater negative impact on human health.

For our study, 6 illegal landfills from northern Serbia were analyzed and 5 samples were taken from each landfill. The aim of our study was to assess the risk to human health due to inhalation, oral or dermal intake of contaminated soil from landfills. Both carcinogenic (R) and non-carcinogenic risk (HQ) were investigated. The following potentially toxic elements (PTEs) were analyzed: As, Cd, Co, Cr, Cu, Ni, Pb, Zn and Hg. Samples were prepared by microwave digestion and the PTE concentrations were measured by inductively coupled plasma optical emission spectroscopy (ICP-OES).

The results showed the following order of HQ levels (median) of PTEs in landfills' soil: Pb (5.49E+02) > Cr (3.21) > Ni (2.93E-01) > Co (1.61E-01) > Hg (9.37E-02) > As (1.10E-02) > Cu (2.97E-03) > Cd (2.28E-03) > Zn (8.62E-04). These values show that there is a high risk of damage to the brain and central nervous system due to chronic exposure to high concentration of Pb, in addition to other diseases that can occur due to the synergistic toxic effect of other PTEs. For carcinogenic risk values (median), the order is as follows: Cr (8.01E-04) > As (2.90E-06) > Pb (4.22E-07). The results show that there is a medium to high risk to human health because of the chronic exposure to soil from landfills in agricultural areas. The potential non-carcinogenic risks followed the order of inhalation > ingestion > dermal absorption, but the order of exposure routes for carcinogenic risk was ingestion > dermal absorption > inhalation.

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EA PP 10

In silico eco-toxicity evaluation of novel coumarin-1,2,4-triazole hybrids

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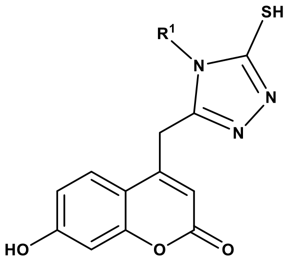
Pesticides are known for their high environmental persistence, affecting the environment and living organisms in multiple ways depending on their nature, chemical structure, dose, and targeted action. Therefore, it is of great importance to assess the eco-toxicity of potential pesticide candidates and the danger they may pose to non-target plants, fish or animal species. To avoid testing on animals, the use of *in silico* methods for the initial screening is highly encouraged. Recently, several coumarin-1,2,4-triazole hybrids (Fig.1.) were synthesized. QSAR models, implemented in the freely available Java application VEGA 1.2.3., were used to evaluate their possible toxic effects on the environment. The obtained data indicated that tested coumarin-1,2,4-triazole hybrids have a low chance for bioconcentration, low persistence in water but moderate in soil, are mostly readily biodegradable, and exhibit moderate toxic effects towards the water-dwelling organisms. Thus, if shown to exhibit desirable biological activities against pests, these compounds could be considered as new pesticide candidates.



1a - 1k

1a; R^1 = Me
1b; R^1 = Allyl
1c; R^1 = Benzyl
1d; R^1 = 3-OMePh
1e; R^1 = 3-ClPh
1f; R^1 = 4-ClPh
1g; R^1 = 4-BrPh
1h; R^1 = 4-OMePh
1i; R^1 = 4-MePh
1j; R^1 = Et
1k; R^1 = Ph

Figure 1. General structure of coumarin-1,2,4-triazole hybrids.

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EA PP 11

Toxicity evaluation of coumarin 1,2,4-triazole derivatives on honey bees (*Apis mellifera*)

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Extensive usage of pesticides has contributed to the rapid decline of pollinator species, including honey bees (*Apis mellifera*). Recently, new coumarin 1,2,4-triazole derivatives were synthesized for use as potential eco-friendly pesticides. A total of 8 compounds along with a positive and a negative control were tested for determination of oral toxicity on honey bees. The compounds were mixed with the standard sugar syrup feed, not exceeding a total concentration of 100 ppm. Experiment was conducted on caged bees in triplicates, with each cage containing approximately 30 bees during a period of an average lifespan of honey bees (around 30 days). The sugar syrup was weighted and exchanged every 24 h. Mesured parameters included the mortality rate, mass of the sugar syrup along with an approximate daily intake of a certain compound per bee (μg/bee).

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EA PP 12

Promising Phosphonium-Based Ionic Liquids aqueous biphasic systems for metal extraction

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Ionic liquid-based aqueous biphasic systems (IL-ABSs) have gained significant attention as extraction media for metal extraction and separation due to their enhanced tailoring ability in terms of specific interactions and eco-friendly characteristics. In this context, the design of task-specific and functionalized ionic liquids has become crucial for the development of efficient and selective ABS. Phosphonium-based ionic liquids (ILs) have emerged as highly promising candidates for various applications, due to their unique properties such as non-volatility, low toxicity, possibility to combine with different anions and thermoresponsivity [1]. This research focuses on the synthesis and characterization of novel hydrophilic phosphonium-based ILs with anions derived from natural acids that are well-known complexing agents, including acetate, lactate, glycolate, and propionate. By combining phosphonium cations with selected anions, ILs with tunable polarity and hydrophilicity are obtained. The work aims to investigate liquid-liquid equilibria of a ternary aqueous biphasic system by determining the phase diagrams under different temperatures. As the second ABS constituent, ammonium sulfate was chosen as a salting-out agent because of its acidic pH, low cost and wide availability. Phase diagrams were determined by the well-established cloud point method at 25°C and 35°C, while tie lines were ascertained analytically in order to gain insight into exact phases' compositions. These parameters are very important in order to select operational conditions for potential application in metal recovery. The results obtained from the phase diagrams show that the formation of ABS is favored in the following order of anions: Acetate < Glycolate < Lactate < Propionate. Propionate-based phosphonium ILs showed the highest ability to form ABS while acetate-IL is the most hydrophobic leading to low ability to salt-out ammonium sulfate. From these results is obvious that the choice of anionic species in designing phosphonium-based ionic liquids plays a crucial role in the formation of ABS as well as for their future application.

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EA PP 13

Determination of the adsorption capacity of zeolites for capturing CO_2 from the air

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Human activities, including modern agriculture and industry, contribute to the production of greenhouse gases, whose prevalence is increasing significantly. The three most important gases that are potentially most responsible for the greenhouse effect are CO_2 (57%), while CH_4 and N_2O account for 27% and 16%. The impact of anthropogenic activity on the increased concentration of CO_2 in the atmosphere and the global climate has been discussed for more than 100 years. Chemical absorption is one of the most promising technologies for CO_2 capture. One of the latest techniques for removing large amounts of CO_2 is direct air capture technology, the principle of which is based on CO_2 capture, its treatment with certain sorbents, regeneration and reuse. The main goal is CCU as carbon capture and utilization (as opposed to CCUS which also includes sequestration (storage) of carbon), so that the adsorbed CO_2 can later be desorbed and used as a potentially clean compound to produce some other component. In this work, zeolites were used as potential materials for CO_2 adsorption. The method used for testing was based on the simulation of air flow of a certain composition using a test station, where it is possible to measure the flow and air humidity. The results obtained are presented in graphs together with adsorption capacities. For the applied conditions in this research, satisfactory results were obtained in a high percentage.

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EA PP 14

Trace elements in soil intended for grass cultivation

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Trace elements include microelements and heavy metals. Some of them are essential for plant nourishment, but when used in greater amounts, they are harmful to the environment. There are also trace amounts of other elements (Cd, Hg, and Pb) in the soil, although these are not essential to plants and are major soil pollutants. Microelements are crucial to plant nutrition and are necessary for healthy plant growth and development. They have a role as cofactors and take part in a number of metabolic activities, including respiration and photosynthesis. Rocks (minerals), the fundamental substrate on which the soils were formed, are where microelements and heavy metals in the soil originate. The majority of the time, the naturally occurring concentration of heavy metals in soil is modest and has no effect on the agro-ecosystem's pollution. Trace elements can reach the soil in a variety of ways, and how they behave there depends on the kind and source of the substance. Most frequently, they enter the soil through a variety of anthropogenic methods, including transportation, burning fossil fuels, extraction and smelting, the production of non-ferrous metals, collection of urban and industrial waste, use of waste sludge and other waste as fertilizer, irrigation, atmospheric deposition from industrialand urban emissions, as well as the use of mineral fertilizers and pesticides in agriculture. This research was conducted in order to determine trace elements in soil intended for growing grass in the territory of Vojvodina, Sremski district, geographical coordinates 44.96003149334459, 20.27415379860020. Trace elements were determined using Atomic Absorption Spectroscopy using PinAAcle 900T (PerkinElmer, US). The results of the test gave the average level of the content of trace elements, which is: Cd (0.15 ± 0.03), Cu (12.08 ± 3.04), Pb (26.46 ± 5.45), Zn (24.74 ± 1.24), Hg (0.03 ± 0.01), As (4.68 ± 0.87), and Fe (89.30 ± 17.51) mg/kg. On the basis of this research, it can be concluded that the concentration of trace elements in the tested soil was below the established maximum allowed values according to national and European regulations.

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EA PP 15

Investigation of the possibility of binding ciprofloxacin from wastewater using surface-modified zeolite

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Wastewater containing pharmaceutically active components (PhAC) represents a major hazard due to potential adverse effects on human health. PhACs can not be removed from water by conventional treatment methods. Efficient, economically profitable and environmentally acceptable adsorbents for the removal of PhAC are the subject of intensive research [1]. Zeolites are microporous crystalline aluminosilicates that show good adsorption properties in water purification processes [2]. The aim of this work is the preparation of two adsorbents based on natural zeolite for the removal of ciprofloxacin, one of the most commonly used broad-spectrum antibiotics. The crystal lattice of zeolite is negatively charged and it does not have the ability to adsorb anions and nonpolar organic molecules. The surface of the zeolite can be adapted for the adsorption of organic molecules in two ways: by modification using an aqueous solution of benzalkonium chloride and hydrothermal synthesis of calcium hydroxyapatite on the surface of the zeolite. ADS1 was obtained by hydrothermal crystallization of calcium hydroxyapatite in the presence of natural zeolite at 160 °C for 4 hours. ADS2 was obtained by surface modification of Na-enriched zeolite with benzalkonium chloride solution. The resulting powders were characterized before and after adsorption by X-ray powder diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), thermogravimetric analysis and scanning electron microscopy. The concentration of ciprofloxacin in the solution was determined by UV spectrophotometry. XRD determined that the hydrothermal synthesis of hydroxyapatite on the surface of zeolite did not disturb its crystallinity. Structural analysis confirmed the presence of calcium hydroxyapatite in ADS1. FTIR and thermal analysis of ADS2 showed that a double layer was formed on the surface of the zeolite. The efficiency of ciprofloxacin binding with these two adsorbents was good. After 3 hours of contact, more than 80% of PhAC was removed from solution. These adsorbents showed good results in the removal of ciprofloxacin from aqueous solutions and can potentially be used in the treatment of municipal wastewater.

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EA PP 16

Biological degradation of recycled jute used as an adsorbent for crude oil

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In the fight against oil and it's derivatives pollution, adsorbents play a crucial role in efficient removal of these harmful substances from the environment. Jute, a natural plant fiber, is gaining increasing attention as a potential adsorbent for oil due to high porosity, good physical and chemical characteristics, biodegradability, and sustainability [1]. The aim of this study was to investigate the biodegradable properties of jute used as an absorbent for oil in a liquid medium and model compost. **Materials and methods:** The study monitored weight loss in oil-contaminated jute (NWSO) and compared it with control jute (NWS). Morphological changes in jute fibers were observed with optical microscopy and SEM analysis. Gas chromatography (GC-MS) was used for the detection of hydrocarbons in degraded jute. Enzymatic activity changes in compost soil were tracked. Bacterial strain isolation was done to assess growth on pure and oil-contaminated jute, with subsequent taxonomic identification. **Results:** NWSO samples were degraded more efficiently compared to clean jute with a weight reduction of 20% in NWSO compared to 5% in NWS. Microscopic and SEM analyses confirmed morphological changes in jute fibers after degradation. A decrease in hydrocarbon concentration after degradation was shown. Enzymatic activity tests provided additional insights into the composting process. The study also identified diverse bacterial strains capable of oil degradation, primarily belonging to *Bacillus* and *Microbacterium* genera. **Conclusion:** The study demonstrates the superior biodegradation of NWSO compared to NWS. The promising role of jute in sustainable bioremediation strategies leading to reduced harm from oil pollution has been demonstrated.

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Physical and computational chemistry

PCC PP 01

Rhodium-enhanced electrocatalysis of hydrogen and oxygen electrode reactions on polycrystalline nickel in alkaline media

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As hydrogen and oxygen electrode reactions are key figures regarding water-splitting and fuel cell technologies, developing advanced electrocatalysts is critical for addressing the energy needs of modern society that will foster a cleaner and greener future. Therefore, we present comprehensive research on rhodium-enhanced electrocatalysis of hydrogen and oxygen electrode reactions on polycrystalline nickel in alkaline media. The surface modification of the nickel electrode involves a simple and fast (up to 30 seconds) galvanic displacement utilizing a highly concentrated acidic Rh^{3+} solution. Our findings reveal a remarkable improvement in electrocatalytic activity for the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) on rhodium-enhanced nickel electrodes, highlighting the potential of galvanic displacement as an applicable route for designing advanced electrocatalysts. While the HER and OER reactions, primarily occurring on metallic Rh and conductive RhO_2, show high activities, the hydrogen oxidation reaction (HOR) and oxygen reduction reaction (ORR) activities of the rhodium-modified electrodes are lower compared to polycrystalline platinum. This discrepancy can be attributed to the detrimental role of semiconducting Rh_2O_3 formed on the surface, which pertains to the HOR and ORR relevant potentials. This research offers valuable insights into the mechanisms underlying the enhanced electrode kinetics observed on rhodium-modified nickel electrodes and contributes to the understanding of efficient and cost-effective electrocatalyst development, thereby contributing to the advancement of renewable energy technologies.

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PCC PP 02

DFT screening of the adhesion affinity of transition metals on TiO_2 (001) surface

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The rapid development of the materials science implies a need for efficient, practical and economical screening methods to predict and tailor required material properties. *Ab initio* screening of calculable target material properties has emerged in the last decade with the development of computational speed, particularly in the field of electrocatalysis [1], photochemistry, and adsorption [2]. Calculation of adhesion energies of metals is a common approach in investigation of the stability of metallic overlayers on various supports. In this contribution, we present a screening of adhesion energies of several transition metals on high-symmetry sites of rutile TiO_2(001) surface model, using spin-restricted DFT – GGA calculations, with *ultrasoft* pseudopotentials in a plane-wave basis set (Figure 1).

According to the general trends obtained, adsorption energy decreases from 8th to 10th group in periode, and also decreases in group with the increase of atomic number. To confirm these prepositions and get more precise results, spin-polarized calculations should be performed instead of spin-restricted.

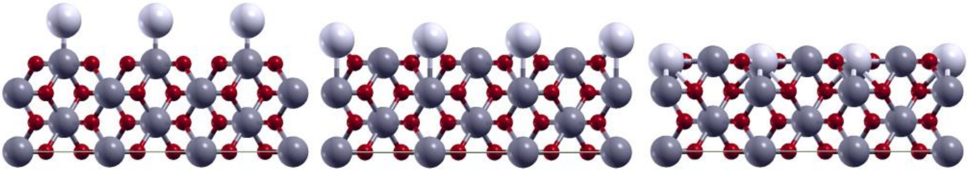

Figure 1. Metal adsorption of high-symmetry adsorption sites of TiO_2(001) surface (“top” - left, “bridge” - in the middle, “hollow” - right.

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PCC PP 03

In silico assessment of the bioavailability of newly synthesized spirohydantoins

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Analyzing properties of molecules, such as membrane permeability and oral bioavailability, a preliminary selection of molecules that have a higher potential to be drug candidates is possible. [1] Lipinski's rule was applied to check whether newly synthesized spirohydantoin derivatives have good (theoretical) oral bioavailability and whether they possess pharmacokinetic activity.[2] The values for the molecular descriptors log P (logarithm of the partition coefficient), MW (molecular weight), nHDon, and nHAcc (the maximum number of proton-donor and proton-acceptor groups when building a hydrogen bond) were determined by applying the appropriate software. In addition to the mentioned molecular descriptors, two more descriptors were considered, drug-like properties of the investigated compounds and drug score.

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PCC PP 04

Nickel polyoxometalates deposited on reduced graphene oxide catalyst for metal-air battery application

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The unique and specific structure of polyoxometalates (POMs) could enable their application in the metal-air battery (MAB) [1]. Herein we showed the catalytic activity of nickel-POM combined with reduced graphene oxide (Ni-POM/rGO) for oxygen evolution reaction (OER) in alkaline media (Fig. 1). Ni-POM/rGO shows high OER current density of 50 mA cm^{-2} at 1.7 V (Fig. 1A). The OER polarization curve shows an onset potential of 1.55 V with an overpotential of 350 mV at 1 mA cm^{-2}. The Tafel slope of 88 mV dec^{-1} was calculated for Ni-POM/rGO which is significantly lower than similar literature reports [1,2]. Fig. 1B shows the Nyquist plot of the Ni-POM/rGO electrocatalyst where the charge-transfer resistance was found to be as low as 22 Ω. Ni-POM/rGO with these catalytic performances was presented as promising candidates for MAB.

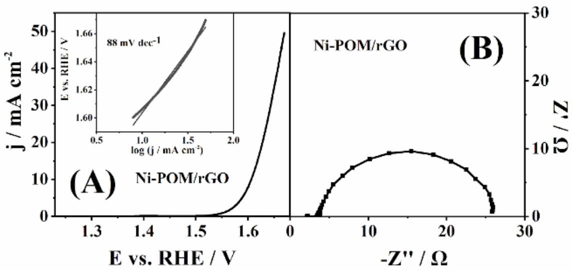

Figure 1. The IR-corrected OER polarization curve of Ni-POM/rGO in 1 M KOH solution at 5 mV s^{-1} with the corresponding Tafel plot inset, and Nyquist plot of Ni-POM/rGO recorded at 1.57 V.

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PCC PP 05

Application of LIBS in elemental analysis of pig shoulder bone

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The LIBS technique based on low pulse energy TEA CO_2 laser was used for the elemental analysis of pig shoulder bone. The spectra showed atomic and single-charged ionic lines of bone matrix elements (Ca and P) and other elements (e.g., Mg, Zn, Na, K, and C) with a good signal-to-noise ratio suitable for chemical analysis. The detection limits for Mg and Zn were 16 ppm and 12 ppm. Respectively (Figure 1). Carbon and H_α lines were used for plasma diagnostics (electron concentration of 2.9×10^{17} cm^{-3} and 1.9×10^{17} cm^{-3}; ionization temperature in the range from 10500 to 18100 K) and optical profilometry for depth profile analysis.

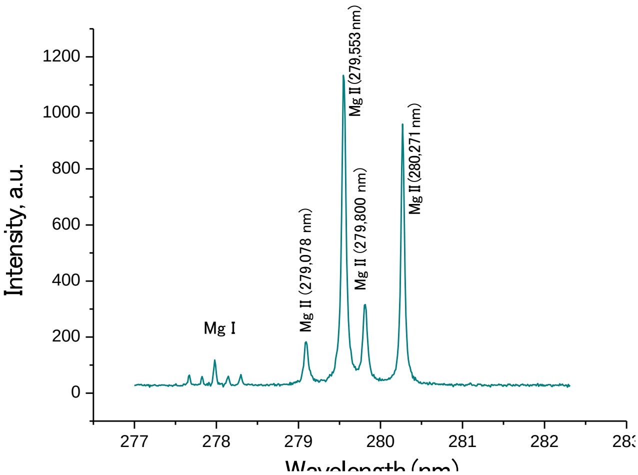

Figure 1. Part of LIBS spectra of the pig shoulder bone sample: Mg I and Mg II lines

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PCC PP 06

Spectrofluorimetric and molecular docking investigation of the BSA/HSA binding affinity of differently substituted 3-methoxycarbonylcoumarin derivatives

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Coumarin derivatives represent compounds with pronounced biological activities that depend significantly on the present substituents [1,2]. In this contribution, the Bovine Serum Albumin (BSA) binding affinities of four 3-methoxycarbonylcoumarin derivatives with –Br, -NO_2, -OH, and –OMe substituents in position 6 (denoted as **6-Br**, **6-NO2**, **6-OH**, and **6-OMe**) were determined by spectrofluorimetric titration at three temperatures. Thermodynamic parameters governing the binding process were calculated from the van't Hoff's plots. The binding process was spontaneous for all four derivatives. The decrease in change of Gibbs free energy of binding with the increase in temperature was observed for **6-OH** (between -32.0 and -24.6 kJ mol^{-1}) and **6-OMe** (between -30.5 and -23.7 kJ mol^{-1}) due to the decrease in flexibility of groups that are important for the interactions with surrounding amino acids. On the other hand, **6-Br** and **6-NO_2** showed the opposite behaviour with the increase in temperatures. Overall, the affinity order at 37°C was **6-NO_2** > **6-Br** > **6-OH** > **6-OMe**. The substituent effect and formation of hydrogen bonds at the active site were responsible for these differences. The molecular docking study was performed on the Human Serum Albumin (HSA) as a more relevant transport protein. The binding affinities of coumarin derivatives at Sudlow I and II sites were compared to those of site-specific markers, warfarin and ibuprofen. The affinity order of compounds at the Sudlow II site was the same as the one experimentally observed, and the process's spontaneity was higher than that of ibuprofen. Coumarin derivatives showed lower binding affinity than warfarin at Sudlow I. These findings were explained by the intermolecular interactions formed at the binding site.

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PCC PP 07

Influence of the number of halogen substituents and their type on the electrostatic potential of TNB molecules

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It is known that positive potentials above the central regions of molecular surfaces are indicators of the sensitivity towards detonation of molecules.[1] The higher the value is, the more sensitive the molecule is considered to be. The presence of halogens in the molecule significantly affects the charge distribution, and thus the sensitivity. However, the exact influence depends on the type of halogen due to their different strength of electron-withdrawing effect.[2]

In this work, electrostatic potential maps were calculated for the optimized geometries of 1-halo-2,4,6-trinitrobenzene, 1,3-dihalo-2,4,6-trinitrobenzene and 1,3,5-trihalo-2,4,6 -trinitrobenzene. The geometry optimizations were obtained using the PBEPBE/6-311G** level of theory in the Gaussian program. Calculations were made with and without the inclusion of GD3BJ dispersion. The wfn files used in the WFA-SAS program to obtain electrostatic potential maps for the mentioned molecules were obtained using the same combination of method and basis set.

The results showed that within groups of molecules containing the same number of halogen substituents, the value of the positive potential above the central region of the molecule is the highest in cases where the substituent is fluorine. There is a decrease in value as the substituents change in the direction from fluorine to iodine, with the largest decrease being recorded in the case of 1,3,5-trihalo-2,4,6-trinitrobenzene. The obtained results are in accordance with the strength of electron-withdrawing effect of the halogen elements. There is also a noticeable trend of the increase in positive electrostatic potential values with the increase in the number of halogen substituents (with the exception of the sequence in which chlorine is the substituent).

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PCC PP 08

Simultaneous determination of dopamine and folic acid using chitosan-carrageenan polyelectrolyte complex/graphene oxide modified glassy carbon electrode

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Dopamine and folic acid are compounds co-existing in biological fluids, playing crucial roles in metabolism and the central nervous system [1]. In this study, a novel electrochemical sensor was developed, obtained through the modification of a glassy carbon electrode. This sensor was applied for the simultaneous quantification of the abovementioned biologically active substances, using adsorptive square wave voltammetry as the basic analytical method. The electrode was modified with a polyelectrolyte complex composed of biopolymers chitosan and carrageenan, complemented by the addition of a catalytically active material, graphene oxide. This modification process significantly enhanced the adsorption of the target analytes onto the electrode surface, facilitated by favourable electrostatic interactions. These interactions primarily occurred between chitosan and folic acid, as well as between dopamine and carrageenan. Furthermore, the presence of the polyelectrolyte complex and graphene oxide increased the active surface area of the electrode and improved its electrical conductivity. Consequently, this resulted in enhanced electrochemical detection of dopamine and folic acid, at the optimal pH value of 5.5. The sensor exhibited a linear response of the anodic current concerning the concentration of dopamine and folic acid, both when measured individually and simultaneously. This developed sensor was effectively applied for detecting these compounds in synthetic urine and commercial products. Key advantages of this sensor include the achieved low detection limits for both compounds, electrode stability, selectivity, good reproducibility of results, and the convenience of renewing the electrode surface for subsequent measurements. These qualities indicate the significant potential of this sensor for the determination of dopamine and folic acid in various samples.

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PCC PP 09

Synthesis and characterization of novel Co-PWB bronze using TGA/DTA, XRPD, FTIR and SEM-EDS methods

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Phosphate tungsten bronzes (PWBs) constantly attract a lot of attention due to their interesting chemical, electrical, optical, and mechanical features [1]. Heteropoly acid hydrate H3PW12O40×29H2O (PWA) was obtained by dissolving Na2WO4×2H2O in a H3PO4-HCl mixture and by extracting the precipitate with ether at room temperature. The dehydration process of H3PW12O40×29H2O (PWA) to H3PW12O40×6H2O (6-PWA) is done by heating of PWA in a kiln at 80 °C. An aqueous solution of H3PW12O40×6H2O is then mixed with an aqueous solution of CoCl2×6H2O, gently heated to initiate the crystallization process, and left overnight to complete crystallization. The obtained with (CoHPW12O40×nH2O, CoPWA) is then heated in a furnace, from room temperature to 600 °C, during which cobalt phosphate tungsten bronze crystals are formed. Obtained CoPWB was further characterized by FTIR, XRPD and SEM-EDS methods which confirmed the formation of the desired structure. In this work, cobalt phosphate tungsten bronze was synthesized and characterized for the first time in order to obtain more information about its structure, chemical characteristics and potential practical application. A potential practical application of Co-PWB is in its incorporation into aqueous lithium-ion batteries and catalysts in the Briggs Rauscher reaction.

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PCC PP 10

Spectroscopic investigation of plasma induced by TEA CO_2 laser on a glass target

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TEA CO_2 laser of low energy was used for investigation of plasma obtained on samples of colored window glass. Spectra with narrow spectral lines of atoms and single charged ions Ca, Mg, Si, Fe, Cr, Co and Ni were obtained, with a favorable ratio of signal to background, suitable for sensitive spectrochemical analysis. Detection limits for metals were determined and values were in the range of 0.5-10 ppm, depending on the element and the selected spectral line. Plasma diagnostics were also performed, by measuring the Stark broadened profiles of spectral lines and measuring the intensity ratio of two spectral lines.

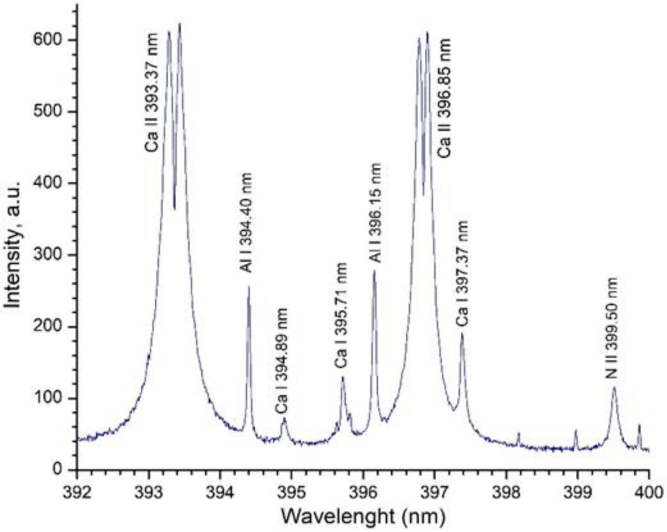

Figure 1. Part of LIBS spectra of window glass

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PCC PP 11

The importance of the metal ion and complex geometry on the interaction between a coordinated amino acid and a free water molecule

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Using quantum chemistry calculations and analysis of crystal structures from the Cambridge Structural Database (CSD), three types of hydrogen bonds, NH/O, O1/HO (hydrogen bond of a coordinated oxygen atom), and O2/HO (hydrogen bond of a non-coordinated oxygen atom) between different metal ion complexes of amino acids and a free water molecule were studied. Octahedral cobalt(III) [1] and nickel(II), square pyramidal copper(II), square planar copper(II), palladium(II), and platinum(II) complexes were investigated at M06L-GD3/def2-TZVPP level, and interaction energies were calculated using basis set superposition error (BSSE) corrected values. The NH/O hydrogen bond of a doubly positive complex has an interaction energy of -16.9 kcal/mol. For singly positive complexes, NH/O hydrogen bonds are weaker, from -8.3 to -12.1 kcal/mol strong, while for neutral complexes their values are the weakest, from -5.2 to -7.2 kcal/mol. In neutral complexes with O1/HO, interaction energies are from -2.2 to -5.1 kcal/mol, while interactions in singly negatively charged complexes are stronger, from -6.9 to 8.2 kcal/mol. Neutral complexes also have weaker O2/HO hydrogen bonds, from -3.7 to -5.0 kcal/mol, than the singly negatively charged systems, which have interaction energy values from -8.0 to -9.0 kcal/mol. Therefore, the results of quantum chemistry calculations showed that the strongest hydrogen bond is the NH/O, followed by O1/HO, and lastly, O2/HO interaction. The results also show a strong influence of the complex charge on the interaction energy. Other factors that influence the interaction energy to a smaller extent are metal oxidation number, coordination number, and metal atomic number. In the crystal structures from the CSD search, the *d* distributions for copper(II) and cobalt(III) amino acid complexes are in good agreement with the quantum chemistry results.

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PCC PP 12

Comparative exploration of the stability of cefoperazone and nadolol through atomistic calculations

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Pharmaceuticals such as nadolol (NAD) and cefoperazone (CEF) have been detected in natural waters and recognized as emerging pollutants with notable adverse effects on living organisms. Thanks to atomistic calculations, it is possible to predict the stability of pollutants and, thus, the efficiency of their removal from water. According to experimental and theoretical research, NAD showed high stability towards autoxidation, hydrolysis, and direct photolysis [1], while for CEF, such data have not yet been determined. To gain insight into the stability of CEF and the possibility of its removal, we studied selected quantum-molecular descriptors and intramolecular noncovalent interactions using density functional theory calculations. Parameters indicating molecular stability and reactivity were addressed using the global and local reactivity descriptors, while intramolecular noncovalent interactions were addressed via the reduced density gradient (RDG) approach (Figure 1). RDG surfaces have been mapped according to the strengths of noncovalent interactions, and the figure obtained in such a way offers identification of the type of intramolecular noncovalent interactions of molecules. A mutual comparison of NAD and CEF molecules indicated a much higher number of noncovalent interactions formed in CEF. These results indicate that the CEF is more stable than NAD and that advanced purification methods, such as photocatalysis, should be applied for removal.

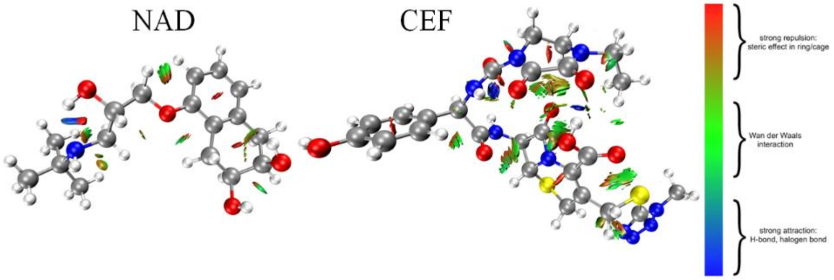

Figure 1. Intramolecular noncovalent interactions of NAD and CEF

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PCC PP 13

Theoretical study of the relationship between molecular geometry and strength of hydrogen bonds in acetylsalicylic acid

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Acetylsalicylic acid is a pharmaceutical drug well-known for its anti-inflammatory and antipyretic effects, and it is commonly used for the treatment of pain and fever caused by different diseases.[1] However, it is well known that pharmaceutical properties highly depend on the geometry of chemical compounds. [2] Herein, we present a theoretical study of the relationship between molecular geometry and chemical properties for various acetylsalicylic acid structures obtained from the Cambridge Structural Database (CSD). It is significant to emphasize that studied structures were synthesized and studied under different experimental conditions, and some of them were classified as different polymorphic structures.

In this work, we used quantum chemical calculations to study the influence of differences in geometries on values of calculated electrostatic potentials in critical points of selected acetylsalicylic acid molecules. The results showed that different crystal structures have significant deviations in electrostatic potential values in critical points above the ortho-Ar hydrogen atom. In addition, we studied the influence of geometry differences on the strength of C-H/O interaction between acetylsalicylic acid and water molecules. The results suggest that minor differences in the molecular geometry of acetylsalicylic acid could significantly influence the strength of C-H/O interaction. In conclusion, the geometry differences could have a crucial effect on the strength of non-covalent interactions and pharmaceutical properties of acetylsalicylic acid.

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PCC PP 14

Platinum nanoparticles on electrochemically exfoliated graphene for efficient hydrogen evolution reaction (HER)

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Although Pt-based materials have been shown to be the most effective HER catalysts, their high cost and lack of availability severely limit their use on a global scale. One strategy for achieving high catalytic activity with minimal metal usage involves reducing the amount of Pt loading on a support material. HER is slower in alkaline electrolytes than in acid, but alkaline media offers enhanced stability, high-purity hydrogen without acid fog, and the potential for transition metal-based catalysts, thereby reducing costs [1]. We have developed an efficient and stable catalyst for HER in a 0.1M KOH solution with low metal loading, specifically platinum supported on electrochemically exfoliated graphene, denoted as Pt/e-rGO. Graphene serves as the catalyst support for platinum nanoparticles (NPs), which were synthesized through anodic electrochemical exfoliation of graphite tape. The Pt NPs were obtained via chemical reduction with formic acid. TEM analysis revealed that most of them fall within the size range of 3-5 nm. Electrochemical active surface area was measured by CO-stripping voltammetry and estimated to be 67,93 m^2/g. Measured mass activity was -5,64 A/mg_{Pt}, on -0.1V vs. RHE, and overpotential at the current density -10 mA/cm^2 was 119 mV.

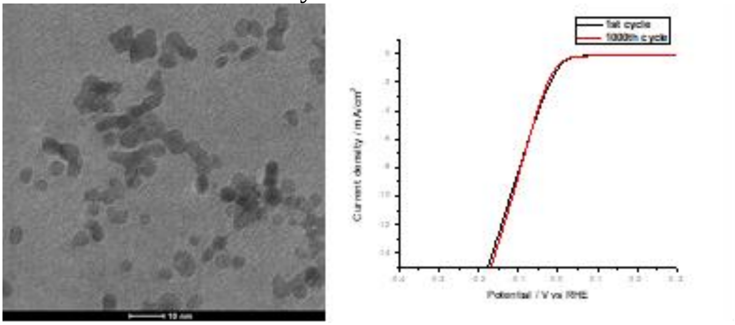

Figure 1. TEM image of Pt/e-rGO (left side) and HER activity of Pt/e-rGO first cycle and after 1000 cycles in 0.1M KOH (right side)

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PCC PP 15

Theoretical study of new hybrid organic-inorganic perovskites: Guanidinium-BX_3 substituted by B = (Sn^{2+}, Ge^{2+}, Ba^{2+}, Zn^{2+}) and X = (I^-, Br^-)

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The development of perovskite solar cells (PSC) has attracted great attention as a “green” energy source that might even replace fossil fuels soon[1]. Conventional perovskite solar cells mostly contain toxic lead, which contributes to environmental pollution, so the solution was found to substitute lead with some non-toxic metal[2]. Our investigation of hybrid organic-inorganic perovskites aims to increase the chemical stability as well as to decrease the band gap value of crystal perovskites which enables better conductivity and shifts the absorbance range, in order to produce the most efficient perovskite solar cells. The *ab initio* calculations of GA-BX_3, where GA is the guanidinium cation $C(NH_2)_3^+$, with several different inorganic cations and anions - specifically: B = (Sn^{2+}, Ge^{2+}, Ba^{2+}, Zn^{2+}) and X = (I^-, Br^-) have been performed using Density Functional Theory (DFT), with several functionals, Local Density Approximation (LDA) and Perdew-Burke-Ernzerhof (PBE), as well as HSE06 (Heyd–Scuseria–Ernzerhof) hybrid functional. Further investigations of structural and electronic properties will provide insights into the potential applications of these new hybrid organic-inorganic perovskite structures.

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PCC PP 16

The influence of vinylene carbonate additive on the electrochemical properties of the V_2O_5/rGO composite in $LiNO_3$ aqueous solution

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The lithium-ion batteries are widely implemented in everyday life. However, there is still a need to improve their characteristics, primarily in terms of safety, capacity, longer service life and cost [1]. For example, to replace the organic electrolyte with an aqueous electrolyte that is more environmentally friendly is one way to improve safety. The most used anodic material in aqueous batteries is vanadium pentoxide (V_2O_5). In this work, the composite of V_2O_5 and graphene oxide (GO) was synthesized by the sol-gel method. The synthesized composite V_2O_5/GO was characterized by X-Ray diffraction analysis (XRD) and Field emission scanning electron microscopy (FE-SEM). After the electrochemical reduction of GO, the electrochemical characteristics of V_2O_5/rGO xerogel were analyzed by chronopotentiometry at various current densities in a saturated $LiNO_3$ aqueous solution containing 0.5 % vinylene carbonate (VC) and without any additive.

XRD confirmed the amorphous structure of the V_2O_5/GO xerogel, i.e. the existence of only short-range ordering. The FE-SEM image shows that V_2O_5/GO has a uniform and wrinkled surface. Fig. 1 shows that adding VC to the electrolyte significantly increases the discharge capacity of the V_2O_5/rGO, which is noticeable even after 50 charge-discharge cycles. The easy, fast and low-cost synthesis of this V_2O_5/rGO composite could make it a potentially good electrode material for application in aqueous lithium-ion batteries.

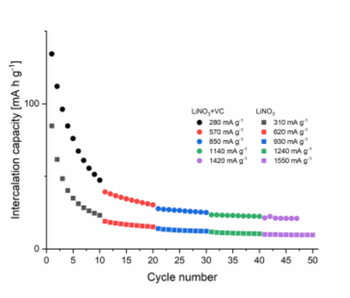

Figure 1. Specific capacity of V_2O_5/rGO in saturated $LiNO_3$ with and without VC

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PCC PP 17

Investigation of hydrogen evolution reaction on ZnO/rGO

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The hydrogen evolution reaction (HER) is one of the indispensable parts of the water splitting process and is increasingly being researched [1]. The main goal of this study was to enhance the electrochemical properties of nanostructured zinc oxide (ZnO) particles toward HER. In order to enhance their electrochemical properties, ZnO nanoparticles were precipitated onto graphene oxide (GO) to form a ZnO/GO composite which was *in situ* reduced before electrochemical measurements toward HER.

A composite of ZnO/GO (0.1 and 0.5 wt.%) was synthesized using a microwave processing of a precipitate. X-ray diffraction analysis (XRD), Raman spectroscopy, and field emission scanning electron microscopy (FESEM) were used to investigate the structural and morphological characteristics of composite materials. The diffractograms showed narrow reflections with relatively high intensities, which implies high crystallinity of composite materials. Raman spectra of ZnO/GO_0.5 shows a higher intensity D- and G-bands, attributed to GO, than ZnO/GO_0.1 confirming a larger amount of graphene oxide. FESEM images of composite samples show nanostructured particles. Before HER measurements, the electrode prepared by a mixture of ZnO/GO composite, nafion and ethanol/water solvent, was in situ reduced at potential -1.4 V in 0.1 M KCl to get ZnO/rGO. HER activity was investigated in NaOH by linear voltammetry. ZnO/rGO_0.5 showed increased electrochemical activity as a result of the evolution of hydrogen starting earlier and the higher current density.

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PCC PP 18

Relationship between geometry and energy of interactions in S_8 dimers

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Elemental sulfur exists in several allotropes, including α-S_8, β-S_8, and γ-S_8, wherein the arrangement of cyclic S_8 molecules varies according to the specific allotrope [1]. Intermolecular interactions among S_8 molecules have been detected within crystal structures extracted from the Cambridge Structural Database (CSD) and the Inorganic Crystal Structure Database (ICSD). Within these structures, S_8 molecules assume a parallel-displaced alignment, as illustrated in Figure 1a.

Quantum chemical calculations confirm that the parallel-displaced orientation represents the most stable geometry for two S_8 molecules. The interaction energy for the most stable geometry is calculated to be $\Delta E_{CCSD(T)/CBS}$= -8.70 kcal/mol (Figure 1b). According to the energy decomposition analysis performed using the SAPT 2+(3) method, the dominant attractive force between two S_8 molecules arises from dispersion interactions with the significant contribution of electrostatics.

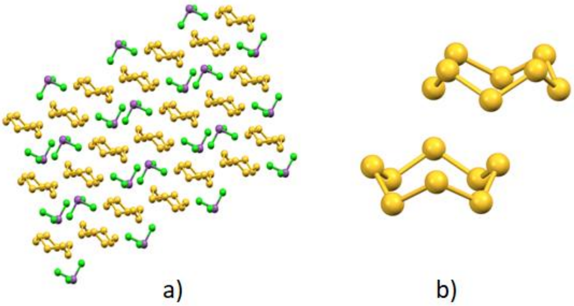

Figure 1. Parallel-displaced interactions between S_8 rings in a) Cl_3S_8Sb compound (ICSD ID: 35741) and the most stable geometry of S_8 dimer obtained by quantum chemical calculations.

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Phytochemistry and Food Chemistry

PFC PP 01

Physicochemical properties of honey samples with added freeze-dried fruit

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Honey is a supersaturated aqueous solution of different carbohydrates, including fructose, glucose, maltose, sucrose and other oligo-and polysaccharides [1]. Honey is usually used in the original form and as comb honey, but also enriched with pollen, propolis, royal jelly, or other primary bee products. Besides these types of honey, honey with freeze-dried fruits is also prepared and consumed as a tasty dessert [2]. The aim of this study was to assess the physicochemical properties and quality of honey with different freeze-dried fruit added. Seven honey samples, each with added freeze-dried fruit (cherry, strawberry, blueberry, raspberry, pineapple, orange, blackberry) were collected. One polyfloral honey sample was used as control. The acidity of these samples were analysed by titrimetic method. Also, electrical conductivity, pH, water content and hydroxymethylfurfural (HMF) concentration were determined for all studied samples. The results shown the acceptable range of acidity (6.0–30.7 meq/kg). Electrical conductivity varied from 0.23–0.48 mS/cm, while the pH value ranged between 3.60–3.97. The water content of honey samples was in the range 16.2–21.4%. Regarding hydroxymethylfurfural concentration, honey with added orange exhibited the highest value (7.10 mg/kg) while the lowest HMF content was found in honey with added raspberry (2.02 mg/kg). All measured physicochemical parameters were in agreement with the EU and national regulation standards except for water content (one sample). However, the honey quality varied based on added freeze-dried fruit, but also depends on handling, transportation and storage conditions.

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PFC PP 02

Isolation and structure determination of a flavonol glycoside from the roots of *Euphorbia amygdaloides*

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Euphorbia amygdaloides, known as wood spurge, is a bushy, evergreen, compact, free-branching spurge that typically grows up to 50 cm. The habitats of *E. amygdaloides* are woodland margins in Europe, western Asia and the Mediterranean. Previous researches have shown that the metabolites of *E. amygdaloides* are jatrophanes and tiglianes [1,2]. In this study, the roots of *E. amygdaloides* were examined. Using standard chromatographic techniques, the metabolite quercetin-3-*O*-rhamnoside was isolated. The structure of the compound was determined using 1D and 2D NMR methods.

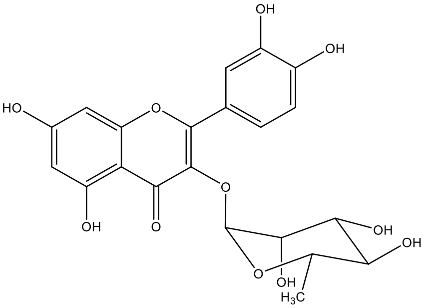

Figure 1. Stucture of quercetin-3-O-rhamnoside.

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PFC PP 03

Extraction of the protein fraction of sugar beet leaves

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Nowadays, with the intensive growth of the world's population, there is a need for alternative plant-based protein sources. Sugar beet leaves, with their high protein content, can be a good source for the production of proteins, and the leaf processing can revalorize this agro-industrial waste. The aim this research is to determine the most effective and economical method for extracting the protein sources found in sugar beet leaves. During a previous research, the isoelectric precipitation method was tested, but in this research, the goal is to test the efficiency of 2 new methods. The protein content of the protein concentrates obtained during the extraction processes was determined using the Kjedahl method. The obtained protein yield was 0.072 and 0.09%, and the isolate contained 7.1% proteins. Since a low yield was achieved during both extractions, the obtained protein concentrates were subjected to FTIR analysis in order to determine the contaminating substances found in them. In addition to the proteins, a large number of polysaccharide, lipid and amide compounds are found in the isolates, so further separation must be performed in order to purify the proteins. In addition to all of this, the dry matter content of the leaves and of the cake left after pressing of the leaves was also determined. Based on the measurements, the initial leaf sample contained 93.4% and the cake contained 93.1% dry matter. Since the obtained protein yield is considered low, further improvements must be made to ensure its use on an industrial scale (e.g. testing of new extraction processes, temperature, inhibitors). Furthermore, there are great opportunities in the investigation of the properties of proteins and in the potential use of the left-over leaf cake in industry.

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PFC PP 04

The content of selected phytochemicals and antioxidant activity of raspberry (*Rubus idaeus* L.) fruits

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The raspberry (*Rubus idaeus* L.) is one of the most popular berries in the world due to its attractive color, excellent taste, and aroma. This fruit is a rich source of natural antioxidants such as polyphenols, carotenoids, vitamins, and minerals that help to remove toxic substances and mutagens from the body, thus reducing the risk of diseases such as cancer, cardiovascular diseases, and many others [1,2]. In this study, the total polyphenols and flavonoids content of the raspberry methanolic extracts was determined *via* standard spectrophotometric methods. In addition, the antioxidant activity of analysed samples was evaluated through the ability to scavenge DPPH (2,2-diphenyl-1-picrylhydraziyl) free radicals and FRAP (Ferric Reducing Antioxidant Power) assays.

The obtained results demonstrated that the raspberry sample had a significant total polyphenols and flavonoids content, 5.91±0.17 mg gallic acid equivalent/g dry weight (mg GAE/g DW) and 4.84±1.68 mg quercetin equivalent/g dry weight (mg QE/g DW), respectively. Additionally, the samples showed a high antioxidant potential measured by DPPH and FRAP assays: 6.06±0.34 and 5.84±0.23 mg ascorbic acid equivalent/g dry weight (mg AAE/g DW), respectively. Based on the content of selected bioactive compounds and the antioxidant activity, it can be considered that the consumption of analyzed fruits may benefit human health.

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PFC PP 05

Determination of Theobromine in Chocolate with Screen-Printed Boron-Doped Diamond Electrode

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Theobromine, (3,7-dimethylxanthine; TB) is a naturally occurring alkaloid found in various food products, such as chocolate. TB exerts stimulating effects on the central nervous system. Its potential health benefits have garnered significant research interest, including its positive effects on cardiovascular health. Furthermore, TB has been investigated as a potential cough suppressant and its ability to enhance cognitive function [1]. The boron-doped diamond (BDD) is a very attractive material that shows excellent electroanalytical performance and is considered a green electrochemical sensor. It is an extremely hard and chemically inert material, which makes it highly resistant to degradation and fouling. This sensor has a wide potential window and a low background current, electrochemical stability, and fouling resistance, which makes it ideal for a range of applications, from sensing and electroanalysis to environmental monitoring.

This study examines the utilization of a novel screen-printed sensor with chemically deposited boron-doped diamond electrode [2] as an electrochemical sensor for accurate detection and quantification of TB in a simple, fast, and reliable manner. By employing cyclic voltammetry (CV), TB was observed to exhibit a distinct irreversible oxidation peak at relatively high potentials +0.90 V vs. Ag/AgCl reference electrode, in the presence of 0.5M H_2SO_4 and 0.1M KCl. Optimal experimental conditions were selected, and linear calibration curves were generated using differential pulse voltammetry (DPV), within the concentration range of 1 to 60 μM. The interference study confirmed selectivity. To verify the practical applicability of BDD SPE, it was utilized to analyze commercially available chocolate products with varying cocoa percentages (30% and 70%) using differential pulse voltammetry (DPV). The results indicated that the electrochemical sensor based on BDD SPE holds promise as a suitable choice for practical applications in food quality control.

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PFC PP 06

Assessment of the antioxidant potential of blackberry (*Rubus fruticosus* L.) and sour cherry (*Prunus cerasus* L.) fruits

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The health benefits of consuming certain foods have been commonly known since ancient times. However, the study of foods as a source of healthy bioactive compounds has been gaining interest over recent decades. At present, berries have received considerable attention due to their high content of flavonoids, anthocyanins, tannins and vitamin *C*, among others. Sour cherry (*Prunus cerasus* L.) and blackberry (*Rubus fructicosus* L.) are recommended in a healthy diet due to the rich selection of the mentioned bioactive components and their antioxidant activity. Bioactive components, known as plant secondary metabolites, are the main antioxidants in plant materials, and it is known to be effective in preventing obesity, diabetes, and cardiovascular disease as well as in improving cognitive function [1,2].

This study aimed to investigate the antioxidant potential of blackberry and cherry samples using two extraction solvents, methanol and ethanol. The evaluation of the antioxidant capacity of the tested extracts was performed using the CUPRAC (Cupric Reducing Antioxidant Capacity) assay and the results were expressed as µmol ascorbic acid equivalents per gram of fresh weight of the sample (µmol AAE/g FW). The obtained results indicate that both blackberry extract samples had higher antioxidant activity compared to the cherry extracts, with the difference that ethanol was a better extraction agent for studying the antioxidant properties of the blackberry extracts (ethanol: 100.05±1.30; methanol: 78.14±1.30 µmol AAE/g FW), while the cherry samples extracted with methanol showed higher antioxidant activity (74.98±0.47 µmol/g AAE) than those extracted with ethanol (71.57±0.16 µmol AAE/g fw). In view of the results, it should be noted that the consumption of berry fruits may have positive effects on human health.

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PFC PP 07

Complete assignment of ^{1}H- and ^{13}C-NMR spectra of salvipisone isolated from *Salvia aethiopis* L. (Lamiaceae)

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We report on a detailed NMR spectral analysis of salvipisone isolated from the roots of *Salvia aethiopis* L. (Lamiaceae). The structural elucidation was accomplished by extensive spectroscopic methods including 1D and 2D NMR experiments. According to a literature survey, there is limited, unassigned, or even incorrectly assigned data for this compound [1]. In order to correct the situation, a complete assignment of ^{1}H- and ^{13}C-NMR spectra of this compound recorded in $CHCl_3$, based on a combination of 1D and 2D-NMR experiments, including ^{1}H-^{1}H COSY, DEPT, HSQC, HMBC, and NOESY, was performed.

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PFC PP 08

Preparation of NiO supported carbon paste electrode for sensitive and selective determination of Gallic acid in plant samples

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Gallic acid (GA), namely 3,4,5-trihydroxy benzoic acid, is a natural phenolic compound present in tea, wine, fruits, beverages, and various medicinal plants [1]. Due to their ability to scavenge free radicals and act as antioxidants, gallic acid and its derivatives, including lauryl-, propyl-, octyl-, tetradecyl-, hexadecyl-gallate, can prevent the oxidation and rancidity of oils and fats, and as a result, they are used as food additives [2]. There are numerous scientific reports on the biological and pharmacological activities of GA, with an emphasis on antioxidant, antimicrobial, anti-inflammatory, anticancer, cardioprotective, gastroprotective, and neuroprotective effects [1,2].

In this work, nickel oxide (NiO) nanoparticles were synthesized by the chemical coprecipitation method and used for modification of the carbon paste electrode for GA detection and determination. Morphological properties of prepared material were investigated using ICP-OES (inductively coupled plasma–optical emission spectrometry), XRD (X-ray diffraction), SEM and TEM (Scanning and Transmission Electron Microscopy). The electrochemical properties of the prepared electrode and the behavior of GA over the modified electrode were examined using CV (Cyclic Voltammetry), EIS (Electrochemical impedance spectroscopy), and SWV (Square Wave Voltammetry). The prepared electrode showed better electrocatalytic response than the bare carbon paste electrode. After square wave voltammetry (SWV) optimization, the electrode showed a wide linear working range from 0.2 to 100 μM at pH 3 of Britton–Robinson buffer solution (BRBS) as the supporting electrolyte. The excellent selectivity of the proposed method, with good repeatability and reproducibility, strongly suggests a potential application of the method for the determination of GA in plant samples.

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PFC PP 09

Robust predictor for consumer's acceptance of newly bred strawberry varieties based on Brix/acidity ratio

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Strawberry (*Fragaria x ananassa* Duch.) is widely known for its nutritional value, richness in polyphenols and antioxidant capacity. In abundance of numerous ongoing strawberry breeding programs worldwide, some of the main parameters for breeding and selection are fruit quality, flavour and aroma which are directly affecting commercial acceptance [1]. These could be easily identified with some of objective measurements such as soluble solids concentration (°Brix), acid contents (titratable acidity, TA) and Brix/acid ratio, which could be strong predictors of quality in terms of consumer acceptability [1,2].

In this trial, we compared 24 strawberry genotypes, including 12 parental varieties and 12 perspective candidates obtained by crossing these particular parental varieties. Results of °Brix, titratable acidity and °Brix/acid ratio measurements indicated that new perspective candidates have had higher °Brix/acid ratio than the parental varieties, leading to conclusion that those genotypes had better flavour. Therefore, this ratio could potentially be used as indicator for distinguishing consumer acceptance.

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PFC PP 10

Assessment of microplastics content in (sub)urban soils of Serbia and its correlation with Cd, As, and Pb mobility to the Capsella bursa-pastoris (L.) Medic

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This study investigates the presence of microplastics (MP) in the soil of (sub)urban areas of Serbia and its correlation with the mobility of toxic metals (Cd, As, Pb) to the plant species Capsella bursa-pastoris (L.) Medic. The density separation method with two-phase digestion (H_2O_2 and NaClO) was employed to optimize MP detection in soil samples. Eight different types of polymers were identified through ATR-FTIR spectroscopy analysis, consequently polystyrene and phosphorylated cardanol prepolymers being the most prevalent.

The results of this study reveal significant positive correlations between the presence of MP and the availability of Cd, As, and Pb to plant, suggesting a potential role of MP in the mobility of these heavy metals in soil. Additionally, a connection was established between concentration of cadmium (Cd) in under and above-ground tissues of C. bursa-pastoris and the concurrent presence of microplastics (MP) within the soil. This correlation indicates an increased mobility of cadmium in the presence of microplastics. Conversely, the Pb content in plants showed a negative correlation with the presence of MP in the soil, indicating complex interactions between these factors.

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PFC PP 11

Citrus fruit peel waste as a fruitful source of natural antioxidants for industry purposes

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Thanks to their pleasant aromas and attractive colours, citrus fruits are one of the most cultivated fruit crops in the world. 20% of cultivated citrus fruits are industrially processed, mainly for juice production. During industrial processing, only 45% of the total fruit mass is used, while the rest (peel, pulp, and seeds) is discarded as waste creating about 120 million tons of waste per year [1,2].

The aim of this study was to evaluate the potential of citrus fruit waste as a source of natural antioxidants. Oranges, lemons, mandarins, and grapefruits were purchased in January 2021 at a local supermarket in Novi Sad. Peel and endocarp were separated, lyophilized and macerated with 80% EtOH. Extracts were examined by determination of total phenolic (TPC), flavonoid (TFC), tannin (TTC) and vitamin C contents, while the antioxidant activity was evaluated by DPPH and FRAP assays[2].

Peel contained more phenolics (TPC – 16.5-49.8 mg GAE/g d.w., TFC – 3.4-8.8 mg QE/g d.w. and TTC – 4.7-17.0 mg GAE/g d.w.) compared to endocarp extract (TPC – 3.2-15.5, TFC – 0.4-3.4 mg QE/g d.w. and TTC – 0.7-6.9 mg GAE/g d.w.). Also peel contained more vitamin C (3.3-4.8 mg/g d.w.) than the endocarp (0.5-2.0 mg/g d.w.) of the same fruit. Additionally, peel extracts showed higher antioxidant activity (FRAP – 10.8-21.5 mg AAE/g d.w. and EC_{50} – 0.13-0.18 mg/mL in DPPH assay) compared to endocarp extracts (FRAP – 2.6-7.3 mg AAE/g d.w. and EC_{50} – 0.26-1.00 mg/mL in DPPH assay). The highest amounts of TPC, TFC, and TTC were detected in grapefruit peel, while the highest concentration of vitamin C was detected in orange peel. These results support more extensive utilization of citrus fruit peel waste in food, cosmetics and other industries as a fruitful source of natural antioxidants, thus supporting circular economy.

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PFC PP 12

Mycorrhizal and edible mushroom species *Hydnum repandum* L. 1753 as a great source of natural antioxidants

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Mushrooms possess great nutritional value since they are rich sources of many bioactive compounds: proteins, fibers, fatty and amino acids, vitamins, especially B and D, and micro- and macronutrients (K, P, Se, Mg, Cu, Zn, Fe). It is known that various mushroom species, both saprotrophic and mycorrhizal have positive impact on human health, enhance immune system, express antioxidative properties, protect against atherosclerosis, and support nervous system [1,2].

The aim of this study was to evaluate the antioxidant potential of the mycorrhizal and edible mushroom *Hydnum repandum*. The mushroom was extracted with different solvents: $CHCl_3$, acetone, 70% EtOH, 80% MeOH and hot water (infusion). In order to evaluate total phenolic content (TP) of the extracts, Folin-Ciolcateu procedure was applied, while the antioxidant potential was evaluated by DPPH, ABTS, and FRAP assays [2].

The ethanol and methanol extracts exhibited higher amounts of TP (27.26±0.03 and 27.13±0.26 mg GAE/g d.w., respectively) compared to the other analyzed extracts. *Hydnum repandum* demonstrates notable antioxidant properties (FRAP – 58.0-197.9 mg AAE/g d.w., ABTS – 5.6-30.3 mg TE/g d.w., and IC_{50} = 0.08-0.3 mg/mL for DPPH assay), with good correlation with TP. The strongest activity exhibited acetone extract in FRAP and DPPH assays, while acetone and ethanol extracts showed the highest ability to scavenge ABTS radicals (29.37±0.43 and 30.27±0.91 mg TAE/g d.w.).

Based on the results of this study *Hydnum repandum* is a good source of antioxidants, and after further mycochemical characterisation it could be considered as a valuable nutraceutical.

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PFC PP 13

Phenolic and multi-elemental profiles as a tool for quality assessment of Serbian blackberry wines

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Blackberry wine is produced by a yeast fermentation of natural saccharides present in blackberry juice. This wine is traditionally consumed in Balkans, mostly as a dessert wine, but in recent years it is gaining more attention due to unique flavour and potential health benefits. Blackberries are a natural source of many minerals and bioactive phytochemicals such as vitamins, folic acid, anthocyanins, and phenolics [1,2]. Considering biological potential of blackberries and their products aim of this study was to evaluate quality of Serbian blackberry wines. This quality assessment was achieved through determination of: (a) the phenolic profile by high-performance thin layer chromatography (HPTLC); (b) total phenolic (TPC) and anthocyanin content (TAC); (c) *in vitro* antioxidant activity by DPPH and ABTS radical scavenging assays and total antioxidant capacity (d) *in vitro* antimicrobial activity by the agar diffusion test; and (e) the content of macro, micro and toxic elements by inductively coupled plasma mass spectrometry (ICP-MS). Twelve blackberry wines from different geographical regions were tested indicating various phenolic profiles and great antioxidant and antimicrobial activity. Strong positive correlation was confirmed between TPC and antioxidant activity determined by DPPH and ABTS assays. Additionally, high levels of antibacterial activity were shown against all six tested strains, but primarily against *Staphylococcus aureus* and *Micrococcus lysodeikticus*. Samples were rich in macroelements, such as Ca, K, Mg, Na, P and Zn, and microelements Cu and Fe, while Mn was present in higher concentration only in one sample. Toxic metals Cd and Pb were present in low concertation in all samples. These results indicate great quality of Serbian blackberry wines concerning minerals, phenolics, antioxidant and antimicrobial activity, which support its health potential.

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PFC PP 14

HPTLC based approach for assessment of antibacterial effects of selected *Lamiaceae* family plants

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The *Lamiaceae* family stands out as one of the most diverse and common plant families in terms of ethnomedicine. Their potential therapeutic effects stem from a wide array of secondary metabolites synthesized as defense mechanisms against pathogens, herbivores, UV radiation or any other environmental stress [1]. The aim of the present study was the development of a high-performance thin-layer chromatography (HPTLC) based approach for the bioassay-guided assessment of antibacterial activities of specialized metabolites extracted from selected plants against two reference strains (*Escherichia coli* ATCC 35218 and *Staphylococcus aureus* ATCC 6538). The detection of separated metabolites was achieved through chemical derivatization with the *p*-anisaldehyde/sulfuric acid reagent, and the visualization of bioactive components was carried out through direct bioautographic assays. Images of the chromatographic plates were recorded under white light and processed using ImageJ software. The working range of the calibration curve was determined by plotting chromatographic peak areas against standard concentrations (µg/band). The antibacterial activity was expressed as mg streptomycin equivalents/g of dry plant material, while the total terpenoid content as mg linalool equivalents/g. Among the various species studied, *Salvia officinalis* L. and *Lavandula angustifolia* Mill. exhibited the highest terpenoid content and demonstrated the highest antibacterial potential. A paired t-test revealed no statistically significant difference in the activity of a given plant species, indicating that the components of a particular species exhibited consistent activity against both bacterial strains. In addition to other *in vitro* antimicrobial assays, the HPTLC approach described here has potential in exploring alternative antibacterial agents derived from natural sources. These compounds can have a crucial role in combating infections and the increasing resistance to existing antibiotic therapies.

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PFC PP 15

Elastase and tyrosinase inhibitory activity of plant petals cultivated in Serbia

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The cosmetic industry is currently experiencing substantial growth, accompanied by a surge in the number of consumers. Due to natural ingredients' safety and efficiency, an increasingly prominent trend in this industry is the design of herbal-based cosmetic products and formulations. To meet demand, integrating innovative natural resources like plant-based formulations is essential [1]. Skin ageing-related enzymes, elastase and tyrosinase, contribute to the emergence of aesthetic issues such as wrinkles, freckles, and loss of elasticity, as well as hyperpigmentation and melasma [2]. Hence, there is an increasing focus on finding inhibitors for enzymes associated with skin ageing. The fact is that plant metabolites, particularly phenolic acids and flavonoids, are frequently concentrated in plant leaves and flowers. Accordingly, we assessed the inhibitory effects on elastase and tyrosinase in seventeen particularly selected methanolic extracts obtained from various flower petal varieties cultivated in Serbia. Our analysis revealed that petals exhibit significantly more pronounced inhibitory effects, expressed as IC_{50} values, on elastase compared to tyrosinase. White peony (*Paeonia lactifora*) (230 ± 1 μg/mL), pelargonium (*Pelargonium peltatum*) (206 ± 3 μg/mL) and purple rose (*Rosa centifolia, purple*) (222 ± 8 μg/mL) emerged as the most potent elastase inhibitors, surpassing the reference compound epigallocatechin gallate (348 ± 9 μg/mL). Additionally, the lowest IC_{50} value for tyrosinase inhibition was attributed to lilac (*Syringa vulgaris*) petal extract (272 ± 28 μg/mL), which was compared to the standard compound kojic acid (50 ± 14 μg/mL). In conclusion, white peony, pelargonium, purple rose, and lilac represent promising candidates for further investigation and incorporation into cosmetic products, showcasing their potential to effectively address skin-related concerns.

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PFC PP 16

Characteristics of the fruit of different walnut cultivars (*Juglans regia* L.)

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Walnut is one of the most important stone fruits in Serbia and modern cultivation technology and a new walnut assortment is a great opportunity for fruit production. The fruits of different walnut cultivars (*Juglans regia* L.) may differ in several characteristics, including size, shape, flavor, and thickness of the shell. Therefore, the aim of this work is to analyze the characteristics of the fruits of different walnut cultivars. Eight cultivars were examined: Chandler, Pieral Lara, Tulare, Champion, Rasna, Šejnovo, Gazenheim 139, and Ovčar. The Champion cultivar has the highest fruit weight (15.13 g), and the Šejnovo cultivar has the lowest fruit weight (11.27 g). The Tulare cultivar has the highest kernel yield, (53.88%), and the Rasna cultivar has the lowest yield, (44.26%). Half of the examined cultivars had light (Chandler, Pieral Lara, Tulare and Ovčar), and the other half of the cultivars had dark kernel color (Šampion, Rasna, Šejnovo and Gazenheim 139). In Chandler and Tulare cultivars, the kernel was slightly easier to separate from the shell, while all other cultivars had medium kernel separation. The highest percentage of crude oil, 53%, was obtained when pressing the Gazenheim 139 cultivar. Chandler (34%) and Šejnovo (34%) cultivars had the highest percentage of clear oil. The analysis of the sensory characteristics of the cold-pressed oils revealed that cold-pressed oils of three cultivars: Chandler, Pieral Lara, and Champion had the best characteristics and belonged to the excellent quality category. The Gazenheim 139 cultivar had the highest kernel oil content, 68.17%, while the Chandler cultivar had the lowest 56.80%.

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PFC PP 17

Proposal of thermogravimetric method for determining oxidative stability of cold pressed oils

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The aim of this study was to develop the quick and rapid method for assessing the oxidative stability of vegetable cold pressed oils by utilizing thermogravimetric (TG) analyzer (model TGA701, LECO Corporation, USA). The method is based on measurement of sample weight changes as a function of temperature in a controlled environment [1]. The main goal is to investigate if aforementioned robust TG analyzer can be used for recording weight gain due to oxygen caption of oil sample which occurs as a result of the oxidation, similar as *Coni et al.* (2004) presented. Several different cold pressed oils (rapeseed, soybean and olive) were analyzed by putting 0.5 g of sample in crucible which was then put in a furnace of TG analyzer. The samples were heated up to 95 °C (rate 5 °C/min), held for five minutes and further heated up to 210 °C (rate 5 °C/min) while the mass of samples was automatically weighed by incorporated analytical balance and the oxygen was used as purge gas (flow rate 3.5 l/min). The obtained TG curve (Fig. 1) showed that sample weight gain was recorded but it was also possible to determine temperatures at which oxidation starts and finishes. Further development of method is required in order to enhance the applicability of proposed method.

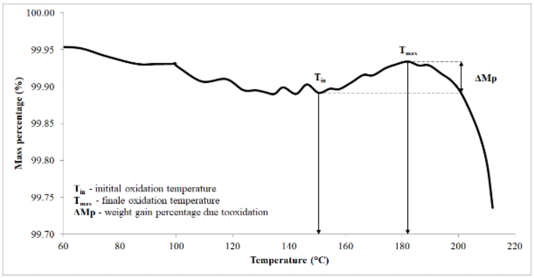

Figure 1. Thermogravimetric curve of rapeseed oil.

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PFC PP 18

Properties of glucose syrup and application in the production of jelly beans

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Glucose syrup is obtained by acid or enzymatic hydrolysis of starch and in addition to glucose, it also contains maltose and dextrins of different molecular weight. This paper analyzed the properties of glucose syrup, which is the primary raw material for the production of jelly beans in the company "Swisslion Takovo" from Gornji Milanovac, and also described the technological procedure for the production of jelly candies. The analyses are done in the laboratory of the Faculty of Agronomy in Čačak and gave results that describe the quality of the tested syrup and which are in accordance with the specification and regulations on the quality of this type of product. Based on the tested parameters: reducing power (dextrose equivalent) and dry matter it is clear that glucose syrup was obtained by acidic hydrolysis. Specific angle of rotation polarized light (130,28 $°\mathrm{mL \cdot g^{-1} dm^{-1}}$) and DE value are not in corelation theoretical values that predict % reducing power about 60 for this specific rotation. On the other hand, by examining the color of the sample using the spectrophotometric method, it is clear that the product has a satisfactory quality, which was also determined by ICUMSA units (9,4 ICUMSA). In order to complete the analysis of the properties of the syrup, chromatographic detection of HMF was also performed, which proved its presence to a lesser extent (with a retention time of 7.5 min) which was expected considering that this type of product is obtained by heat treatment. Finally, a sample of glucose syrup was used in the jelly candies recipe, after which a sensory evaluation of the final product was performed. Jelly candies were produced in with different gelling agents: gelatin and agar agar and identical other ingredients: glucose syrup, water, sucrose, aroma and citric acid with certain differences in the production process. Based on the sensory evaluation, jelly candies with agar agar belong to the very good category, and jelly candies with gelatin belong to the good category.

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PFC PP 19

Amino acid based legume authenticity method: bean and pea

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Because of their richness in nutrients and health benefits, legumes are very important in the human diet. The absence of gluten makes them very popular in the bakery industry lately. The aim of this work was to differentiate 15 bean samples (1-15) and 7 pea samples (16-22) based on amino acid composition. Free amino acids were extracted and derivatized from the legume samples as in [1]. A GC-MS (gas chromatography coupled to mass spectrometry) analysis was performed and the obtained chromatograms were processed in terms of compound identification. Peaks of all identified compounds were semi-quantified and the data were collected into a data matrix. Hierarchical cluster analysis (HCA) was performed as a multivariate statistic tool to differentiate the samples according to their botanical origin [2]. Obtained similarity dendrogram presents a clear separation of the bean and pea samples into two clusters. The results of this paper demonstrates the potential of the proposed method for legume authentication.

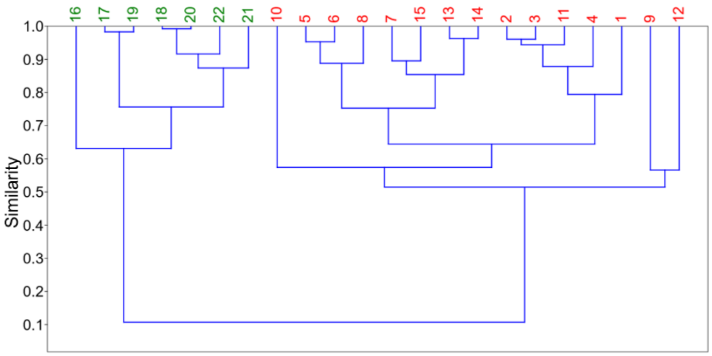

Figure 1. Similarity dendrogram of bean and pea samples differentiation based on free amino acids.

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PFC PP 20

^{1}H NMR iterative full spin analysis of rosin, a secondary metabolite from *Rhodiola rosea* L.

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Rosin (Figure 1) is a glucoside of cinnamyl alcohol unique to the species *Rhodiola rosea* L. (Crassulaceae), a widely used plant in traditional medicine. Assays of rosin content are often used to assess plant material quality and authenticity. ^{1}H NMR is an especially useful technique for quantifying components in complex mixtures [1], provided sufficient analyte spectral data is available. Regrettably, detailed high-field NMR data for rosin are currently lacking.

A sample of rosin obtained by synthesis was used to acquire full ^{1}H and ^{13}C NMR spectral data by utilizing ^{1}H NMR iterative full-spin analysis. Using the spectral simulation capabilities of MestReNova, the iterations were performed manually [2] after a total assignment of resonances by 2D NMR techniques. All values of relevant chemical shifts and scalar coupling constants were determined.

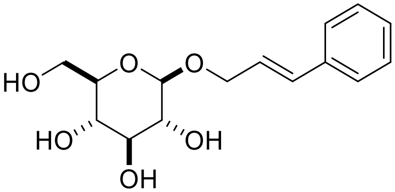

Figure 1. Structure of rosin.

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PFC PP 21

Comparison of chemical composition essential oil of three *Pinus* species

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The Pinus genus, a member of the Pinaceae family, encompasses coniferous trees and shrubs, with a total of 121 recognized species worldwide and are primarily distributed throughout the Northern Hemisphere. In this work, three commercially available pine essential oils, obtained by hydrodistillation of needles of *Pinus nigra Arn.*, *Pinus mugo Turr.*, and *Pinus sylvestris L.,* were analyzed using gas chromatography and gas chromatography-mass spectrometry. The constituents of these oils were identified through mass spectrometry and Retention Index (RI) data and, wherever possible, by co-injection experiments. While the primary components of all three oils exhibited similarities, they varied in their proportions. Among the monoterpenes, which represented the predominant components of these essential oils, the most abundant were *α*-pinene (8.2–26.0%), *β*-pinene (4.5–16.9%), Δ^3-carene (13.1–20.0%), limonene (4.0–12.1%) and *β*-phellandrene (0–16.2%), but also containing significant amounts of terpinolene (0.4–4.1%), and bornyl acetate (4.0–4.4%). Identified sesquiterpenes were less abundant and included (*E*)-Caryophyllene (4.3–9.5%), and others, such as *α*-humulene, germacrene D, *δ*-cadinene and caryophyllene oxide, all ranging from 0.5 to 3.0%. In total, 160 constituents were identified which represented 94.6-98.6% of the total detected GC peak areas.

Acknowledgments

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PFC PP 22

Evaluation of phytochemical constituents and antioxidant potential of leaf of *Petroselinum crispum* L.

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Parsley (*Petroselinum crispum* L.) is an aromatic plant from the *Apiaceae* family. It contains minerals, essential oils, vitamin C, phenolic compounds, flavonoids, non-flavonoids, pigments such as chlorophylls, carotenoids and it shows high antioxidant activity. The plant raw material is a product of the agricultural farm Igrošanac, located in the village of Medveđa near Trstenik, Rasin district.Tests were carried out in the laboratories of the Faculty of Agriculture in Čačak and included the following activities: determination of dry matter and moisture content, of ash content, vitamin C content, the content of photosynthetic pigments, the content of total phenols and antioxidant activity in parsley leaf. Determination of dry matter and ash content was performed by gravimetric method. The estimation of ascorbic acid was determined by titration method with Tillmans reagens. The total phenolic content was determined using a modified Folin-Ciocalteu colorimetric method. Antioxidant properties were determined by the ABTS assay. The content of chlorophyll and carotenoids was determined spectrophotometrically, with absorbance values recorded at wavelengths of 470, 648 and 664 nm. The moisture content in the parsley leaf was 8.22%, the dry matter content 91.78% and the ash content 23.54%. The vitamin C content was 87.5 mg/100 g/g d.m. The content of total phenols was 15.3 mg GAE/g d.m., while the antioxidant activity was 91%, ie. 27.44 µmol TE/g d.m. The content of total chlorophyll was 0.73, while the content of total carotenoids and xanthophylls was 0.10 mg/g d.m.

Based on the study of the characteristics of the parsley leaf, it can be concluded that it is a rich source of vitamin C, phenolic compounds, photosynthetic pigments with high antioxidant activity. Parsley is a good source of phytonutrient components. It is characterized by an exceptional wealth of phytonutrients that have functional value for the human body.

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PFC PP 23

Oil content in seeds of different local pumpkin genotypes

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Pumpkin is one of the oldest cultivated plant species. Common pumpkin (*Cucurbita pepo* L.) is primarily grown for its highly nutritious fruit and seeds, which contain oil. Pumpkin oil is a biologically valuable due to its exceptional composition of fatty acids (about 80% of fatty acids are unsaturated: linoleic and oleic), pigments, tocopherols, fitosterols, phenols and other bioactive components that have a beneficial effect on human health. Local genotypes are adapted to the ecosystem's conditions, allowing them to be traditionally grown with minimal or no agrochemical use. The goal of this study is to analyze the potential of local genotypes of unconventionally grown pumpkins to obtain oil.

The moisture content determined gravimetricaly in ground seed samples with the shell. The crude oil content was determined by extraction with petroleum ether from ground whole pumpkin seeds. Extractions were performed in a Solvent extractor (Velp. Scientifica-SER148, Italy) under the following conditions: immersion 30 min, washing 60 min and recovery 30 min. Extraction in a Solvent extractor saves solvent and time compared to classic Soxhlet extraction. The moisture content ranged from 4.25% to 6.91% (w/w). Low moisture content in the tested pumpkin seeds are favorable from the aspect of sustainability of the seed and the oil in it. Increased humidity would cause the action of lipolytic enzymes, resulting in the hydrolysis of triglycerides and the release of free fatty acids. The oil content ranged from 2.48% to 44%. One genotype stood out with an exceptionally high oil yield of 44%, comparable to high-yield oilseeds. Drought conditions in the 2021 season resulted in low pumpkin yields and reduced oil yields in many samples.

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PFC PP 24

Qualitative and quantitative analysis of lignans from wild chervil (*Anthriscus sylvestris* (L.) Hoffm.)

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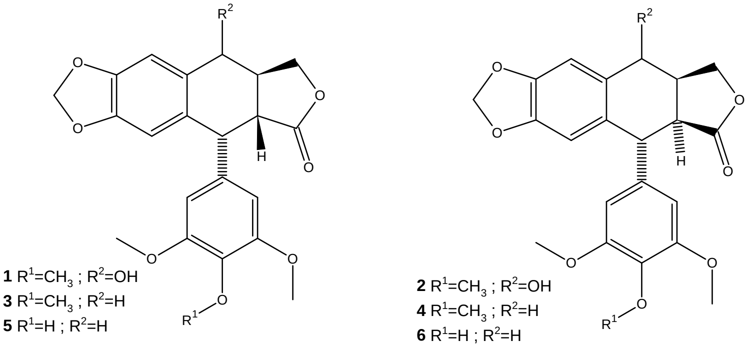
Wild chervil (*Anthriscus sylvestris* (L.) Hoffm.) is a wild-growing plant from Apiaceae family. It has been used as a food in Europe and eastern Asia, but also in traditional medicine to treat headaches, as antipyretic, analgesic, antitussive, tonic, diuretic etc. It is known to be rich in lignans with antitumor and antiproliferative, anti-inflammatory, antiviral, antioxidant, cardiovascular and insecticidal activity [1,2]. As a part of our on-going comprehensive study of *A. sylvestris*, we have employed LC-DAD-MS to identify six lignans from fruit extract (Figure 1): podophyllotoxin (**1**), picropodophyllotoxin (**2**), deoxypodophyllotoxin (**3**), deoxypicropodophyllotoxin (**4**), 4'-*O*-demethyldeoxypodophyllotoxin (**5**) and 4'-*O*-demethyldeoxypicropodophyllotoxin (**6**). HPLC–MS method was used to evaluate the content of podophyllotoxin, deoxypodophyllotoxin and deoxypicropodophyllotoxin in fruit extract. The most abundant fruit extract component was found to be deoxypodophyllotoxin (86,7% of the extract).



1 $R^1=CH_3$; $R^2=OH$
3 $R^1=CH_3$; $R^2=H$
5 $R^1=H$; $R^2=H$

2 $R^1=CH_3$; $R^2=OH$
4 $R^1=CH_3$; $R^2=H$
6 $R^1=H$; $R^2=H$

Figure 1. Structures of identified compounds.

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PFC PP 25

Assessment of antibacterial activity of *Sempervivum tectorum* L. leaves extracts using HPTLC bioassays and chemometrics

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Sempervivum tectorum L. is a perennial plant with succulent leaves arranged in a rosette. Despite its wide use in traditional medicine for the treatment of various changes on the skin, nervousness, anxiety, menstrual ailments, etc., it still does not have a biography in the European Pharmacopoeia [1]. The antibacterial effect of juice squeezed from the leaves and tea made from dried leaves was tested against bacteria that cause inflammation of the ear and bladder [2]. Direct bioautography on HPTLC plates for the investigation of antibacterial activity of the houseleek leaves extracts was done for the first time. Four HPTLC bioassays were developed for Gram-positive bacteria (*B. subtilis, M. lysodeikticus, MRSA*, and *S. aureus*), and two for Gram-negative bacteria (*E. coli* and *K. pneumoniae*). Antibacterial activity of Gram-positive bacteria comes from active compounds at R_F 0.57 and 0.92. HPTLC bioassays show higher sensitivity for Gram-negative bacteria, as numerous active bands were observed at R_F 0.03, 0.38, 0.42, 0.56, 0.57, 0.86, and 0.92. By applying principal components analysis, the HPTLC bioassays of Gram-positive bacteria were separated into two groups on the scores plot graphic along PC1 axis. The bioassays for *B. subtilis* and *M. lysodeikticus* form a less uniform group in the upper left quadrant, while the bioassays for *MRSA* and *S. aureus* form a homogeneous group in the lower right quadrant. Presence of the active bands at R_F 0.57 and 0.92 affect these separations. The bioassays for the two Gram-negative bacteria are separated along both axes on the scores plot graphic from each other but also from the other bioassays for the Gram-positive bacteria. This separation is influenced by the presence of numerous active bands. For further investigation it is necessary to identify compounds responsible for the antibacterial activity of the houseleek leaves extracts.

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PFC PP 26

Chemical composition of essential oils of two Eucalyptus species

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Eucalyptus is a genus of more than 700 species of flowering plants in the family Myrtaceae. Most species of *Eucalyptus* are native to Australia and islands north of it, and only a few are found wild-growing outside of this continent, while eucalyptus plantations have been grown in many countries. In this work, two commercially available eucalyptus essential oils, obtained by hydrodistillation of *E. Globulus Labill.*, and *E. Smithii R.T.Baker*, were analyzed using gas chromatography and gas chromatography-mass spectrometry. The constituents of these oils were identified through mass spectrometry and retention index (RI) data and, wherever possible, by co-injection experiments. While the major components of these oils exhibited similarities, they varied in their proportions. The most abundant component in both oils was 1,8-cineole (67.6–68.8%), but they also contained significant amounts of *α*-pinene (6.9–8.5%), and other monoterpenes, such as *p*-cymene, *α*-phellandrene, limonene, *γ*-terpinene, terpinolene, and α-terpineol, ranging from 0.1 to 6.0%. The identified sesquiterpenes were much less abundant and included (*E*)-caryophyllene, aromadendrene, and *β*-eudesmol, ranging up to 2.0%. In total, 137 constituents were identified which represented 95,3 and 99.4% of the total detected GC-peak areas.

Acknowledgments

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PFC PP 27

Properties of walnut cold-pressed oils

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Walnut has a long tradition of cultivation in Serbia. Walnut kernel contains significant amounts of oil 52-70% (w/dw) high nutritional and marketable value. Therefore, the aim of the research was to analyze the characteristics of fruits and cold-pressed oil of local walnut genotypes. Seven different walnut local genotypes were tested. The following morphological characteristics of the fruit were measured: fruit dimensions, mass and randman of the walnut kernel. The results are shown as the mean value of 20 fruits for each genotype. Average fruit weight ranged from 6.72 g to 10.49 g for different walnut genotypes. The yield of walnut kernels ranged from 25.63 to 36.18 %. Walnut oils were obtained by laboratory screw press at a temperature lower than 50 °C (OP650W, Gorenje, Slovenia). Oils obtained by cold pressing retain most of the initial unchanged chemical oil composition, due to the low temperature of the process. The analysis of the oil obtained in this way gives more representative results for characterisation in relation to oils obtained by extraction at high temperatures. Furthermore, cold pressing is an environmentally friendly method. The following parameters were determined for the obtained oil: moisture content and volatile matter (gravimetrically), refractive index (Abbe refractometer, A.KRÜSS, Germany) and recorded UV-Vis spectrum (Cary 3000, Agilent, USA). The moisture content and volatile matter in the analyzed oils were in the range from 0.006 to 0.03 % (w/dw) and were within the Regulations. The refractive index, one of the parameters for oil identification, varied from 1.4610 to 1.4750 at 23 °C, which may indicate differences in their fatty acid composition. All oil samples showed characteristic UV/Vis spectra for walnut oil without significant diferences between samples.

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Acknowledgments

This research was a part of the project "Potential of local pumpkin and walnut genotypes of the Central and Western Serbia for obtaining cold-pressed oils" funded by the Center for Scientific Research of the Serbian Academy of Sciences and Arts and the University of Kragujevac, and also was supported by the Ministry of Science, Technological Development and Innovation of Republic of Serbia under the project 451-03-68/2022-14.

PFC PP 28

Addressing the ambiguity of ^{1}H NMR assignments of testosterone by iterative full-spin analysis

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Steroid molecules exhibit complex ^{1}H NMR spectra due to spin system size and a large number of intricately coupled hydrogen nuclei appearing partially or completely overlapped in the saturated aliphatic region of the spectrum. Albeit complicated, the ^{1}H–^{1}H coupling patterns can be unveiled with adequate data treatment, as steroids are mostly conformationally rigid. Many regularities regarding coupling constans of hydrogen nuclei in particular positions on the steroid backbone have been observed and reviewed previously.

Testosterone (Figure 1) is the primary human male sex hormone, a well-studied analyte in biochemical assays. We were thus surprised to find literature ambiguity for the assignment of its diastereotopic protons at C-16, and consequently, coupling constat values for D-ring protons [1,2]. To address this issue, we performed an ^{1}H NMR iterative full-spin analysis using manual iterations in MestReNova, and obtained results which were in agreement with the work of Hayamizu and coworkers.

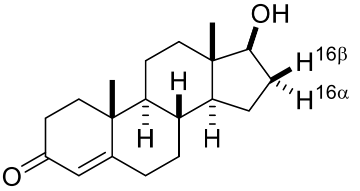

Figure 1. Structure of testosterone with the ambiguously assigned diastereotopic pair of hydrogens indicated.

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PFC PP 29

Polyphenols and antioxidant potential of medlar (*Mespilus germanica* L.) fruit from different locations in Serbia

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Medlar (*Mespilus germanica* L.) is a plant species belonging to the Mespilus genus (Rosaceae family). The plant is well known among folks in the southeastern part of Europe, Turkey, Iran and Iraq. Fruitsa are mostly used for fresh consumption, but also for the preparation of various products (jam, marmalade, jelly, wine, vinegar, juice,etc.) [1,2]. Medlar is becoming increasingly popular due to the unique attributes of its fruit which is a good natural source of bioactive compounds. Medlar fruit has a promissing application in gastronomy, and the food industry for the development of new products and value-added foods. Data about chemical composition of medlar fruits grown in Serbia are scarce [2]. In this regard, the aim of the study was to gain knowledge on the polyphenolic composition and antioxidant properties of fruits originated from different locations in Serbia.

The preliminary results on polyphenolic profile revealed that the fruits were good source of several phenolic acids: cholorgenic (11.61-14.44 µg/g), gallic (11.78-16.26 µg/g), caffeic (10.50-11.32 µg/g) and dihydrocaffeic (3-(3,4-dihydroxyphenyl) propionic) (13.96-14.56 µg/g). Ferulic acid was not detected in the fruit samples, whereas coumaric acid was detected in only one sample (11.27 µg/g). The medlar fruits were also rich in flavonoids: catechin (13.12-17.42 µg/g), epicatechin (17.06-64.36 µg/g), naringin (11.30-12.38 µg/g), and naringenin (17.61-18.41 µg/g). Total phenolic content in the fruts varied between 1376.94 and 2894.99 µg/GAE/g), while the values of the antioxidant activity measured in two assays (expressed on fresh fruits), DDPH (2,2-diphenyl-1-picrylhydrazyl) and FRAP (ferric reducing antioxidant power), were in the ranges 1057.56-1637.83 µmol trolox per gram (TE/g) and 603.96-1138.25 µmol Fe^{2+}eq, respectively.

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PFC PP 30

The effect of thermal treatment of hazelnuts on cold-pressed oil and biscuits properties

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Hazelnut oil is a high-value nutritional product, especially the one obtained by cold pressing. But it can undergo oxidative and thermo-oxidative changes due to its characteristic chemical composition, especially the presence of unsaturated fatty acidsacids. In this research, the influence of thermal treatment on the quality of cold-pressed oil and biscuits with this oil was examined. Hazelnut kernels were exposed to the following thermal treatment: 180 ˚C during 24 minutes. Hazelnut oils were obtained by laboratory screw press at a temperature lower than 50 °C (OP650W, Gorenje, Slovenia). Changes in hazelnut oil were determined by analyzing the following quality parameters:. content of water and volatile matter (gravimetricaly), refractive index (Abbe refractometer, A.KRÜSS, Germany), acid and peroxide values (volumetrically), specific absorbance and appearance of the UV-Vis spectrum (Cary 3000, Agilent, USA). Thermal treatment did not affect the content of water and volatile matter in the oil (for fresh and thermally treated hazelnut oil it was same value 0,04%) and the peroxide value (in both case it was 0 mmol O_2/kg oil). On the other hand, thermal treatment affected the deterioration of the other quality parameters of cold-pressed hazelnut oil. The value of the refractive index decreased in thermally treated hazelnut oil from 1.4655 to 1.4644. There was an increase in the value of specific absorbances. Increases in specific absorbance in thermally treated hazelnut oil are an indicator of the presence of primary and secondary oxidation products. Also the appearance of the spectra indicated certain oxidative changes.

In contrast, the analysis of the sensory properties showed that the cold-pressed oil obtained from thermally treated hazelnuts, which received a maximum of 20 points, was a preferable option. The same applies for buiscuits made from cold-pressed oil of thermally treated raw material, which proved to be very effective, with 18.08 points. All quality parameters of cold-pressed hazelnut oils in accordance with the regulations, regardless of the application of heat treatment and observed changes.

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Solution chemistry and Chemical equilibrium

SCCE PP 01

Physicochemical characterization and volumetric properties of the newly synthesized ionic liquid, 1-butyl-3-methylimidazolium benzoate

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In the 21st century, serious infections caused by microorganisms resistant to commonly used antimicrobial agents, have become a global healthcare problem. In 2019, the outbreak of the COVID-19 pandemic reinforced the importance of synthesis and characterization of the new antimicrobial substances. Designing new compounds such as ionic liquids (ILs) which show antibacterial activities is of great importance. ILs are compounds composed of organic cation and organic or inorganic anion. Their physicochemical properties can easily be tuned through a careful choice of the cation and anion. ILs have a melting point below 100°C and unique properties such as low flammability, wide liquid range, high thermal stability etc. Due to these unique properties ILs have generated attention for their potential use as green solvents. Most of the ILs show good antibacterial properties, but ILs that consist of the imidazolium cation were even more antibacterial as compared to positive control. Benzoic acid is commonly used as food preservatives. This is due to the low price and a wide spectrum of antimicrobial activity. Because of these properties, we chose these components for the synthesis of ionic liquid.

In this work, IL was synthesized, formed by combination of cation (1-butyl-3-methylimidazolium) and anion (benzoate), which individually showed a significant antimicrobial effect. The structure of 1-butyl-3-methylimidazolium benzoate [Bmim][Ben] was confirmed by FTIR and NMR spectra. Based on the measured density, viscosity and conductivity interactions between cation and anion were discussed. Also, to determine the influence of the newly synthesized IL on the structure of water, aqueous solutions of IL were prepared and the densities of solutions were measured. Results of density measurements could be used to describe the character of ionic solutions in terms of kosmotropic and chaotropic behaviour. Investigation of the antimicrobial effect of this IL is the next step of this research.

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Supramolecular Chemistry and Functional Materials

SCFM PP 01

A novel carbon paste electrode modified by NP-Y_2O_3 doped with the g-C_3N_4 for sensitive electrochemical detection of herbicide bentazone in river, soil, and vegetable samples.

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Pesticides have a significant role in the world food chain in the setting of rising agricultural output demand and rising climate change impacts on agricultural productivity. Pesticide contamination across the world is not just a pressing issue; it also has the potential to get worse, for instance, because of movements in global production to nations with laxer environmental regulations. [1]

In this work, we have designed a new electrochemical sensor for detecting bentazone (BZT) by using NP-Y_2O_3/g-C_3N_4 modified carbon paste electrode (CP). For the first time, the Pechini method was employed to synthesize the Y_2O_3 nanocomposite. The nanomaterial was characterized by X-ray powder diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). In order to create an analytical technique for identifying and measuring BZT, the electrocatalytic characteristics of the suggested Y_2O_3/g-C_3N_4 modified CP electrode were examined. Using the CV and DPV approaches, the electrochemical behavior of BZT at the Y_2O_3/g-C_3N_4 sensor was investigated. The proposed electrochemical sensor exhibited excellent electrochemical response toward BZT with a wide linear range of 1 to 100 µM, with a detection limit of 0.68 µM. The effect of possible interfering agents is negligible, confirming the good selectivity of the method. The sensor also displayed excellent sensitivity, reproducibility, and stability. Additionally, the Y_2O_3/g-C_3N_4 sensor was utilized for the detection of BZT in water and soil samples, and also in red and green pepper samples, and it exhibited good recovery results.

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SCFM PP 02

A novel gallium activated macroporous glycidyl methacrylate based copolymer and its antimicrobial potential

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Cross-linked macroporous copolymers based on glycidyl methacrylate (GMA) have been used as sorbents for metals, support for enzymes, as biomaterials etc. In this research GMA copolymer was prepared by copolymerization of GMA (glycidyl methacrylate) and EGDMA (ethylene glycol dimethacrylate), in the presence of inert component (90 mass% of cyclohexanol and 10 mass% of dodecanol), and functionalized with diethylenetriamine (DETA). Presence of epoxy groups in GMA-based copolymers allows chemical modifications on the polymer in order to achieve its different applications. GMA-based copolymer was activated with 0.1 M solution of $Ga(NO_3)_3$, at pH 3, and 25 °C [1].

Antimicrobial activity of functionalized and activated GMA-based copolymer, GMA/Ga, was analyzed against *Staphylococcus aureus* (Gram positive bacteria), *Escherichia coli* (Gram negative bacteria), *Candida albicans* (yeast) and *Aspergillus niger* (fungi) [2]. The agar-well diffusion method was used to evaluate antimicrobial activity of GMA/Ga polymer. Nutrient agar plates were inoculated with broth of 1 MFU microbial suspensions. Wells of 5 mm diameter were punched in the inoculated plates using a sterile metallic borer, and then filled with 100 µL of water solution containing nanoparticles of GMA/Ga copolymer, at various concentrations: 10, 20, and 30 mg/mL. Control wells were filled with 100 µL of distilled water. Inoculated plates were incubated at 37 °C/24 h for bacteria and yeast, and at 30 °C/48 h for fungus. Antimicrobial activity of Ga activated copolymer was evaluated by measuring the inhibition zone diameter around the wells. The GMA/Ga copolymer displayed good antimicrobial activity against *Escherichia coli* and *Candida albicans,* which makes it selective for Gram negative bacteria and yeasts, and as a material that can be potentially used for biomedical applications, in food industry etc.

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SCFM PP 03

Methacrylate-based hydrogels as sorbents for the removal of Mn^{+2} from aqueous solutions

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One of today's imperatives is the effective removal of pollutants from the biosphere, particularly from natural and wastewater sources. The removal of metal ions from solutions has long been a goal of numerous investigations, and hydrogels have been utilized as sorbent materials for this purpose. [1,2] This research was performed in order to create a new class of poly(oligo(propylene glycol methacrylate)/oligo(ethylene glycol methacrylate))/acid), abbreviated as p(OPGMA/OEGMA/acid), temperature-responsive copolymeric hydrogels and to analyze the influence of different acids on the volume phase transition temperature (VPTT) of the obtained hydrogels and on the efficiency of Mn^{+2} removal from the water. In this work, three acids were used: itaconic (IA), acrylic (AA), and methacrylate (MA), which were incorporated into the composition of the hydrogel in the monomer feed ratio OPGMA/OEGMA/acid of 95:2:3.

Henceforth, the obtained hydrogels p(OPGMA/OEGMA/acid) were synthesized for the first time by γ-irradiation polymerization and crosslinking of monomers from a water/ethanol solution. The hydrogels were put through swelling analysis and testing as potential sorbents once the high level of gel content was confirmed.

Taking into account the size of the metal ions, their concentration in the solution, and the porosity of the gel, the results show that hydrogels can be employed to remove manganese ions from solutions.

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SCFM PP 04

The synthesis, characterization, behavior in the Briggs-Rauscher reaction, and photoluminescence properties of newly created phosphate tungsten bronzes doped with cerium and praseodymium

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Phosphate tungsten bronzes (PWBs), due to their intriguing and potentially valuable properties, have consistently garnered research attention [1]. In this study, we introduced two rare-earth metallic elements, namely cerium and praseodymium, as dopants for PWBs. This led to the successful synthesis of novel PWBs doped with cerium and praseodymium, which were subsequently subjected to various characterization techniques, including thermal analyses (TA), Fourier-transform infrared spectroscopy (FTIR), X-ray powder diffraction (XRPD), scanning electron microscopy with energy-dispersive X-ray spectrometry (SEM-EDX), and photoluminescence spectroscopy (PL).

The behavior of cerium and praseodymium doped phosphate tungsten bronzes (Ce-PWB and Pr-PWB) [2], was investigated in the Briggs-Rauscher (BR) oscillatory reaction. The alterations in the oscillatory dynamics, brought about by the incorporation of cerium and praseodymium dopants, served as a means to distinguish between these bronzes. Additionally, this approach provided a method for assessing the catalytic properties of the bronzes. Apart from their nonlinear behavior, these bronzes also exhibited photoluminescence in the visible spectrum, specifically in the blue region.

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SCFM PP 05

p(AMPS)-Ni(0) hydrogel composite: Synthesis and catalytic activity investigation on the reduction of 4-nitroaniline

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The reduction of nitro aromatic compounds to their corresponding amines is an important process in the industrial production of many products, such as dyes, pharmaceuticals and agricultural chemicals. However, traditional methods of reducing nitro aromatic compounds generate a large amount of oxide sludge. This sludge causes a serious environmental concern. Therefore, it is necessary to develop alternative methods [1]. Metal nanoparticles have been used extensively as efficient catalysts for these reactions due to their high surface area to volume ratio. However, metallic nanoparticles are not stable due to their high surface energy, which strongly favors their aggregation, decomposition, and oxidation. Thus, to increase stability, metallic nanoparticles are generally prepared on various carriers [2]. Hydrogels can be suitable support materials in the preparation of metal particles. Additionally, they enable the flow of the reaction mixture and constant contact with the nanoparticles [1].

In this research, a composite of Ni(0) and poly(2-acrylamido-2-methyl-1-propanesulfonic) acid was synthesized in situ. Its catalytic effect on the reduction of 4-nitroaniline to p-phenylenediamine using sodium borohydride was investigated. The investigation was performed by monitoring the absorbance of the reaction mixture in the presence of the synthesized composite. The synthesized composite has shown an efficient catalytic effect on the reduction of 4-nitroaniline. The reduction efficiency was 63.2% after 90 minutes and the yield of the catalyzed reaction was nearly 6 times that of the uncatalyzed reaction.

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SCFM PP 06

Selection of deep eutectic solvent as a modifier of molecular imprinted polymer for aniline sorption

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Deep eutectic solvents (DESs) have been recognized as promising solvents due to their purity, high conductivity, bio-degradability, thermal stability[1]. These environmentally friendly solvents are important tools in the creation of green and sustainable technologies. The use of DES in polymer science is highly promising for the development of novel green materials. Therefore, DESs have been used in molecular imprinting in order to improve the properties of molecularly imprinted polymers (MIP). DES are most often prepared by combining two classes of compounds: hydrogen bond donor, HBD (such as amide) and hydrogen bond acceptor, HBA (such as quaternary ammonium salt) in different molar ratios[2]. By mixing these components in with appropriate molar ratios, eutectic mixtures are formed in a liquid state at temperatures below 100 °C. This study reports the ability of DES-MIP as a sorbent for the removal of aromatic amine from plastic packaging. In order to obtain the most effective sorbent, DESs are prepared by combining choline chloride as HBA with different HBDs, such as urea, glycerol, and ethylene glycol. The results showed that choline chloride:urea was the most suitable DES as modifier of MIP.

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SCFM PP 07

The influence of irradiation modalities and preparation conditions on different properties of irradiated low-density polyethylene and isotactic polypropylene

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The current study reveals the impact of different irradiation modalities, gamma and electron beam (EB) radiation, diverse initial preparation conditions (quenching and slow cooling of the samples following compression molding), and consequential differences in the initial crystallinities on the response of LDPE and iPP samples to the applied ionizing radiation. Gamma and EB radiation of LDPE and iPP libraries in the air at room temperature is performed to a total dose of 25, 50, and 100 kGy. The investigation of microstructure, crystallinity, oxidative degradation, thermal, mechanical and dielectric behavior was performed. The obtained results may be of interest in the practical application of ionizing radiation in various polymer-based technologies, including cable, automotive, packaging, textile, and other industrial uses[1].

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SCFM PP 08

Multifunctional up-converting nanophosphorus: photoluminescent and photocatalytic properties

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In this study, we present the synthesis of a novel multifunctional materials, with particular accent on their photoluminescent and photocatalytic abbilities. $SrGd_2O_4$ powders co-doped with rare earth ions (Yb^{3+}/Er^{3+}, Yb^{3+}/Ho^{3+} and Yb^{3+}/Tm^{3+}) with different mutual ratios are prepared *via* combustion route. X-ray Powder Diffraction patterns proved that all samples crystallize as a pure orthorhombic phase. Luminescence properties were measured and characteristic emission lines were revealed for each dopant system: red emission at 661 nm and two green emissions at 551 and 523 nm for Yb^{3+}/Er^{3+} samples; green emission at 550 nm, red emission at 671 nm and infrared emission at 758 nm for Yb^{3+}/Ho^{3+} samples; two blue emission bands at 450 nm and 474 nm, and red emission band at 650 nm for Yb^{3+}/Tm^{3+} co-doped samples. UV-VIS Diffuse Reflectance Spectroscopy was performed in order to examine materials bandgap. Value of 4.3 eV was obtained for each sample, as well as the additional values from the bands at lower energies, which indicate potentially good photocatalytic properties. UV-VIS Absorption Spectroscopy was used to measure changes of the methylene blue concentration during the photocatalytic degradation process. After 4 h of exposure to the simulating Sun irradiation, more than 60% of the initial dye concentration was decomposed. Reaction parameters (MB concentration and catalyst mass) were altered in order to achieve the best photocatalytic performances of this newly synthesized materials.

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SCFM PP 09

Electrochemical study of Li-ion intercalation into anatase TiO_2 nanotubes at different temperatures

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Lithium-ion batteries (LIBs) are the most promising energy storage devices on the market today. Their importance is reflected in the fact that LIBs power numerous portable devices and that they are being developed for electric and hybrid electric vehicles [1]. Most commercial LIBs are composed of a graphite anode, which cannot meet high performace requirements [2]. Several transition metal-oxide based hosts have been considered as potential alternatives to the graphite anode, including TiO_2. Low cost, high Li-ion insertion potential, low volume expansion and good cycling life make TiO_2 a promising anode material. Different polymorphs of TiO_2 have been investigated, and preference is given to the anatase phase. Herein, anatase TiO_2 nanotube arrays (NTAs) electrode was preapred by anodic oxidation of Ti-foil and subesquent annealing at 400 °C. SEM micrographs show that the nanotubes (NTs) are cylindrical in shape, with an average inner diameter of about 95 nm and wall thickness ~15 nm. In the Raman spectrum, five active modes which correspond to the anatase phase are present. XRD pattern of as-prepared Ti/TiO_2 NTAs electrode was recorded, and the strongest diffraction maximum of anatase phase was used for the claculation of the mean crystallite size. The obtained value is 19 ± 1 nm. Electrochemical experiments, which included cyclic voltammery (CV), electrochemical impedance spectroscopy (EIS) and galvanostatic (GS) cycling, were carried out using a termostat in the temperature range from 25 – 55 °C. The 1 M solution of $LiClO_4$ in propylene carbonate was used as an electrolyte in all cases. CV experiments demonstrated an increase in the redox peak intensity and a decrease in peak-to-peak separation at higher temperatures, indicating improvement in Li-ion storage capability and better reversibilty of Li-ion intercalation/deintercalation process. GS cycling showed a large Li-ion insertion capacity of Ti/TiO_2 NTAs electrode, high Coulombic efficiency (CE) and good capcity retention. Lithiation capacity at 55 °C attains 357 mAh·g^{-1} at current rate 5.3 C, with CE of 97.5% and capacity retention of 98.5% after 50 cycles. EIS showed with increasing temperature a multifold decrease in solid electrolyte interphase (SEI) layer resistance and charge transfer resistance. EDS and FTIR spectra of Ti/TiO_2 NTAs electrode were recoreded to better underastand the nature of the formed SEI film.

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SCFM PP 10

Deposition of Ti/Zr/Ti thin film on laser pre-patterned silicon substrate

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The experimental analysis of the deposited Ti/Zr/Ti thin film system on substrate pre-patterned by femtosecond laser is reported. In order to develop arrayed surface structures for biomedical applications, the design of surface pattering with micrometre features in the form of spikes is being researched. Under 0.65 bar of SF6 ambient pressure, femtosecond laser pulses were employed to acquire black silicon surfaces ornamented with conical structures (spikes) on crystalline silicon surfaces. After irradiation, the silicon surface has high aspect ratio spikes with conical morphologies of about 2 µm height, 40° angle opening, and $13 \cdot 10^6$ cm^{-2} dislocations density, roughly consistent over the treatment area. On such a prepared surface, ion sputtering was used to create a unique composite thin film consisting of Ti thin film with a sub-surface layer of Zr. The deposited system in form of Ti/Zr/Ti has a total thickness of 400 nm. FESEM-EDS and XPS were used to assess the composition and surface morphology. Post deposition of Ti/Zr/Ti onto Si laser-patterned resulted in diffusion of Ti and Zr layers as it was revealed by transmission electron spectroscopy and energy dispersive X-ray spectroscopy.

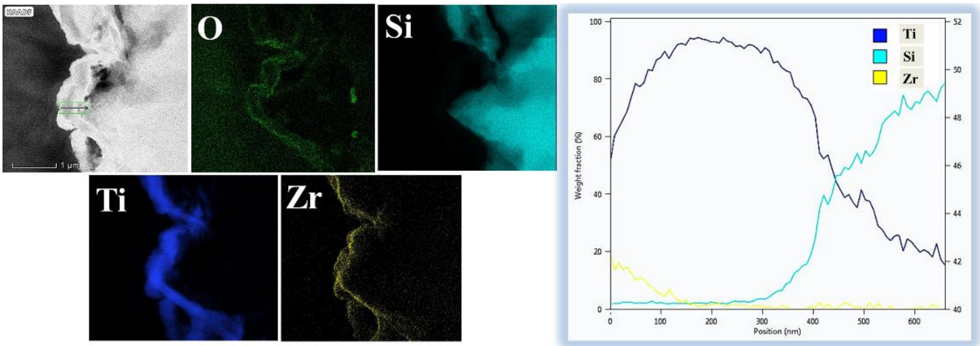

Figure 1. STEM-HAADF image of Ti/Zr/Ti laser-patterned thin film with the 400 nm thick layer with corresponding EDX maps. Elements Ti, O, Si and Zr are highlighted (left side) and elemental line profile along the green line as shown in the HAADF image are shown (right side).

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SCFM PP 11

Starch aerogels impregnated using supercritical CO_2: Application in controlled release of biologically active compounds

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This research explores the potential of starch aerogels impregnated with thymol, carvacrol and eugenol using supercritical CO_2 as systems for controlled release of these biologically active compounds. Systems for controlled release can be used to overcome the problem of inadequate dosing of active substances and to reduce the application frequency with the main purpose of keeping the active substance concentration constant in the target tissue for a long period [1]. Such systems can be made from biocompatible and biodegradable polymers, such as low-cost and widely accessible starch, which was processed into aerogels. Aerogels are highly porous materials with large specific surface area making them of great interest for controlled release of active compounds. Some of the advantages of impregnation using supercritical CO_2, besides avoiding the use of organic solvents, are working at low temperatures, homogenous dispersion of active substances through the polymer matrix, avoiding the drying process, low energy consumption and total separation of the supercritical fluid at the end of the impregnation process [2].

Starch aerogels were prepared by drying of starch alcogels using supercritical CO_2 alternately statically and dynamically during 2 h 40 min. The obtained aerogels were impregnated with thymol, carvacrol and eugenol in a batch mode using supercritical CO_2 during 2 h. The release kinetics of the active compounds was investigated by immersing the impregnated aerogels in a phosphate buffered saline solution at 37 °C during 72 h. The active substance concentration was determined using a UV-Vis spectrophotometer. The active compounds release kinetics was described with Korsmeyer-Peppas, zero-order, Higuchi and first-order models.

All three biologically active compounds were released in a controlled manner during 24 h. The maximum release percentages were 99.8% for thymol, 88.3% for carvacrol and 99.6% for eugenol. The obtained results suggest that developed starch aerogels impregnated in the described manner can potentially be used as systems for controlled delivery of thymol, carvacrol and eugenol during a long period. Due to their properties, such systems could be used for manufacturing wound dressings.

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SCFM PP 12

The effect of mechanical alloying parameters on the copper matrix composite materials

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In powder form, copper (Cu) is the most used element in alloys and composites thanks to its affordability, availability, and capacity to easily improve its properties by adding just a few other elements [1]. It is then of no surprise that Cu composite materials find their application in various industries such as medical devices, aerospace, defense, automotive parts and electronics [2]. In this instance, a hybrid ternary Cu-2wt%Zr-0.6wt%B composite was designed. Mechanical alloying (MA) was used to produce adequate powders for further composite manufacturing. The MA process was conducted in two different devices, Atritor Mill and Turbula Shaker Mixer, to determine the effect that the mixing type has on the final material. The milling parameters were set as (i.) duration for 10 h, 20 h, 30 h, and 40 h, (ii.) ball-to-powder ratio was 10:1, (iii.) inert atmosphere - argon. Electron microscopy and X-ray diffraction were used to investigate the microstructural and morphological properties of the Cu-Zr-B MA powder. Obtained results indicate that MA powders produced in Atritor show lower values of structural parameters (crystallite size, lattice parameter and lattice strain) compared to one in Turbula up to 30 h of milling. It should be noted that values of structural parameters after 40 h of milling in Turbula are lower compared to those in Atritor due to the recrystallization of Cu particles. Based on XRD results, the dislocation densities (ρ) were calculated and exhibited that MA powders milled in Atritor possess lower ρ values compared to MA powders milled in Turbula, except ρ of MA powders after 40 h. Higher values of observed structural parameters of MA powders revealed that during milling in Turbula, powders have been exposed to stronger forces in ball-powder-ball and ball-powder-wall collisions.

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SCFM PP 13

The influence of dopants on anatase-rutile phase transition

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Titanium dioxide exists in three different crystalline forms: anatase, rutile, and brookite. It is well known that on heating, anatase and brookite can be easily transformed to rutile which is considered as the most stable phase [1]. The aim of this study was to investigate the influence of different dopants on anatase-rutile phase transition. Doped TiO_2 samples (TiO_2-M, M = V, Mn, and Cu) containing 5 at% of the dopant were prepared by mixing anatase and appropriate oxide (V_2O_5, MnO_2, and CuO) in agate mortar for 30 min. In order to determine the heat treatment conditions, TG/DTA analysis of the samples was performed. Finally, mixed powders as well as the pure anatase phase (TiO_2) were heat treated at 700 °C for 3 h. XRD analysis was performed to estimate the phase composition, unit cell parameters, and crystallite sizes. Rutile was formed in all samples: 2.8 wt% in TiO_2, 25.5 wt% in TiO_2-Mn, 75.8 wt% in TiO_2-V, and 95.2 wt% in TiO_2-Cu. In TiO_2-Mn, TiO_2-V, and TiO_2, anatase was present beside rutile, while in the case of TiO_2-Cu 4.8 wt% of the unreacted CuO was found. Obtained results revealed that all the dopants accelerated anatase-rutile phase transition in the following order: $Cu^{2+} > V^{5+} > Mn^{4+}$. It is well known that defects are the driving force for the anatase-rutile phase transition and since Ti^{4+} and Mn^{4+} are isovalent, no new defects were formed by incorporating Mn^{4+} ions into TiO_2 lattice. This resulted in the least amount of rutile in TiO_2-Mn comparing to TiO_2-V and TiO_2-Cu where new defects were probably formed. As no initial oxides were found in TiO_2-Mn and TiO_2-V, it can be concluded that Mn^{4+} and V^{5+} ions were incorporated into the anatase lattice. On the other hand, in the case of TiO_2-Cu, even 4.8 wt% of initial CuO was found. The detected residue of CuO can be explained by the fact that the ionic radius of Cu^{2+} for an octahedral environment (0.870 Å) is much larger than that of Ti^{4+} (0.745 Å), unlike those for Mn^{4+} (0.670 Å) and V^{5+} (0.680 Å). Although almost all introduced quantity of CuO, i.e. 96 %, was found in TiO_2-Cu, a small amount was surely necessary to cause the anatase-rutile phase transition. According to calculated crystallite sizes which were in the range of 55 – 90 nm, nanocrystalline samples were prepared.

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SCFM PP 14

Predicting the modulus of elasticity for biocompatible titanium alloys

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Titanium alloys have been present for decades as the main components for the production of various orthopedic and dental elements. However, modern times require titanium alloys of different composition, with lower modulus of elasticity, without the presence of toxic alloying elements such as Al and V [1]. Traditional methods used to detect dependencies between parameters, as well as alloy design, are often not particularly effective and usually require large investments of time and resources. The study introduces the machine learning technique Extra Tree Regression, which, through the analysis of data from 246 biocompatible titanium alloys, identifies factors associated with reduced elastic modulus [2]. The three most influential were: specific heat and mass fraction of titanium and mass fraction of titanium silicon. Using data on the most influential factors, four-component diagrams were designed where certain alloy compositions reach a modulus of up to 54 GPa. In addition, Monte Carlo simulations were used to demonstrate the feasibility of modeling multicomponent alloys with elastic modulus below 70 GPa.

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SCFM PP 15

Development of flexible and cost efficient enzymatic ZnO-based biosensors for glucose detection

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In this study, an amperometric glucose biosensor was fabricated by immobilizing glucose oxidase on ZnO nanoparticle functionalized electrodes, by direct physical adsorption method. Fabrication of biosensor transducer was carried out using e-beam deposition of gold layer on a low-cost and flexible plastic substrate. The desired planar electrode geometry was written in the gold layer with laser ablation technology. A reference electrode was consequently screen printed with commercial Ag/AgCl paste. Functionalization of biosensors working electrode with ZnO layer was performed using screen-printing method and electrochemical deposition. For the screen-printed biosensor, a functional paste with ZnO nanoparticles, ethyl-cellulose as a binder and terpineol as a dispersant, was designed and optimized to obtain a sensitive layer with enhanced specific surface area, suitable for electrochemical detection. Characterization of sensor components (transducer and sensitive layer) was performed with scanning electron microscopy (SEM), X-ray spectroscopy, and Raman spectroscopy. As glucose production is proportional to that of H_2O_2, measuring the H_2O_2 electrochemical reaction current is a convenient method of determining the glucose concentration [1]. Cyclic voltammetry measurements demonstrated that utilized sensor designs are effective in glucose detection. On voltammograms for screen-printed and electrodeposited ZnO-based biosensors characteristic peaks of glucose decomposition into H_2O_2 is clearly observed. In order to determine the performance of biosensors in real time monitoring of glucose levels, chronoamperometry measurements were performed at +0.6 V vs. Ag/AgCl. The present glucose biosensors based on ZnO show that the change in current increases with the rise in glucose concentration, ascribed to the glucose oxidation by glucose oxidase with FAD cofactor, leading to the production of H_2O_2. Subsequently, the H_2O_2 underwent electrochemical oxidation at the electrode surface under constant voltage, releasing electrons, and augmenting the current responsiveness.

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