Society of Chemists and Technologists of Macedonia

Сојуз на хемичарите и технолозите на Македонија

26th Congress of SCTM

with international participation

BOOK of ABSTRACTS

20–23 September 2023
Metropol Lake Resort
Ohrid, R. Macedonia

Сојуз на хемичарите и технолозите на Македонија

Society of Chemists and Technologists of Macedonia

20–23 September 2023, Metropol Lake Resort, Ohrid

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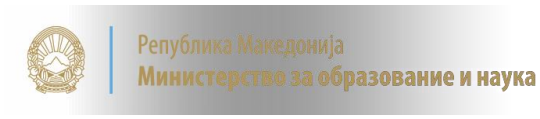

Ss. Cyril and Methodius University, Skopje

Dear Esteemed Colleagues and Participants,

It is with great pleasure that we present the Book of Abstracts for the 26th Congress of the Society Chemists and Technologists of Macedonia, which was originally scheduled for 2020 but, due to the global pandemic caused by Covid-19, has been rescheduled to this momentous occasion. As we gather here in the breathtaking backdrop of the historic city of Ohrid, Macedonia, we reflect not only on the innovative strides made in the field of chemistry and chemical engineering, but also on the unwavering spirit of resilience that has brought us together despite the challenges that have beset us. The world has experienced an unprecedented disruption, testing the limits of our adaptability and resolve. Yet, as chemists and chemical engineers, we have shown that the pursuit of knowledge and advancement knows no bounds. Our ability to transcend obstacles, adapt methodologies, and harness innovation in the face of adversity is a testament to the invincible human spirit.

Within the pages of this Book of Abstracts with 15 invited lecturers and almost 200 presentations from 174 authors and 570 coauthors from the region and much wider making it a really international meeting, you will find a diverse array of topics that reflect the vigor and dedication of the scientific community. From breakthroughs in green chemistry to pioneering developments in materials science, from the forefront of pharmaceutical research to cutting-edge advancements in nanotechnology, each abstract showcases the remarkable flexibility and ingenuity of our colleagues.

We extend our deepest gratitude to Prof. Jadranka Blaževska Gilev and Prof. Biljana Angjuševa, the organizers of this meeting who have dedicated all their efforts and time to make this meeting possible. Our gratitude goes to all members of the scientific and organizational committees who have been in the background making sure things flow seamlessly. Also, our appreciation goes to the reviewers and all participants who have come together to give the substance to this Congress. Your commitment to the scientific endeavor underscores the importance of collaborative efforts in times of uncertainty. It is through the exchange of ideas, the sharing of knowledge, and the fostering of connections that we fortify ourselves and drive the progress of our disciplines. Furthermore, our deepest gratitude goes to the sponsors given in the back cover of this book and most of all to the Organization for the Prohibition of Chemical Weapons who have always given their support to our meetings.

As we come together in Ohrid, we do so with renewed appreciation for the importance of shared experiences and face-to-face interactions. We eagerly anticipate the discussions, debates, and collaborations that will shape the future of our disciplines. Let us seize this opportunity to learn, inspire, and foster connections that will resonate long after the congress concludes.

We hope that this Book of Abstracts serves as a source of inspiration and a record of the remarkable work presented at the 26thCongress of SCTM. Let us seize this opportunity to celebrate not only our achievements, but also our resilience, determination, and enduring commitment to the pursuit of knowledge. Let us navigate the challenges together, and through our collective efforts, continue to inspire innovation that transforms the world in a positive way.

With warm regards,

Prof. Zoran Zdravkovski, president

Society of Chemists and Technologists of Macedonia

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PL 1

Innovative Biobased Polyurethanes from Cradle to Cradle

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Nowadays, the use of renewable biobased carbon feedstock from different resources, such as vegetable oils, is highly taken into consideration because it offers the intrinsic value of a reduced carbon footprint with an improved life cycle analysis, in agreement with a sustainable development. Besides, compared to conventional fossil-based materials, innovative macromolecular architectures with improved or additional properties can be obtained.

In this presentation, we report two decades of active research on the synthesis, characterization, and processing of several innovative and renewable polyurethanes (PUR, PIR, TPU and NIPU)[1,2], with controlled macromolecular architectures to elaborate different designs and morphologies (membranes, foams)[3], for a large range of green applications. These materials are synthesized from different biobased building blocks, which can be directly extracted from biomass or obtained from white biotech (fermentation,): (i) Aliphatic structures from different glycerides and derivate (dimer fatty acids,), sugar-based molecules, bacterial polyesters … (ii) Aromatic structures from lignins[4,5], tannins[6] and furans. A large range of materials with improved properties and durable applications have been developed/synthesized for a greener and durable future. The end of life of these materials is now also considered, by e.g., bio-recycling[7], from cradle to cradle.

Keywords: Polyurethane, Foam, biobased, TPU, NIPU, polymer

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PL 2

Ultrasensitive electrochemiluminescence imaging of single entities: from cells to biomolecules

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Electrochemiluminescence (ECL) is the light emission triggered by an electrochemical reaction at the electrode surface [1-2]. Since ECL is based on an "electro-excitation" process, it does not require any light source to generate the light as in fluorescence. Thus, ECL combines intimately electrochemistry and photophysics. Due to the orthogonal modalities of electrochemical stimulation and optical readout, ECL attracts growing interests in diverse scientific fields, from fundamental research on Marcus inverted region and design of highly efficient ECL fluorophores to original biosensing and imaging strategies.

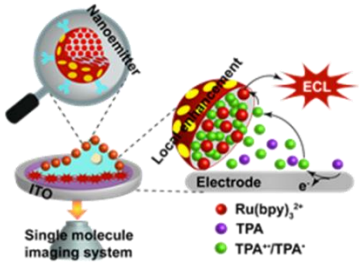

Figure 1. *ECL microscopy at the single molecule level.*

In the first part, the development of coreactant-based ECL as a surface-confined microscopy to image single cells and their membrane proteins down to the single molecule level (Figure 1) will be discussed [3-7]. In a second part, new ECL approaches such as photo-induced ECL based on illuminated semi-conductors will be presented to extend the performances of ECL (bio)sensing and photo-addressable systems [8-10].

Keywords: electrochemistry, luminescence, microscopy, single cells, nanomaterials

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IL 1
Biocompatible Poly(Vinyl Alcohol)-Based Hydrogels For Medical Applications

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The biomaterials field is always evolving towards finding new wound dressing formulations which can provide active protection of the wound from bacterial infections. Hydrogel-based materials are especially interesting for such a purpose, considering their favorable biocompatibility, sorption and mechanical properties, as well as the potential for immobilization and incorporation of antibacterial agents. The synthesis of silver nanoparticles (AgNPs) became very interesting for potential applications in biomedicine, since nanocrystalline silver is proved to be the most efficient antimicrobial agent with a wide inhibiting spectrum towards different types of microorganisms. AgNPs embedded in hydrogel matrices are attractive for biomedical applications due to possibility for their controlled release resulting in antimicrobial activity. Thus, combination of AgNPs with biocompatible hydrogels, poly(vinyl alcohol) (PVA) and chitosan (CHI), provides potential for design of improved medical treatments. Graphene (Gr) has exceptional mechanical properties and has therefore been applied as adequate reinforcing component for composite materials. In this work, we synthesized new composite hydrogels with electrochemically synthesized silver nanoparticles, Ag/PVA/Gr and Ag/PVA/CHI/Gr, aimed for wound dressing materials. Hydrogels were characterized by UV-Vis, CV, FE-SEM, Raman, AAS, FT-IR, MTT cytotoxicity tests and test of antibacterial activity against *Staphylococcus aureus* and *Escherichia coli*. The results indicated that both hydrogels are excellent candidates for soft tissue implants and wound dressings [1-3].

Keywords: hydrogels, poly(vinyl alcohol), silver nanoparticles.

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IL 2

The effect of garment interlayers on evaporation resistance of textile laminates with hydrophilic membranes

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Water vapor permeability, often expressed as evaporation resistance Ret, belongs to the most important thermal comfort parameters of protective, sport and other functional clothing (garments) and related textile fabrics. Water vapor permeability of all textile products should be as high as possible, in order to prevent the accumulation of sweat in the garment system and simultaneously enable efficient cooling of a body by the sweat evaporation. For outdoor or industrial applications, these garments should also exhibit the so-called semipermeability: the textile laminates creating the outside garment fabrics contain micro - or nanoporous membranes, which prevent the penetration of outside liquid water into the laminates, but simultaneously allow the passage of water vapour from the body through the whole fabric system.

In microporous membranes, their semi-permeability is given by their porosity, practically independent of the average moisture level inside the membrane. Contrary to that, water vapor resistance of nanoporous membranes depends strongly on the average moisture level inside the membrane. The average moisture level inside the fiber structure is then proportional to the moisture level (characterized by water vapor partial pressure) on both sides (surfaces) of the nanoporous membranes.

In the study, a new observation based on the above requirement of the highest level of water vapor partial pressure on both membrane surfaces, is presented. It was found, that when a jacket containing a nanoporous membrane is worn over an underwear garment system with high thermal (and also evaporation) resistance, then the average moisture level inside the nanoporous membrane can be significantly lower, then in case of testing the only nanoporous laminate in a testing instrument. This low moisture inside these membranes will significantly reduce WV permeability of the laminates. That is why the effective water vapor permeability of e. g. outdoor jackets with nanoporous membranes, when worn over several fabric layers, can be much lower than marketed levels of these outdoor garments. Clients wearing these clothing may suffer from sweat accumulation and overheating caused by reduced transfer of the evaporated sweat.

Keywords: textile laminates, hydrophilic membranes, water vapor permeability

IL 3

On the properties of perovskites thin films for solar cells

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Structural and morphological properties of $CH_3NH_3PbI_3$ thin films deposited by spin coating, with different spin speeds on glass and ITO patterned substrates were investigated. It results that long length acicular crystals, growth parallel to substrates (> 200μm for spin speeds of 800RPM/min). For low deposition spin speed these crystals are interconnected and deposited films present high electrical conductivity. The XRD investigations indicate the formation generally of the cubic phase, or a mixture between cubic and tetragonal phase. For compact films the absorption is high over a large range of spectral domain (from 200 nm to 2100 nm), the transmission being lower than 20% in IR and less than 15 % in the visible domain. From electrical properties point of view, films are highly sensitive to light. A decrease of the electrical resistivity with three order of magnitude is noticed when films are exposed to a white light of a solar simulator with an intensity of 1000W/m^2, but also an important decrease is observed also when films are exposed to a continuous low intensity ambient light, at least one order of magnitude in less than six seconds. This behavior is identical no matter the films thickness. The variation of the electrical resistivity at exposure to light in function of time and light intensity and the variation of the electrical resistivity in function of temperature were investigated and interpreted. The experimental results, since now, comforting the assumption of a multiband model.

Keywords: $CH_3NH_3PbI_3$, perovskites, electrical conductivity, photoconductivity, band gap

IL 4
Fermentation – from food industry by-products valorization to neurotransmitters production

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Lactic acid bacteria (LAB) are employed as a biotechnological starters to improve the safety and functionality of food and feed, to provide added value and to increase safety of food industry by-products, to design synthesis of functional molecules in fermentable substrates, to moderate the technologies for safer alternative stock incorporation to the main food formulas, to perform conversion of microalgae to valuable molecules possessing neurotransmitters characteristics. The addition of starter cultures under controlled conditions is a highly prospective technology for sustainable food and feed materials preparation. Metabolites of the LAB as well as viable LAB cells in fermented materials leads to desirable changes in mammals digestive tract microbiota *in vivo*. Additionally, the high-functionality fermented food ingredients can be produced by applying LAB for the food industry by-product valorization. Also, fermentation with LAB greatly contribute not only to the flavour, aroma, and texture of the final product but also to functional molecules synthesis, e.g., galactooligosaccharides can be synthesized from the dairy industry by-products containing lactose; gamma-aminobutyric acid (GABA) can be produced from the substrates containing L-glutamic acid (e.g., Spirulina). Additionally, LAB can excrete precursors (L-glutamic acid) for further GABA production in vivo. This type of bioconversion is a very promising technology for food, feed, nutraceuticals, pharmaceuticals, and supplements production. Finally, our works showed, that LAB application in industry is extremely broad: from food industry by-products valorization to neurotransmitters production.

Keywords: Lactic Acid Bacteria; Industrial Biotechnology; Fermentation.

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IL 5

Development of novel bio-based materials with advanced properties

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Development of bio-based materials with advanced properties will enable continued progress and improve human life. The growing pressure for resolving ecological problems, but also to shift research toward circular economy, makes bio-renewable and biodegradable materials, such as poly(lactide) (PLA) very important. Given that a convenient approach can manipulate the structure of PLA at the molecular level, enables the development of different methods for the production of a wide range of PLA with suitable properties. The development of novel polymerization techniques allows the economical production of high molecular weight PLA, resulting in expanded use of PLA in packaging, medical or pharmaceutical applications, in agriculture to prevent freezing, as a system for self-healing of concrete and so on. The architecture of PLA based polymers can be modified by incorporating multifunctional monomers into the polymer chain in order to obtain bio-based materials with advanced properties. PLA can be designed to biodegrade within a reasonable timescale, which makes this polymer an ideal candidate for use in biomedical and pharmaceutical purposes. For drug delivery system, PLA was used as a nanofiber matrix (in dentistry) or microspheres carrier (for oral application). The potential that PLA is showing in newer applications in biomedicine, such as tissue engineering and wound healing, indicates that PLA will become an important material for the future high-value medical market. Special design of PLA nanofibers enables fine tuning of electrical and/or optical properties of PLA based conductive polymers which make them suitable for novel application. Such novel materials are coveted in various fields of biomedicine such as bioengineering, regenerative medicine, and biosensors, and consider as a good platform for future research.

Keywords: polylactide, bio-based materials, advanced polymers, polymeric DDS

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IL 6

Harnessing size segregation effects in film-forming formulations

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The drying process of film-forming formulations such as paints and coatings involves the assembly of micro and nanoparticles and aggregates in suspension into a film as the solvent evaporates. The ways in which these ingredients are assembled will dictate the architecture of the dried coating and therefore its performance. For example, in the case of antibacterial paint, the amount of bactericidal agent that accumulates at the top surface will determine its effectiveness against microorganisms.

We have proven that in drying blends of large and small colloidal particles, small particles can become trapped near the air-water interface as it moves down [1]. This results in a particle concentration gradient from the top to the bottom of the wet film, which drives large particles to diffuse down. As a result, a stratified colloidal film is formed with an enrichment of small particles at the top and most large particles at the bottom. In this talk, I will describe how we can harness and tune this size segregation process to tailor the final structure of bactericidal [2] and abrasion resistant [3] coatings, as well as recent advances to understand the influence of rheology modifiers on this process. These concepts are applicable to other functional coatings as well as to a wider range of products based on the drying of particle suspensions such as inks, adhesives, or cosmetics.

Keywords: colloids; polymers; coatings; formulation; self-assembly

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IL 7

Recycled Aggregate Concrete - Current Challenges

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The construction industry is one of the most resource-intensive economic sectors in the world. In the EU, it is responsible for using around 50% of all raw materials mined. 90% of the raw materials used are non-renewable mineral raw materials such as stones, gravel and sand. Their mining causes extensive interventions in nature and landscape.

At the same time, the construction sector produces one of the most voluminous waste streams. It is responsible for about 30% of the waste generated in the EU. 65% of these are mineral waste (concrete, brick, mortar), with the highest proportion being concrete.

Over 80% of construction and demolition waste is recycled for low-grade reuse in a circular economy (e.g. as loose-fill in road construction) and around 10% ends up in a landfill.

Recycled concrete presents an excellent opportunity to increase resource conservation in the construction industry significantly and to return a significant part of the mineral waste masses to building construction, thus closing material cycles.

This presentation will discuss the current scientific, technical, economic, public and legal barriers and challenges to the broader use of recycled aggregate in concrete.

Keywords: Recycled aggregate, recycled aggregate concrete, challenges, mechanical properties, durability

IL 8

Occurrence of contaminants of emerging concern in water resources and the related analytical challenges

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Numerous chemicals have entered the environment for decades of industrialization and urbanization from a variety of anthropogenic sources. Currently, more than 350,000 chemicals have been registered for commercial use worldwide, with even more new chemicals expected to appear in the future. Only a small fraction of them, accounting for (far) less than 1%, has been routinely monitored in the environmental compartments. Water resources are especially endangered by chemicals in wastewater treatment plant effluents, urban street run-offs and storm waters, leachates from agricultural fields and landfills, etc. This is a cause for concern for water quality, either drinking, underground, or irrigation water. In the last decade particular attention has been focused on organic micropollutants such plasticizers, flame retardants, industrial chemicals, pharmaceuticals, microplastics, personal care products (PPCPs), etc., all considered as contaminants of emerging concern (CECs). Among them there are many persistent and mobile pollutants, which effects can occur over long, intergenerational time scales. Still, the current scale of the occurrence and exposure to CECs is only partly known due to limitation of routine analytical approaches. The aim of this presentation is to give an overview of the problems associated with the CECs' occurrence in water resources and of the available analytical approaches for its determination. It is of special importance to develop and harmonize methods that may enable detection of as many as possible CECs in one analytical run, contributing to the reliable estimates of the CECs' environmental occurrence and the related ecotoxicological and health risks, which are still largely unknown.

Keywords: CECs, target analysis, suspect screening, non-target analysis

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IL 9

Secondary raw materials in line to the circular economy concept for supporting smart specialization strategy

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Smart specialization strategy (S3) presents a modern approach to economic development based on knowledge, research and innovation, thus connecting science and business. Sustainable Development Goals (SDGs) and EU Green Deal present the main pillars of S3. According to the EU Green Deal, there are need, more than any time before, to apply the circular economy concept and the principles for resource efficiency in construction in order to reduce the use of natural resources and protect the environment in the future.

Construction sector has the significant impact on the climate change due to its responsibility for greenhouse gas emissions. Cement industry accounts for about 7% of the total global anthropogenic GHG emissions. Valorization of secondary raw materials in construction presents an approach, among others, to alleviate this problem. Different residues, wastes, and industrial by-products, including coal fly ash and bottom ash, metallurgical slags, red mud, mine, and quarry wastes can be use as secondary raw materials to decrease the CO_2 footprint and reduce their environmental impact.

Significant amounts of secondary raw materials have been use in range of applications, such as: in cement clinker, green cements, as pozzolanic addition in cement, concrete, light weight aggregate, bricks, glass–ceramics as well as for advanced applications as aerogels and geopolymers.

Innovative solutions in construction in terms of valorizing different secondary raw materials for the synthesis of green cements, geopolymers as well as self-healing of mortars, in line to the concept of circular economy supporting the Smart specialization strategy in our country will be present.

Keywords: secondary raw materials, circular economy concept, smart specialization strategy, construction, resources

IL 10
Impact of Food Texture on Food Oral Processing and Sensory Analysis

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In the last decade, the global changes in lifestyle and increased health awareness of the consumers, put pressure on producers to develop or more accurately re-designed food products with reduced glycemic index, lower salt content, lower fat content, lactose free etc to sustain the consumer acceptability. These requirements need a broad knowledge not only of the chemical part and content of the food, but also of food physics and the way that the food will be transformed to bolus and what would be people's sensory reaction to the changes.

Food structure plays an important role in chewing behavior and in consequence in oral processing. Oral processing leads to complex transformations of food where mechanical processes like fragmentation, agglomeration, hydration, and lubrication take place and affect the sensory perceptions of the texture, aroma and flavor in the mouth. Usually, the accent is always on the newly developed product and not on the eating process itself, but recently the new field of study emerged that addresses the connection among the structure – oral-processing – sensory properties.

Bread is a one of the foods that can act as a model of porous structure to establish relationship between oral processing and sensory perception. Therefore, our laboratory started with investigation of the oral processing behavior of different bread and bakery structures (bread, crisps and cookies) and related them to their textural and sensory characteristics. Different bakery samples with similar ingredients but different structures were selected. Samples were chewed by healthy subjects, and the masticatory performance (time, biting rate, sample weight, saliva content) was analyzed. In vivo food boluses were collected at the swallowing point and their textural properties were analyzed immediately after collection. Finally, food texture and structure were analyzed using descriptive sensory analysis. Bolus analysis showed different texture characteristics depending on the sample's characteristics and subjects. Data obtained from sensory analysis revealed correlations with instrumental results. The study provided better understanding of

food oral processing and the impact of food structure in mastication behavior and sensory perception.

Keywords: food structure, food texture, food oral processing, sensory perception

IL 11

Quantum dot solids with tunable optical properties on glass substrates

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The focus of nanoscience and nanotechnology is gradually shifting from individual nanostructures to their assemblies in which these nanostructures mutually interact and organize into nanostructured materials with new collective properties and remarkable applications in a wide range of fields (such as medical diagnostics, drug delivery, sensors, electronic devices etc.). Currently, in this context, self-assembly of nanoparticles is a hot topic in nanotechnology and a key tool in construction of novel nanodevices.

In this talk, tunable optical properties of several QD solids will be of primary focus, including materials built up by core-shell nanostructures. Band gap energy of QD solids was size-tuned using a bottom-up approach, based on the ultrasound-assisted colloidal mechanism. Coupled with sonoluminescence, this approach provides fine control of the QD size. Along with this, optical properties were additionally modified implementing doping procedure which led to creation of doped QDs and core-shell nanostructures. Since self-assembly of QDs is driven by interactions between them, depending on the experimental conditions under which the synthesis has been taken, QD solids with different degree of ordering have been created. Their optical properties, including sub-band gap absorption and photoluminescence, were considered as a complex interplay of the structural disorder on an individual QD level and on a superlattice scale. Structural inferences have been derived from advanced analysis of X-ray diffraction patterns of the synthesized QD solids, as well as from electron diffraction technique, while superlattice-scale morphology has been studied by SEM and AFM in conjunction with image-analysis techniques.

Keywords: quantum dots (QDs), QD solid, self-assembly, tunable optical properties, band gap energy, sub-band gap absorption, photoluminescence properties, ultrasound-assisted synthesis, bottom-up approach, sonoluminescence.

IL 12

Phytochemical analysis: extraction, characterization and diversity of bioactive secondary plant metabolites

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Phytochemicals are essential components of traditional knowledge systems in complementary and alternative medicine, nutraceutical, food supplements, and pharmaceuticals. Bioactive secondary metabolites can be classified as phenolics, terpenes and steroids, and nitrogen compounds including alkaloids. Each of these classes contains a very large and diverse set of compounds that have a very wide range of biological activities.

The use and benefits of bioactive phytochemicals largely depend on a thorough understanding of their structure and properties. Hence, it is necessary to establish methodology for efficient extraction, identification and quantification of the active compounds present in the extracts and plant material that should be further studied for their biological activities. The extraction processes are based on the difference in solubility of the target compounds for which a variety of solvents and their mixtures can be used. During extraction of target bioactive compounds from plant material, it is important to minimize interferences from compounds that may co-extract with the target compounds and to enable maximum yield and prevent decomposition of important metabolites.

Separation, identification and quantification of secondary metabolites is a complex analytical task owing to their huge number and diversity between various classes of compounds and numerous representatives within each class. The choice of method depends on the sensitivity required for the purpose at hand, the complexity of the matrix related to the time spent on sample pretreatment prior to analysis, the required chromatographic resolution and the preferred detection method. Liquid chromatography coupled to mass spectrometry (LC/DAD/MS) is the technique of choice because it is highly effective for characterizing complex

samples that would be difficult to analyze by conventional LC/UV analysis. Results from characterization of bioactive secondary metabolites from the groups of flavonoids, phenolic acids and alkaloids will be discussed and specific points from using tandem mass spectrometry for their identification and quantification highlighted.

Keywords: polyphenols, xanthones, alkaloids, extraction efficiency, LC/DAD/MS.

IL 13
Nanomaterial-Based Chemical Sensors

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Due to their high surface-to-volume ratio nanomaterials are highly interesting candidates as functional materials for chemical sensors. Furthermore, using composites enable tuning of the materials properties to allow the formation of sensor arrays, and that can be used for many different applications including industrial process, food and environmental monitoring as well as for medical diagnosis. Due to the ease of the measurement and easy device and materials integration options amperometric, potentiometric and resistive sensors are the preferred choice for application-oriented devices. In this talk several examples for chemical sensing in the gas and liquid phase are given to show the extraordinary properties of the investigated sensing materials (e.g. Nanocarbon composites, Nanoparticle composites, semiconductor fibers, Metal organic frameworks) in various applications.

Keywords: nanomaterials, composites, chemical sensors

ICTM O-1
Calcium Containing $ReAlO_3$ (Re = La, Gd) Perovskites. Mechynosynthesis, Morphology and Electrochemical properties

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Rare-earth aluminates ($LaAlO_3$ and $GdAlO_3$) and their calcium-substituted derivates ($La_{1-x}Ca_xAlO_{3-\delta}$; x = 0.05, 0.10, 0.15 and 0.20; $Gd_{1-x}Ca_xAlO_{3-\delta}$; x = 0.05, 0.10 and 0.15) were prepared via one-step mechanochemical processing of simple oxide precursors at ambient temperature. In the case of mechanochemical formation of the $GdAlO_3$, the reaction is accompanied by Gd_2O_3 phase transformation. The as-prepared and sintered materials were characterized by X-ray diffraction and scanning electron microscopy. Sintering at 1450°C resulted in different porosity of the samples, i.e. dense $LaAlO_3$ (density <95% of theoretical value) relatively porous $GdAlO_3$ ceramics (density <90% of theoretical value) except sintered $Gd_{0.85}Ca_{0.15}AlO_{2.925}$. The electrical conductivity of the sintered samples was investigated by impedance spectroscopy in the temperature range ~350-1000°C in air. Acceptor-type substitution of lanthanum and gadolinium by calcium results in ~3 orders of magnitude increase in both total and bulk conductivity associated with a substantial enhancement in oxygen-ionic transport. Further doping has a limited effect on the electrical transport properties, and electrical conductivity remains nearly composition-independent in the range x = 0.05-0.20 for $La_{1-x}Ca_xAlO_{3-\delta}$ and x = 0.05-0.15 for $Gd_{1-x}Ca_xAlO_{3-\delta}$, respectively. Grain boundaries were demonstrated to have a significant contribution to the total resistivity of prepared calcium-substituted ceramics with grain sizes in the range up to 1.5 μm.

Keywords: Lanthanum/Gadolinium aluminates, Perovskites, Mechanosynthesis, Conductivity, Solid electrolyte

Acknowledgement: This work was supported by the Slovak Scientific Grant Agency VEGA (2/0058/23) and Slovak Research and Development Agency APVV (contracts No. 19-0526 and SK-PT 18-0039).

ICTM O-2

Modification of Mechanical and Thermal properties of Epoxy-Inorganic Composites

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Epoxy resin has wide applications due to its exceptional chemical resistance, toughness characteristics, and bonding effects. The epoxy-matrix composites are predominantly used in the design of high-performance materials[1]. Thus, studying the properties of composite materials based on epoxy resin matrix is highly suggested in order to enhance their characteristics.

The effect of modified epoxy resin with micronized inorganic-additive (mineral mixture) used as a matrix in the production of impregnated composite materials was examined and compared. A set of various series was realized by variation of the inorganic-additive quantity.

The main focus was set on the improvement of the mechanical and thermal properties of the composite materials. The thermal properties of the composite samples were characterized by means of differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA), while the mechanical properties were examined using 3-point flexural tests, tensile strength and compression strength measurements.

Keywords: epoxy-matrix composites, inorganic additive, impregnation, mechanical properties, thermal properties

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ICTM O-3
The Process of Production of FeMn and SiMn in R.Ž "TOPILNICA" JSC Skopje

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R.Ž Topilnica j.s.c-Skopje as production plant consists of 3 basic production units:

1) Receiving bunkers and homogenization of ore

2) Mini agglomeration (Dellattre Levier / CRESOT-LOIRE) which collects all the fines of ore, slag, coke, fines of ferromanganese and silicomanganese finished product, finesse of the thyssen hole of the furnace cooling systems that collects all the dust, because the stove has a chimney that serves only as a reserve.

3) Silicomanganese crushing and sowing machine (finished product)

The agglomeration process takes place on a sinter tape consisting of 2 parts:

-Sintering zone

-Cooling zone

The thickness of the sintering mixture is 460 mm, where the sinter is heated with fuel oil or gas (by-pass).

Sinter capacity can produce up to 1,200 tons / 24 hours a day. This is emphasized, because the mini agglomeration is a collector of all waste raw materials and thus sums up all operating losses, and most importantly and environmentally positively affects the protection of the environment because there is no need to look for a landfill for waste materials.

Keywords: silicomanganese, sinter plant, production FeMn, SiMn, waste materials

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ICTM O-4

Frost resistance and biocorrosion of ceramic composites

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Frost resistance mechanisms and biocorrosion as major processes that leads to weathering of ceramics are of great practical and scientific interest upon their exposure to surrounding environmental conditions.

The aim of this work was to define the influence of different deterioration mechanisms regarding both frost and biocorrosion actions on ceramic composites in which a significant part of the clay (40 wt.%) was replaced with fly ash. The ceramic composites made of local clay and fly ash from thermal power plant "REK" Bitola, were fabricated in laboratory conditions by pressing (P = 45 MPa) and sintering at 1100°C, with heating rates of 3 and 10 °/min.

The frost resistance investigation was conveyed through a double approach: calculating durability through textural characteristics (obtained by mercury intrusion porosimetry and low-temperature nitrogen adsorption method) and performing low-temperature dilatation measurements on water saturated and dray samples.

Based on the obtained results and estimated susceptibility to different frost action mechanisms (closed container, micro ice lens and hydraulic pressure) it can be concluded that the balance of all three mechanisms indicates good frost resistance and that the ceramic structure was capable for regulating and compensating possible local stresses during the freezing. In addition, the ceramic composite sintered at 1100°C with heating rate of 10°/min showed slightly higher stability to frost action deterioration and it was used for biocorrosion investigation.

The biocorrosion was performed by following Aspergillus niger colonization on ceramic composite. Only aesthetic changes on the surface of the ceramic composite without any internal and chemical degradation were detected.

In summary, the obtained durability investigations are encouraging, showing that utilization of fly ash (40 wt.%) in ceramic composites is possible, without significant negative impact on their frost resistance and biocorrosion properties.

Keywords: ceramic, frost action mechanisms, biocorrosion, porosity, fly ash

ICTM O-5

Silver Nanoplates: Morphology Exhibiting Strong Plasmonic and Catalytic Properties

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Silver nanoplates, either in trigonal or hexagonal morphology, are crystals formed due to the stacking faults in a crystal lattice, resulting in highly asymmetric crystals of otherwise cubic silver morphology. Because of that they exhibit pronounced plasmonic properties also in visible spectra. As such they are attractive material for various applications like enhance sensors or as catalysts.

In this work we present novel method to prepare sliver nanoplates in gram quantities. The method is seedless, consists of few reagents, enables preparation of silver nanoplates with desired optical properties in high concentration, is scalable and allows their long-term storage. The developed method is based on silver nitrate, sodium borohydride, polyvinylpyrrolidone and H2O2 as the main reagents, while antifoam A204 is implemented to achieve better product quality on larger scale. Prepared nanoplates was dried and spontaneously dispersed after at least one month of storage in the dark without any change in plasmonic properties.

Their application for catalysis is demonstrated by preparing the catalytic reactor silver nanoplates by depositing them on positively charged high internal phase emulsion monoliths via their negative zeta potential. Such reactor was used in a

flow-through mode for catalytic reduction of 4-nitrophenol and demonstrated to be stable under various elution conditions, even after prolonged usage.

Furthermore, their plasmonic effect in visible spectra was exploited for potential use in modern art by drying silver nanoplates on different surfaces, resulting in a variety of colors but, more importantly, patterns of varying complexity, from simple multi-coffee-rings structures to dendritic forms and complex multi-level Sierpiński triangle fractals.

Keywords: silver nanoplates, plasmon, catalysis, tubular reactor

ICTM P-1

Microstructural Analysis of Thermally Treated Geopolymer Incorporated with Neodymium

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The following investigation presents the thermal treatment of geopolymer based on metakaolin, with the addition of 1% and 5% of neodymium in the form Nd_2O_3, at 300˚C, 600˚C and 900˚C. Six samples were synthesized in total. Samples GT1 and GT2 containing 1% and 5% of Nd_2O_3, and they were treated at 300˚C, while the samples GT3 and GT4 also had the same percentage composition of Nd_2O_3 and were treated at 600˚C, and the samples GT5 and GT6 were treated at 900˚C with the same percentage of Nd_2O_3. Physical and chemical changes in the aluminosilicate geopolymer matrix were monitored. The incorporation of rare earths into the polymer network of aluminosilicates has been proven to disrupt the basic structure of geopolymers, however, with increased temperature, these materials show even more unusual properties. DRIFT was employed to investigate the structural properties of thermally treated geopolymers. Additionally, TEM provided further insight into the structural changes induced by thermal treatment and Nd_2O_3 doping. SEM was used to observe the effect of thermal treatment temperature (300˚C and 600˚C) on geopolymer porosity, which resulted in the appearance of large pores and cracks in the material. The UV/Vis spectra of the synthesized Nd_3^+

doped geopolymers exhibited attractive optical properties. The photoexcitation of electrons from the valence band to the conduction band in the geopolymer structure is responsible for the absorbance observed at 260 nm, while the minor peaks at slightly longer wavelengths can be linked to Nd^{3+}.

Keywords: Geopolymers, Rare earth, Neodymium, Metakaolin, DRIFT, UV/Vis

ICTM P-2

Physicochemical, Radiological and Structural Properties of Alkali Activated Materials – Future Trends and Applications

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The aim of this study was determination of physical-chemical, radiological and structural characteristics of kaolin, fly ash and the products of alkali-activated as well as thermally treated kaolin (alkali activated materials). Kaolin (raw material) and fly ash (industrial waste) used in the investigation showed the great potential for obtaining alkali activated materials as relatively new products to be used in construction and civil engineering as green cements. Physical-chemical and structural characterization was conducted using X ray diffraction (XRD), Fourier transform infra-red (FTIR) and X ray photoelectron spectroscopy (XPS), Scanning electron microscopy (SEM) and High-resolution transmission electron microscopy (HR-TEM). Activity concentration of naturally occurring radionuclides in kaolin, metakaolin, fly ash and alkali activated materials were determined. The absorbed dose rate (D) and the annual effective dose rate (EDR), were calculated in accordance to the UNSCEAR 2000 report. Kaolin was thermally treated on 750°C, and specific activity of natural radionuclides in metakaolin increased up to 1.6, while specific activities in alkali activated materials were significantly reduced.

Keywords: Alkali activated materials, kaolin, fly ash, XPS, HR-TEM, natural radioactivity

ICTM P-3
Investigation of $Co_{0.9}Ho_{0.1}MoO_4$ Nanopowders Obtained by Glycine Nitrate Procedure

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Nanometric size $Co_{0.9}Ho_{0.1}MoO_4$ powder particles were obtained by applying glycine nitrate procedure (GNP). Powder properties have been studied by DTA, X-ray diffraction (XRD), Fourier transform infrared (FT-IR) spectra, Spectroscopy, Field emission scanning electron microscopy (FESEM), and nitrogen adsorption method. The photocatalytic activity of acquiring $Co_{0.9}Ho_{0.1}MoO_4$ nanopowders was estimated by the photocatalytic degradation of crystal violet in an aqueous solution. We present a simple and effective method for controlling the composition and morphology of $Co_{0.9}Ho_{0.1}MoO_4$, as well as a possible new approach in inorganic synthesis methodology. During photocatalytic testing, the studied nanoparticle powder indicated a potentially promising solution in photocatalytic processes toward green chemistry and sustainable development.

Keywords: X-ray diffraction, Electron microscopy, Nanostructured materials

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ICTM P-4

Green Alkali Activated Materials Based on The Different Precursors

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The main goal of this study was the evaluation of physical–chemical, as well as radiological properties of residual materials used for synthesis of alkali activated materials (AAMs) for the possible application as new materials in a civil engineering industry. Also, the purpose of this research was to investigate the hydrophobicity of new alumino-silicate materials and the influence of Si/Al ratio on their surface properties. Contact angle measurement (CAM) as reliable indicator of hydrophobicity was determined for synthesized AAMs using water and ethylene glycol as reference liquids.

Alkali-activated materials were synthesized from various precursors: kaolin, bentonite and diatomite. Characterization of phase structure and microstructure was performed by X-ray diffraction (XRD), Fourier transform infra-red (FTIR) spectroscopy, Scanning electron microscopy and Energy-dispersive X-

ray (SEM/EDX) spectroscopy. Contact angle measurements confirmed that the alkali-activated materials synthesized from metakaolin are the most porous, which can be explained by the smallest Si/Al ratio. The maximum value of contact angle and free surface energy (110.2 mJ/m^2) has been achieved for alkali-activated materials synthesized by diatomite (GPMD). Concentration of ^{40}K and radionuclides from the ^{238}U and ^{232}Th decay series in waste precursors, their metaphases and AAM samples synthetized by alkali activation were determined together with corresponding absorbed dose rate ($\dot{D}$) and the annual effective dose rate. Natural activity concentrations in the alkali-activated materials were found to be lower than that of both residual materials and calcined ones.

Keywords: Alkali activated materials, metakaolin, contact angle measurement, absorbed dose rate

ICTM P-5

Preparation and Performance of Low Content Carbon Geopolymer

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Due to the low CO_2 emission of geopolymers compared to Portland cement, interest in their use as binding cement has increased in recent years. The main goal of this research is to relate the green and sustainable characteristics to the good mechanical and chemical properties of fly ash-based geopolymers. For those purposes, samples of different ratios of fly ash (FA) and metakaolin (MK) were prepared. Mineralogical characterization of the geopolymer samples conducted using X-ray powder diffraction (XRD) showed that in the geopolymer synthesis reaction new amorphous phase was formed. Diffuse reflectance infrared Fourier transform spectroscopy (DRIFT) confirmed characteristic bands of Si-O and O-Si-O groups at 1045 cm^{-1}. Compressive strength analysis revealed that the optimal ratio of FA and MK is 50:50 and exhibits the highest value, while X-ray photoelectron

spectroscopy (XPS) analysis revealed the total reduction of carbon content in the alkali activated geopolymer with optimal stoichiometry 50:50. The results of this research indicates the possibility to obtain a geopolymer material with almost complete absence of carbon, which implies further application as a material with very high environmental potential and zero carbon emission.

Keywords: carbon reduction; compressive strength; geopolymer; metakaolin; fly ash.

ICTM P-6

Molecular and Crystal Structure of the Bis(Acetato)-Bis(4-Methyl-1h-Pyrazole)-Zinc(Ii)

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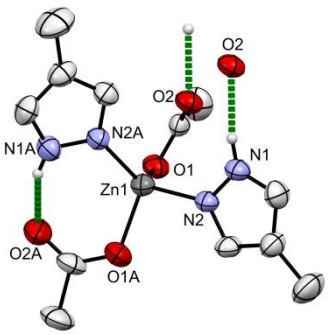

Ligands with multiple coordination sites are often used in the synthesis of the extended metallo-organic structures. Both pyrazolyl and acetato ligands can have a role of a "bridge" between the metallo-organic fragments. As a part of the study of the coordination capabilities of pyrazole-based ligands we are reporting the molecular and crystal structure of the bis(acetato)-bis(4-methyl-1H-pyrazole)-zinc(ii). Zn is coordinated by two methyl-pyrazole and two acetato ligands, in a

distorted tetrahedral environment. Different pattern of non-bonding interactions involving chemically equivalent ligands influence the overall shape of the complex molecule. This is evident in different mutual position of the pyrazolyl and acetato ligands, which is associated with different hydrogen bonds. Two neighboring complex molecules forms hydrogen bonded dimer. There are no significant inter-molecular contacts between dimmers.

Keywords: pyrazole complexes; fomepizole; Zn complex; structure

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ICTM P-7

Semiconducting Co_3O_4 Nanocatalyst Prepared by Eco-Friendly Thermal Decomposition

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The cobalt oxide (Co_3O_4) is a very attractive material for optoelectronic applications due to the intense absorption of visible light and p-type semiconducting properties. On the other hand, conventional synthesis methods for its preparation could be either time- and energy-consuming or relying on toxic chemicals. To address this issue, spinel Co_3O_4 nanoparticles were prepared by a simple, facile, and eco-friendly method of synthesis. Such method is based on the thermal decomposition of hexaaquacobalt(II) D-camphor10-sulfonate at 900 °C. This synthesis route avoids the use of toxic organic solvents which overcomes the disadvantages of many combustion methods. In order to assess the potential use of synthesized powder, the characterization methods were performed in detail. The purity and semiconducting properties of the Co_3O_4 were confirmed by UV/Vis spectroscopy which indicated the presence of two band gaps (2.10 eV and 1.22 eV). A noteworthy improvement in the electron transfer kinetics with the addition of the prepared sample to the carbon-paste electrode led to an enhanced electrocatalytic performance. Such remarkable functional properties are suitable for a wide range of

technological applications, open the way for the implementation of this preparation procedure for the synthesis of Co_3O_4 on a larger industrial scale.[1]

Keywords: Co_3O_4; nanocatalyst; semiconducting properties; eco-frinedly thermal decomposition

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ICTM P-8

Production of Silver Salts in Alkaloid AD Skopje

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Alkaloid AD Skopje, within the Chemistry Program has a long tradition in the production of pure chemicals. This group of products, also includes silver salts. Currently we manufacture the following silver salts: silver nitrate, silver sulfate, silver iodide and silver cyanide. The quality of these products ranges from reagent grade, pro analysi, Ph.Eur., USP and special quality requirements specified by the customers.

During the years our Research and Development team, alongside with Production and Quality control have made a series of improvements which include an integrated production process which is optimized to yield high quality products. This is achieved by using unique technology process and substantial improvements in the analytical techniques in the Quality control laboratory. The result of these improvements is a reliable and efficient process, which is at the same time flexible and tunable and can provide high quality silver salts, depending on the market demand.

Summary of the process: Silver metal is oxidized to silver nitrate with the action of nitric acid. The resulting solution can be concentrated by evaporation and crystallized to yield silver nitrate. Alternatively, the silver nitrate solution can be

reacted with sulfuric acid to yield silver sulfate, or with potassium iodide to yield silver iodide, or with potassium cyanide to yield silver cyanide.[1]

Keywords: silver nitrate, silver sulfate, silver iodide, silver cyanide, redox, synthesis, quality

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ICTM P-9

Synthesis and Characterization of New Copper(II) and Palladium(II) Complexes with S, O-Tetradentate Ligand as Derivative of Thiosalicylic and Thiopropionic Acids

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Complexes of copper(II) and palladium(II) with different types of ligands (S, O and N donor ligands) have significant antiviral, antibacterial, antifungal and antitumor activity.[1-2] In this work we report synthesis and characterization of two new transition metal complexes (copper(II) and palladium(II)) with S, O-ligand as derivative of thiosalicylic and thiopropionic acid.

The transition metal complexes were obtained by direct reaction of S,O-tetradentate ligand as derivative of thiosalicylic and thiopropionic acid with starting metal salt (copper(II)-nitrate or potassium-tetrachloridopaladate(II)) in molar ratio 1:1 with addition aqueous solution of equimolar amount of lithium-hydroxide with satisfactory yields. The composition of obtained compounds was

confirmed based on the results of elemental analysis. The structure and coordination of metal ions to donor atoms were predicted by spectroscopy methods (UV-Vis, IR and H^1 and C^{13} NMR) and magnetic measurements.

Keywords: Synthesis; Characterization; Copper(II) and Palladium(II)-complexes

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ICTM P-10

Structural Characteristics and Adsorption Properties of Alkali Activated Blends Ashes/Metakaolin

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The aim of this paper is to show the possibility of using waste materials, blends of (wood ash, fly ash, from thermal power plant, and metakaolin) for the production of alkali activated materials that can be used to purify wastewater from different kinds of pollutants such as heavy metals. Heavy metals are toxic, especially cadmium, so they must be removed from wastewater to prevent or minimize contact with the environment and humans. The synthesis of the alkali activated materials was performed by mixing solid precursors with a liquid alkali activator. Two- and three-component systems of wood ash, fly ash and metakaolin (wood ash/fly ash, wood ash/metakaolin, fly ash/metakaolin and wood ash/fly ash/metakaolin) were used as precursor materials. The alkali activator solution was

a mixture of sodium silicate solution and sodium hydroxide solution of concentrations (6M and 12M). The characterization of alkali activated materials was studied by X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy, Scanning electron microscopy and energy-dispersive X-ray spectroscopy (SEM/EDS). XRD measurements of investigated samples showed a characteristic halo between 18□ and 35º 2□ with a dominant crystal phase of quartz. FTIR spectroscopy showed that the main vibration band of all investigated samples appeared between 1037-996 cm-1, and corresponds to Si-O-Si/Si-O-Al bands. SEM/EDS analysis was used to determine the microstructure of the samples. The adsorption efficiency of the investigated alkali activated materials for removing cadmium ions from aqueous solution was tested under different conditions: initial concentration of cadmium ions in the range of 20-100 mg/l, pH values from 3 to 7 and mass of adsorbents from 0.02-0.05 g.

Keywords: wood ash, fly ash, metakaolin, alkali activated materials, adsorption, cadmium

ICTM P-11

Improving the Surface Consolidation of Historical Material Using Calcium-Based Consolidants

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The aim of the work is to improve an advanced consolidation system for cultural heritage materials in order to accelerate the carbonation of the consolidation process. The research represents a step towards a circular economy, as it is expected to increase the sustainability of the historical material thus consolidated and to improve the carbonation of the consolidation process, which will allow a faster restoration process and thus a reduction in restoration costs. Due to the shorter and faster curing process, it has an economic advantage over established methods. The selection of suitable materials and processes is designed to generate as little waste as possible and to have less impact on the environment than conventional processes.[1]

Based on the tests conducted, we found that Consolidant Formulation Water (CFW) is the most effective and suitable consolidation agent for heritage consolidation compared to other agents (Calosil in ethanol, Calosil in isopropanol, and Nanorestore). In this study, the effects of consolidation with different consolidants are investigated: one based on calcium acetoacetate (CFW) solution and the other based on alcoholic dispersions of $Ca(OH)_2$ nanoparticles. Their synergistic effects on the final consolidation result are also investigated in a presented study. Monitoring of carbonation progress using FTIR spectroscopy, X-ray powder diffraction (XRD), electron scanning microscopy (FE-SEM) is presented.

Keywords: consolidation, materials, synergy effect, characterisation

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ICTM P-12

Heterogeneity of Adsorption and Reaction Sites on Silica Supported (10%Co+0.5%Pd) Catalyst Surfaces During CO Hydrogenation

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Heterogeneity of adsorption and reaction sites of Co-Pd/SiO_2 catalysts for CO hydrogenation was studied by chemisorption, TPD, and DRIFTS. Precursor materials were treated in H_2, Ar, or air and named respectively as (red), (inert), or (ox). CO conversion changed in low extent due to effect of preliminary treatment. Activity of samples in synthesis of CH_4 ranged as (inert)<(ox)<(red) and decrease of 18-24% was registered. H_2 adsorption showed similar heterogeneity of (red) and (inert) samples as their low-energy sites were weaker than those of (ox) one. The most hindered H_2 adsorption was registered on (ox) catalyst. High-temperature TPD region analysis revealed (inert)-type of catalyst as an owner of more stable H_2

adsorption sites compared to the other materials. Thus, heterogeneity was also of same type. Infrared bands of linear CO-Co^0/$Co^{\delta+}$ species were of high almost constant intensity in the row (red)<(ox)<(inert) and low-temperature desorption peak T_{max} ranged as (inert)<(red)<(ox). Increased formation of mono- and bidentate carbonates and formate species was found with process progress. Respective CO-TPD region showed that the intermediate compounds on (inert) sample were more reactive in comparison to those from other samples. The observations allowed generalization that various linear CO species were formed on the surface; adsorption sites were strong; processes of adsorption, dissociation and hydrogenation on the surface were to a great extent balanced; adsorption site working as reaction center reduced its activity with time in CO hydrogenation and occurring of WGSR got more advantageous. Comparative analysis concerning carbonate-like species showed that adsorption sites/intermediates in case of (ox) sample were weak sites/unstable complexes and (inert) sample had adsorption centers/carbonate-like complexes of average strength/stability.

Keywords: CO hydrogenation; Co-Pd catalysts; adsorption and reaction sites

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ICTM P-13

Physico-Chemical Properties of Geopolymers Based on Metakaolin with The Addition of Organic Phase PVA

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Recently, there has been a growing interest in mixing two different systems, organic and inorganic, which would contribute to some improved properties, such as adjustment time, reduced shrinkage, improved mechanical properties and durability. A new class of geopolymer composites with an organic matrix has been

developed with the main goal of improving the fire resistance of organic polymers and reducing the production of smoke resulting from their combustion, as well as improving mechanical properties.

For the synthesis of hybrid geopolymer materials, metakaolin with the addition of organic phase poly (vinyl alcohol) (PVA) was used as the starting material. For the synthesis of alkaline activator, a solution of NaOH with a molarity of 12 mol / dm3 was used. The chemical composition of the samples was determined by XRF analysis. Structural and phase characterization of hybrid and reference materials were analyzed using X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FTIR), which revealed new phases in the PVA-added samples. The results show that the content of added PVA in the reaction mixture affects the phase composition of the synthesized materials. The morphology was analyzed using a scanning electron microscope with energy dispersive spectroscopy (SEM/EDS), where efflorescence was observed and identified. After characterizing the geopolymer with the addition of PVA, we obtained a material that is far more porous than the basic sample, and we can conclude that we have synthesized a material that shows good mechanical properties.

Keywords: metakaolin, geopolymer materials, organic polymer, organic phase, PVA

ICTM P-14

Development of High Entropy Spinel Oxides Prepared *via* Ball Milling

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In this work, high entropy oxides with MAl_2O_4 spinel structure, i.e. $(Zn_{0.25}Cu_{0.25}Co_{0.25}Mg_{0.25})Al_2O_4$, were successfully synthesized *via* one-step mechanochemical method. Moreover, their lithiated derivates of the final composition:

$Li_{0.5}(Zn_{0.125}Cu_{0.125}Co_{0.125}Mg_{0.125})_{0.5}Al_2O_{3.5}F_{0.5}$,$Li_{0.5}(Zn_{0.125}Cu_{0.125}Co_{0.125}Mg_{0.125})_{0.5}Al_2O_{3.5}Cl_{0.5}$ were prepared by mechanochemical reaction between oxide precursors and LiF and LiCl, respectively. The phase evolution as well as the structure of the prepared oxides were controlled by XRD. The morphology of the samples was studied by STEM and HR-TEM and supported by EDX elemental analyses. The STEM images showed nanocrystalline nature of as-prepared samples with average crystalline size in the range of 6 to 17 nm. The analyses of HR-TEM micrographs of samples showed excellent agreement of the average interplanar distances in comparison to the XRD analyses. The EDX analyses demonstrated a homogeneous distribution of the elements. The influence of the preparation method on the oxidation state of elements was investigated by XPS. The electrochemical properties were studied by cyclic voltammetry of Li insertion in the potential window of 0.01–3.0 V vs Li^+/Li at scan rate of 0.1 mV s^{-1}. The charge capacity of $(Zn_{0.25}Cu_{0.25}Co_{0.25}Mg_{0.25})Al_2O_4$ was found to be 54 mAh g^{-1}. The charge capacity of $Li_{0.5}(Zn_{0.125}Cu_{0.125}Co_{0.125}Mg_{0.125})_{0.5}Al_2O_{3.5}F_{0.5}$ was shown to be 71 mAh g^{-1} and for $Li_{0.5}(Zn_{0.125}Cu_{0.125}Co_{0.125}Mg_{0.125})_{0.5}Al_2O_{3.5}Cl_{0.5}$ – 52 mAh g^{-1}. According to the achieved results, the mechanochemical method provides the route towards development of novel high entropy oxides.

Keywords: spinel structure, high entropy oxide, nanomaterials, mechanosynthesis

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ICTM P-15

Photocatalytic Activity of Sol-Gel Prepared TiO_2 Thin Films Doped with Degussa Nanoparticles

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Titanium dioxide is a n-type semiconductor and due to its wide optical band gap ($E_g \sim 3.3\ eV$) has numerous applications in various scientific areas such as photocatalysis, sensors, energy harvesting, etc. Its photocatalytic properties have been used in a big number of environmental applications. Degussa P25, is a titania photocatalyst in the form of powder with relatively high levels of activity in many photocatalytic reactions.

Sol-gel grown TiO_2 thin films pure or doped with Degussa were deposited on glass substrates by spin-coating under different conditions. The films were thermally treated at 500 °C, to obtain the anatase phase. The film properties were fully characterized. The photocatalytic activity of all films was evaluated by measuring the rate of atrazine decomposition under UV-A irradiation. All films show significant photocatalytic activity but the film doped with Degussa showed more than double decomposition rate.

Keywords: Sol-gel; TiO_2; Degussa; Photocatalysis; Spin coating; Anatase

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ICTM P-16

Application of Zeolite in Agriculture

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Zeolites are three-dimensional crystalline compounds that are built from AlO4 and SiO4 tetrahedra. The tetrahedral structures of zeolites can be further linked into different rings. Such structures are called secondary building units. They can contain more than 16 atoms in the ring (only the atoms located in the center of the tetrahedron (Si and Al) are considered). By interconnecting eight of the six members, a polyoctahedron (known as a beta-cage) can be formed. The selectivity

on the surface of zeolite as an adsorbent depends on the SiO2/Al2O3 ratio. Aluminum-rich zeolites adsorb polar molecules in their structure and are therefore used as desiccants. A higher proportion of silicon in the structure increases the hydrophobic character of the zeolite. The transition from hydrophilic to hydrophobic form is in the ratio SiO2 / Al2O3 of about 20. The skeleton of zeolites is built from [SiO4] and [AlO4] tetrahedra, they are connected to each other, occupying one or more corners forming a ring through the oxygen atoms. The specific and unique structure of zeolites allows them to have a variety of applications. This is a new application of zeolite in growing a plant whose properties are improved thanks to the water that zeolites have in their structure. Soils that are mixed with zeolite for growing plants have a higher yield and retain their moisture for a longer time.

Our research was performed on plants that were tested on soil without zeolite and soil with added zeolite. The plant grown with added zeolite has better characteristics and a better yield.

Zeolite should be added to the soil every five years, and the yield of plants increases up to 50% and their resistance to various diseases. The root system with added zeolite becomes more powerful, seed germination increases. In our tests, it was shown that plants with zeolite require less watering than plants without zeolite. The result of that is the structure of the zeolite that retains water in its cavities and channels.

Keywords: zeolite, application, agriculture, plant, soil

ICTM P-17

Characterization of Pottery Vessels Excavated at The Archaeological Site Stobi in Republic of North Macedonia

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The primary goal of this study was to characterize three pottery vessels excavated at the archaeological site Stobi. The significance of the study lies in the fact that it presents an initial publication of research conducted on these objects, encompassing multiple analytical aspects such as chronology, technology and experimental analysis.

Based on comprehensive investigations, the examined objects exhibit distinct characteristics. Two of the analyzed vessels were chronologically attributed to the I to II century AD. One of these vessels demonstrates an original Terra Sigillata imported to Stobi, while the other suggests a locally made imitation of this type of pottery. The third sample originates from a bowl with imprinted decoration, which was characteristic of local ceramic production at Stobi during the Middle Roman Times, dating from the II to III century AD.

Three samples collected from each vessel underwent physical examinations (density and porosity), chemical analysis (SEM coupled with EDS) and mineralogical examination using XRD and FTIR techniques.

The sample of the original Terra Sigillata object exhibited the highest density (1.99% porosity), while the second and third samples displayed porosities of 10.01% and 11.20%, respectively. Regarding the mineralogical analysis, it is noteworthy that calcite was identified in all samples, following quartz and feldspar. The presence of calcite could be attributed to the used raw materials, but also to the post-production processes. The absence of certain clay minerals (kaolinite and chlorite) and the presence of neoformed high-temperature minerals such as anorthite, sanidine and diopside assess the conditions and sintering temperature (> 700 ˚C).

Keywords: pottery, conservation, porosity, Terra Sigillata, SEM-EDS, XRD and FTIR

ICTM P-18

Electrospun $BaTiO_3$ Nanofibers

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$BaTiO_3$ is a ceramic lead-free material which is extensively investigated due to its ferroelectricity and piezoelectricity, which opens a wide applications in many electronic devices such as capacitors and nanogenerators.[1] In comparison with

nanoparticles, the 1D nanostructured $BaTiO_3$ such as wires, tubes and fibers have attracted substantial attention due to their high aspect ratio and unique physical and chemical properties.[2] Electrospinning, as a simple and versatile technique, can be used for production of both organic and inorganic continuous fibers with diameters of several nanometers.[3]

In this work, $BaTiO_3$ nanofibers were prepared by electrospinning technique via polymer assisted sol-gel precursor solution, in order to adjust the viscosity which is a key parameter for successful electrospinning. The obtained fibers were spun onto a rotating collector, which resulted in production of aligned nanofiber mat. Additionally, the effects of calcination temperature and time on crystal structure were examined by XRD, Raman and FTIR analysis. SEM study showed that the obtained $BaTiO_3$ nanofibers have smooth morphology and hollow diameters.

Keywords: $BaTiO_3$, electrospinning, nanofibers, SEM, XRD

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ICTM P-19

Synthesis and Investigation of Complex Perovskites with Manganese

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The rare-earth perovskite oxides containing 3d transition metals are considered as important materials due to their specific electronic, magnetic, optical and catalytic properties. These properties are even more pronounced in complex perovskites, particularly those with manganese in the B-position. Continuing our work on complex perovskites, in this work we present the synthesis and characterization of new double perovskites with the general formula $PrMn_{0.5}M_{0.5}O_3$ (M = Cr, Fe, Co, Ni).

The synthesis was conducted by solution combustion method using glycine as fuel. The fuel quantity was calculated by setting the fuel/oxidant ratio to 1. The obtained powders were additionally heated in a furnace for 8 hours at 800 °C. Perovskites with iron were also synthesized by the method of sol-gel combustion with citric acid as fuel.

The obtained compounds were investigated by powder XRD, vibrational spectroscopy, SEM, and EDX analysis. The XRD patterns showed that the compounds are pure and isostructural to each other. The comparison of the obtained diffractograms with the ones of simple Pr-perovskites with the constituent metals, indicated that the synthetized perovskites are orthorhombic. The EDX analysis confirmed the 1:1 ratio of Mn/M that corresponds to the general formula $PrMn_{0.5}M_{0.5}O_3$ (M = Cr, Fe, Co, Ni). The recorded diffractograms of the iron-containing perovskites obtained by the two different methods are identical, thus indicating that both methods can be used for synthesis of this type of perovskites. In order to determine the way the applied method of synthesis affects the morphology and dimensions of the particles, SEM images were recorded. The compounds within the series are of the same polycrystalline porous morphology, typical for perovskites obtained by solution-combustion method.

Keywords: complex perovskites, manganese, solution combustion, sol-gel combustion, PXRD, vibrational spectroscopy, SEM, EDX.

ICTM P-20

Synthesis and Investigation of $Ln_{1-x}Er_xFe_{0.5}Mn_{0.5}O_3$ (Ln = La, Sm; x = 0.2 and 0.4)

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In recent years, perovskites that contain two different lanthanides in the A-position have garnered significant attention due to the ability of these elements to introduce exceptional properties and functionalities to the versatile perovskite framework. Lanthanides, which exhibit unique and distinctive electronic configurations and magnetic moments, offer opportunities for precise tuning of optical, electric, magnetic, and catalytic properties of perovskite materials. In this work the synthesis and characterization of complex perovskites with general formulas $Ln_{1-x}Er_xFe_{0.5}Mn_{0.5}O_3$ (Ln = La, Sm; x = 0.2 and 0.4) is presented.

The proposed perovskites were synthesized using the sol-gel combustion method with citric acid as a fuel/chelating agent. In this procedure, the pH value of the initial mixture was controlled using NH_4OH. After the combustion, the obtained perovskite precursors were annealed for 8 hours at 900 °C.

For the identification of the obtained powders, PXRD was used. The XRD patterns confirmed their purity and crystallinity and showed that the sol-gel combustion method is an appropriate method for the synthesis of this type of compounds. The comparison of the recorded XRD patterns to the ones of the pristine La/Sm/Er-perovskites indicated that the partial substitution was successfully done. The structural analysis implied that the synthesized $Sm_{1-x}Er_xFe_{0.5}Mn_{0.5}O_3$ perovskites are orthorhombic, but $La_{1-x}Er_xFe_{0.5}Mn_{0.5}O_3$ are cubic. The two samarium perovskites are isostructural to each other, as well as, the two lanthanum perovskites.

The influence of the lanthanide substitution on metal-oxygen bonds in the investigated perovskites was studied by Fourier Transform Infrared Spectroscopy (FTIR). The infrared spectra showed the presence of characteristic modes of stretching and banding metal-oxygen vibrations.

Keywords: complex perovskites, lanthanides, sol-gel combustion, citric acid, PXRD, FTIR spectroscopy

ICTM P-21

Synthesis and Characterization of Hybrid Organic-Inorganic Perovskites with Morpholinium as an Organic Cation

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Hybrid organic-inorganic perovskites (HOIPs) have been an intensely studied class of materials since the synthesis of the seminal compound $(CH_3NH_3)PbI_3$, due to their promising optoelectronic properties and their potential application in the design of diodes, photosensors and photovoltaic cells. In this work, we describe the synthesis and characterization of a class of iodide organic-inorganic perovskite with morpholinium as an organic cation, while the second cations are varied (B = Bi^{3+}, Sb^{3+}, and Pb^{2+}). The emphasis of the research is in the direction towards their application as semiconductors, estimated through the direct and indirect band gap energies.

The synthesis of the perovskites was conducted in acetonitrile as a solvent, to which corresponding iodide salts of the organic cations were added. The reaction mixtures were heated for 30 minutes to an hour. Crystallization of the lead perovskite was observed almost instantaneously. However, in the case of Bi and Sb perovskites, the solutions had to be evaporated almost completely, before lighter-colored crystals precipitated from the solution. The crystals were left overnight, that lead to the formation of a darker crystalline phase. Studies were conducted on these darker phases of each of the studied perovskite.

The obtained compounds were investigated by powder XRD and vibrational spectroscopy (IR and Raman) in a wide temperature range (liquid nitrogen temperature to 20 °C). Thin films of the HOIPs were obtained with the use of spin coating techniques, and they were investigated by UV-vis spectroscopy. These data were used to construct the Tauc plots, from which the direct and indirect band gaps were determined.

Keywords: hybrid organic-inorganic perovskites, morpholinium, thin films, PXRD, vibrational spectroscopy, UV-vis spectroscopy.

ICTM P-22

Calcium Phosphate Ceramic Tablets for Studying De- and Remineralization Processes

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Calcium orthophosphates are of particular interest among the other phosphorus inorganic compounds because calcium orthophosphates are the mineral basis of the bone tissues. The latest requirements not to test new materials on living organisms pose a challenge to finding suitable artificial substitutes.

In this work, the possibility of using ceramic tablets based on hydroxyapatite (HA), which represent an approximate model for studying biomimetic processes in an environment free of biological macromolecules, was investigated.

Poorly crystalline carbonate apatite powder was obtained via wet precipitation method from 1M solution of $Ca(NO_3)_2$ and 0.6M solution of $(NH_4)_2HPO_4$ at a Ca/P ratio of 1.67 and pH 12 (keeping with NH_4OH). The resulting precipitate was matured for 24 h, centrifuged, washed and dried at 90ºC for 15 h. Tablets with a diameter of 13 mm and a height of 2.2 mm were prepared at a pressure of 6.5 t for 1 min and sintered at 1000ºC for 1 h. The degradation ability of the tablets was tested by immersion in a 0.1% solution of lactic acid containing 2.2 mM $CaCl_2$ and 2.2 mM NaH_2PO_4 for different duration. Lactic acid was chosen as demineralized agent because it was produced by the bacteria in the oral cavity and participates in the dental biofilm causing caries. Remineralization was examined in the presence of artificial saliva after biostimulating of the tablet surface with polycarboxybetaine. XRD, SEM and EDX analysis of all samples were performed and obtained results were discussed.

Keywords: hydroxyapatite, ceramic tablets, demineralization, remineralization

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ICTM P-23

Polycarboxy/Sulfo Betaine Functionalized Calcium Phosphates Obtained by Adsorption Process

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The adsorption of polycarboxy or polysulfo betaine on the double doped (with Zn and Mg) amorphous calcium phosphate (ACP) was studied with the aim of preparation of functionalized materials with improved remineralizing activity for dental applications. ACP is a precursor for the formation of the teeth and bone mineral phase. Mg and Zn are essential for the building and growth of hard tissues while polycarboxy (PCB) and polysulfo (PSB) betaines mimic the naturally occurring betaine form of amino acids as well as the polar groups of phospholipids.

The Mg (6.6 mol %) and Zn (1.2 mol %) doped calcium phosphates ($\Sigma Me^{2+}/P$ = 1.44 (Mg, Zn-ACP) were biomimeticaly prepared in the media of simulated body fluid and saturated solution of glycine that provides bone like composition and high specific surface area (100-180 m^2/g). The functionalized materials were prepared in dynamic conditions, PCB/PSB to Mg, Zn-ACP ratio of 1:10 g/g and solid to liquid ratio of 1:6.25 g/ml, 36^oC and duration 6 and 24 hours.

It was established that the chosen method for obtaining the materials leads to the transformation of the initial amorphous calcium phosphate phase into poorly crystalline hydroxyapatite. This process occurs faster in the presence of PSB, with the amount of PSB in the final material being less than the amount of PCB. Under the conditions of the experiment, increasing the time from 6 to 24 h has no effect on the amount of adsorbed polymer.

Observed differences in the two materials can be explained by the different nature of the negatively charged functional groups of the polymers, which results in different polymer/calcium phosphate interactions.

Keywords: calcium phosphates, poly carboxybetaine, poly sulfobetaine

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ICTM P-24

Morphological and Thermal Characteristics of the Mechanochemicaly Activated Calcium Phosphates

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Mechanochemical activation is an effective method for obtaining uniform, nano-sized and surface-activated powders. It increases the energy of the system, affecting the morphology of the particles, and hence the thermal properties of the materials and often leads to the formation of new phases.

The effect of the revolutions and duration of the mechanochemical activation on the properties of equimolar mixtures of $Ca(OH)_2$ and $CaHPO_4$ was investigated in order to clarify the nature of ongoing processes. Experiments were performed in FRITSCH 6 ball mill with 300, 450 and 600 rpm and duration of 5, 11, 24, 48 and 120 h.

The results show different behavior of the two starting substances. The $CaHPO_4$ particles considerably decrease in size with increasing revolutions and grinding time (from 89.9 nm to 24 nm at 300rpm (120 h); to 28.8 nm at 450 rpm (24h) and to 42.2 nm at 600rpm (11h)), which leads to a decrease in the temperature effects of its phase transformations in the DTA curves. For $Ca(OH)_2$ the effect is less pronounced. A new phase of nonstoichiometric poorly crystalline hydroxyapatite was identified at 120 h at 300 rpm, at 24 h at 450 rpm, and at 5 h at 600 rpm. Higher revolutions create conditions for obtaining more and larger defects in the crystal structure of $CaHPO_4$, which accelerates the transformation to hydroxyapatite. Identical fragments in the structures of $CaHPO_4$ and $Ca_5(PO_4)_3OH$, stimulates additionally the phase transformation. The amount and crystallinity of hydroxyapatite increases with increasing milling time and reaches 94% after 48 h activation at 600 rpm, a quantity that no longer changes.

Keywords: mechanochemical activation, calcium phosphate, morphological characteristics, thermal properties

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ICTM P-25

Comparative Crystallization Behaviour of Glass-Ceramics Derived from Raw and Modified Coal Fly Ash

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The production of glass ceramics from coal fly ash represents a sustainable and innovative approach to waste utilization and material development. Glass-ceramics based on $CaO\text{-}Al_2O_3\text{-}SiO_2$ system were produced by controlled crystallization of three types of vitrified fly ash: a raw fly ash (RFA), and the two types of pre-treated fly ash: physically modified (PM) and chemically modified (CM). The fly ash samples were heated up to 1500ºC, in the furnace, until they melted and formed a molten glass and then quenched to a room temperature where they solidified in an amorphous state. The glass was subjected to controlled heat treatment, at specific temperature regime, to induce controlled crystallization. Crystallization behavior of the parent glasses was investigated by differential thermal analysis. Glass transition temperature (Tg), peak temperature (Tp) and melting temperature (Tm) of parent glasses were determined. The crystallization tendency of the parent glasses estimated by Hruby-coefficient was between 4,6-2,3. The dominant crystalline phases determined by XRD were calcium aluminum silicate (anorthite) and hematite. SEM and EDS analysis were performed on the selected glass-ceramic samples in order to investigate their microstructure.

By transforming coal fly ash into glass ceramics, we not only tackle the environmental problems associated with waste disposal, but also contribute to the creation of valuable materials with a variety of applications.

Keywords: coal fly ash, parent glass, quenching, vitrification, glass-ceramics

ICTM P-26

Alkali Activation of Coal Fly Ash and Construction and Demolition Waste: A Sustainable Path to Innovative Materials

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Alkali activated synthesis (AAS) of coal fly ash (CFA) and construction and demolition waste (CDW) presents a sustainable solution for fabrication of construction materials. AAS utilizes industrial byproducts like CFA and CDW as precursors, offering an environmentally-friendly alternative in comparison to the traditional cement-based materials. CFA, a fine powder produced from coal combustion in the thermal power plant REK Bitola, and CDW generated from construction activities, were collected and processed to remove impurities. CFA and CDW were characterized from physical, chemical, mineralogical, thermal and morphological aspect. The precursors were mixed in different ratios with the alkaline solutions based on Na_2SiO_3 and NaOH. Scanning electron microscopy equiped with energy-dispersive X-ray spectroscopy (SEM/EDS) were used to determine the microstructure of final products. The compressive strength of the alkali activated products vares from 6,14 to 25,5 MPa, depending on the CFA/CDW ratio and the solid/liquid content.

In conclusion, the AAS from CFA and CDW exemplifies the synergy of sustainable materials engineering and waste management. This innovative approach addresses not only the waste disposal challenges, but also yields materials with a lower environmental footprint and superior properties, positioning AAS as a compelling solution for a greener and more resilient construction industry.

Keywords: coal fly ash, CDW, alkali activation, mechanical properties

ICTM P-27

Examination of the Characteristics of Tufa from the Piplići Locality and Their Possible Applications

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Tuff is a type of volcaniclastic rock formed by the deposition of finer volcaniclastic material. Zeolitic tuffs are rocks that contain zeolites as well as various other crystalline or amorphous phases. In the Piplići deposit located 5 km southeast of Prnjavor, the average thickness of the only tuff layer is about 10 m, and it is interstratified within a complex of gray clayey sandstones deposited conformably over layered fossiliferous limestones.

Sample characterization was performed using the following methods: low-temperature nitrogen adsorption (LTNA), thermogravimetric analysis and differential thermogravimetric analysis, Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy and energy-dispersive X-ray spectroscopy (SEM-EDS), X-ray diffraction analysis (XRD), and cation exchange capacity (CEC) determination. The results of the analysis showed that the tested samples are mesoporous materials, that they are thermally stable materials that do not change their structure when heated up to 800°C. FTIR spectra of the samples shows characteristic peaks of aluminosilicates. SEM-EDS surface investigations of all samples revealed the presence of structural cations (silicon and aluminum) as well as additional cations such as Na^+, Mg^{2+}, K^+, and Ca^{2+}, while XRD analysis showed that the tested samples consist of feldspar, clinoptilolite/heulandite, mordenite, smectite, quartz, and calcite. Cation exchange capacity (CEC) determinations showed that samples 1 and 2 have CEC values of 30.15 and 25.26 mmol M^+/100g of sample, respectively.

Due to their adsorption properties and ion exchange capabilities, scientists have explored their potential applications in addressing pressing environmental issues, particularly in processes involving the removal of various pollutants from water streams.

Keywords: zeolite, tuff, adsorption, ion exchange, polutants

OBPC O-1

Effect of Pure Anethole and Synergistic Interaction of Anethole with Different Essential Oils- Potential Alternative Biocontrol Products Against Plant Pathogens

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The development of natural protective agents against plant fungal pathogens as alternatives to chemical fungicides is currently in the spotlight all over the world. In the present investigation, antifungal activities of anethole alone, as well as synergism of its possible double combinations with nine other essential oils (EOs) were investigated. For determination of antifungal activity, a disk diffusion and a broth microdilution method were used.

The data reported in this study show that EOs exhibited promising antimicrobial activity against tested fungi and they might provide an alternative way to fight with plant fungal pathogens, so they can be considered safe for plants because originate from them. Generally, it is possible to recommend the use of EOs for replacement of synthestic fungicides in agriculture. The results of this study provided an important contribution to development of potential ingredients for natural antimicrobial agents.

Keywords: essential oils, fungistatic, fungicidal, phytopathogens

OBPC O-2

Phenol Biodegradation Using Native and Granulated Microorganisms Adapted from Petroleum Wastewater

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Toxic phenolic wastewater has become a significant environmental issue due to the overuse of phenol-containing products and their uncontrolled discharge. The aim of the present study is to determine the viability, resistance, and potential application of native and granulated microorganisms in an efficient phenol biodegradation process. The screening was carried out by providing phenol concentrations between 100 to 2000 mgL^{-1}, which are increased progressively. pH, biomass, COD, oil materials, NH_4^+, NO_3, chlorides, sulphates, phosphates, and phenol tolerance were all analyzed. Microorganism resistance decreased dramatically as phenol concentration increased. When all the sample strains were used in combination, the results were better. Citrobacter sp., Raoultella sp., Leclerciasp., and two species of yeasts were adapted from oil refinery effluent and synthetic water. The study examines the adaption, granulation, and characterization of native and granulated microorganisms from petroleum wastewater for the biodegradation of high phenol concentration and its potential as an alternative for the phenol bioremediation method.

Keywords: Biodegradation, Phenol degradation, Wastewater.

OBPC O-3

New 17α-picolyl Androstane Derivatives: Synthesis, *In Vitro* Biological Activity and *In Silico* ADME/T Properties

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Oxyimino ethers are compounds very often used in organic synthesis to obtain various products such as amino alcohols, hydroxylamines and amines, but they have also shown promising anticancer activity.[1] Bearing this in mind, we have efficiently synthesized a new *O*-alkylated oxime derivative in the androstane series, which was then used as a precursor for preparing a 3-hydrazinocarbonylmethyloxyimino derivative.

New androstane derivatives were evaluated for relative binding affinities to the ligand-binding domains of selected steroid receptors (ERα, ERβ, AR and GR) and inhibition potential against recombinant enzymes from aldo-keto reductase 1C subfamily, promising drug targets for cancer treatment. Our results showed the lack of estrogenic or androgenic properties of the tested compounds, suggesting they could be suitable candidates for the development of anticancer agents against hormone-dependent cancers. In addition, *in silico* ADME/T profile and physicochemical properties were determined using the online web tools, where parameters for both compounds were within the optimal range, suggesting them as drug-like molecules.

Keywords: androstane; *O*-alkylated oximes; hormone receptors; AKR1C4

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OBPC O-4

The Role of Chemistry in the Development of the Radiosynthesis Methods for Fluorine-18 Radiopharmaceuticals

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Fluorine-18 radiopharmaceuticals are drug molecules that contain the positron-emitting (β+) radioisotope [18F] F. As a favorable halogen atom in radiopharmaceutical chemistry, [18F] F is suitable for the development of many radiopharmaceuticals, intended for investigating tumors by positron emission tomography (PET).

The utilization of nucleophilic [18F]F−ions in the fluorine-18 radiopharmaceutical synthesis processhas many advantages over fluorine gas[18F]F2. The radiosynthesisis fully automated using a chemical synthesizer in a lead-shielded hot cell because of handling with radioisotopes. Therefore, during the radiosynthesis method development, sampling at different reaction steps to follow reaction progress can be a challenge. Finding a solution may demand the efforts of many research experiments wherefore operator radiation exposure increases, so applications of [19F]F− chemistry would be practical.

This study aimed to discuss [19F]F− chemistry practices in developing of radiosynthesis method and to adapt suitable reaction conditions with the most common radioisotope used in PET, short-lived fluorine-18 (t1/2 = 109.77 min). The experiments were carried out using the stable isotope, [19F]F−or radioisotope [18F]F−in an aqueous solution. Analysis of the reaction mixture at different steps of synthesis (before/after fluorination reaction, unhydrolyzed/hydrolyzed intermediate mixture, unpurified product mixture) as well as in the final purified product were performed. The samples were analyzed with HPLC method.

The radiosynthesis development was facilitated by using this experimental chemistry approach. Also, the results obtained can help overcome the challenges, which can impede the reactions or lead to unwanted chemical impurities during radiosynthesis.

Keywords: Radiopharmaceutical, ^{18}F-chemistry, radiosynthesis, developing, analysis

OBPC O-5

Model of G-quadruplex Interactions with Heterocyclic Ligands

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We offer a contribution to methodology of targeting important regulatory nucleic acid structures, G-quadruplexes. A model of their interaction with potentially anticancer hetero-polycyclic molecules is developed using methods of its precision computation by quantum chemistry.[1] Further we use quantitative characterizations of biological activity of studied heterocycles.[2] We find meaningful relationships of computed molecular energetic values, namely affinity of heterocyclic ligands to a model G-quadruplex, and experimental values of pharmacological characteristics, e.g. **IC_{50}.**[3] **Applied quantum chemistry theories are DFT, e.g. using wB97XD/6-31G*, and explicitly correlated MO theory,[1,3] e.g. in the RI-MP2 form. These types of QSAR may be** significant in the quest for novel anticancer and other medications, provided G-quadruplex regulation of the key biological process is involved.

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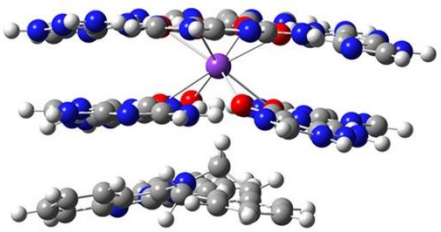

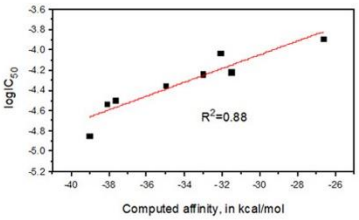

Keywords: G-quadruplexes, quantum chemical model, ligand affinity, cancer IC_{50}

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OBPC O-6

Electrochemical Biosensor Based on NAD(P)H-dependent Quinone Reductase for Rapid and Efficient Detection of Vitamin K_3

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Vitamin K refers to a group of vitamins that play an important role in blood coagulation and regulation of bone and vascular metabolism. However, vitamin K3 may give severe side effects in animals and humans when improperly added to food and feed due to its toxicity. An electrochemical biosensor was developed based on the YaiB NADPH-dependent quinone reductase from Lactococcus lactis (YaiB) to achieve rapid and redox probe-free detection of vitamin K3. First, the ability of the carbon electrode to distinguish between 1,4-benzoquinone and hydroquinone was developed. Then, YaiB immobilized at the electrode to work as a bioreceptor was engineered and its sensitivity and specificity to reduce vitamin K3 was demonstrated. Finally, the biosensor's practical potential was tested directly in spiked milk samples achieving quantification of the vitamin K3 for 15 minutes. The limit of detection was 0.18µM and 0.86 µM in buffer and milk, respectively.

Keywords: Enzymatic sensor; Carbon Screen Printed Electrode; Voltammetry; Food quality; Vitamin detection.

OBPC O-7

Method for Analysis of Terpenes in *C. Sativa* Using Headspace GC-FID and GC-QQQ

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Terpenes are cannabis secondary metabolites that provide not only beneficial biological properties for the plant, but also are found to have synergic and/or enhancing effects of the cannabinoids[1]. Therefore, they are extremely important in the production of pharmaceuticals significant for the improvement of human health[1]. To emphasize, terpenes are volatile compounds that produce the plant its aroma and flavor, characterize the specific cannabis strains, and are primary constituents of the essential oils[1,2]. Hence, the analysis of terpene profile, that includes the terpene composition, chemistry, diversity, quantity, and biosynthesis, in the various products obtained from cannabis, is of primary importance[2].

We present method for identification and quantification of terpenes in *C. Sativa* using Agilent 7967A headspace sampler for sample introduction, Agilent 8890 gas chromatograph for terpene separation and Agilent Flame Ionization Detector accompanied with Agilent Triple Quadrupole 7000D for their detection and quantification. Namely, the headspace technique is perfect for analysis of the volatile terpenes, and it can provide better separation, faster analysis, and reduced matrix effect, compared to the traditional automatic liquid sampler[3]. Moreover, we present a comparison of the separation capabilities of two different GC columns, Agilent DB-Select 624 UI and Agilent HP-5. Finally, we optimized the process of sample preparation, without any significant losses because of the terpene volatility.

Keywords: terpene, cannabis, headspace, gas chromatography

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OBPC O-8

New Thiazole Androstane Derivatives: Synthesis and Cytotoxic Activity

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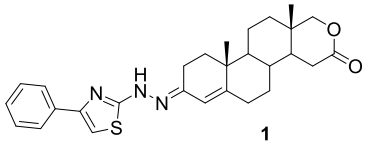
Hybrid molecules created by combining a steroid with a thiazole core may be potential candidates for drug design, with improved biological activity and bioavailability. This work describes the synthesis of new thiazole androstane derivatives. The starting compound was dehydroepiandrosterone, which was modified in a multiphase synthesis into 3- or 6-thiosemicarbazone androstane derivatives, direct precursors in the synthesis of thiazole androstane derivatives **1** and **2**. Their cytotoxicity was tested on five cancer cell lines: breast adenocarcinoma cells (MCF-7), acute lymphoblastic leukemia (CCRF-CEM), cervical carcinoma cells (HeLa), hormonal insensitive prostate cancer cells (DU-145), hormonal sensitive prostate cancer cells (LNCaP), as well as on one healthy line: normal skin fibroblasts (BJ). Compound **1** showed strong cytotoxic activity against cervical carcinoma cells (HeLa), while compound **2** was highly cytotoxic against acute lymphoblastic leukemia (CCRF-CEM).



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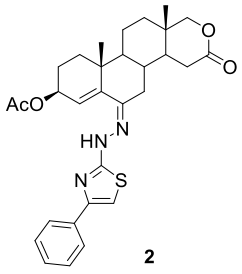

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Keywords: steroids, thiazole, cancer, cytotoxicity

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Development and Innovation of the Republic of Serbia (Grant No. 451-03-47/2023-01/200125).

OBPC O-9

Comparative Analysis of Marjoram Essential Oils from Serbia and Egypt

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The chemical composition of essential oils from commercial marjoram (*Origanum majorana* L.) sourced from southeastern Serbia and Egypt was investigated using GC and GC-MS techniques. The major volatile compounds in both oils were terpinen-4-ol and *γ*-terpinene, constituting approximately 50% of the oils based on GC peak areas. However, significant differences between the two oils in terms of their *cis*- and *trans*-sabinene hydrate content, which are commercially important monoterpenes were determined. The Egyptian oil contained 12.1% *trans*-sabinene hydrate and 3.5% *cis*-sabinene hydrate, while the Serbian oil contained a total of 7.2% *cis*- and *trans*-sabinene hydrates in a 1:1.7 ratio. We also performed a complete and comprehensive ^{1}H and ^{13}C NMR assignment of sabinene hydrates, that includes *J*-values obtained by computer spin simulation and molecular modeling. Interestingly, we found that the literature NMR data on these compounds were mostly incomplete and usually lacked a thorough multiplet analysis.

Keywords: *Origanum majorana* L., *trans*-sabinene hydrate, *cis*-sabinene hydrate, NMR, spin simulation.

Acknowledgement: This work was supported by the Ministry of Science, Technological Development and Innovations of the Republic of Serbia (Contract Number 451-03-47/2023-01/ 200124).

OBPC P-1

Biologically Active Fibers with the Sorption Tramadol

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Biologically active fibers as drug carriers have improved characteristics in comparison with conventional medical therapies. Cellulose as a hydrophilic and biocompatible, nontoxic and eco-friendly material, makes a good polymer matrix for obtaining biologically active fibers.

The aim of this study was to investigate the possibility of obtaining biologically active materials by sorption of tramadol on oxidized cellulose fibers. For this purpose, samples of oxidized cellulose (OC) with 0.547 and 1.163 mmol/g of COOH groups and a sample of OC with 0.547 mmol/g activated Na+ ion were used

The bonding was performed in analgesic water solution concentration of c=1,7·10-3 2,5·10-3 3,4·10-3 4,3·10-3 5,1·10-3 mol/L at temperature 26±1 °C, while desorption was performed in physiological solution. The amounts of bonded and released antibiotic were determined spectrophotometrically in UV range. Maximum amount of the bound drug (0,2232 mmol/g) was obtained during the sorption on the oxidized bandage with 1,163 mmol/g COOH from a tramadol solution with a concentration of c=5.1·10-3 mol/L after 24 hours. The amount of tramadol bound to the activated OC fiber was significantly higher and amounted to 0.5297 mmol/g from a tramadol solution with a concentration of c=5.1·10-3 mol/L after 24 hours. The maximum amount of the released drug was 0.0524 mmol/g.

The paper studies the influence of tramadol's chemical structure and the duration of sorption on the amount of the bound drug. It was determined that the drug bonding was achieved through ionic hydrogen bonds and π-π interactions of the drug functional groups with the oxidized cellulose bandage.

Keywords: oxidized cellulose, tramadol, biologically active cellulosic fibers.

OBPC P-2

Method Validation for *in Situ* Identification of Diazepam with Raman Spectroscopy in Pharmaceutical Industry

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Raman spectroscopy in its hand held version is one of the most advanced and used analytical techniques used for routine, *in situ* identification on incoming raw materials in the warehouses of the pharmaceutical industry.

The main objective of the validation of the analytical procedure is to demonstrate that the procedure is suitable for its intended purpose. This is performed according to the Guidance on validation of analytical procedures (CPMP/ICH/701/95) and USP Monograph ⟨1225⟩ Validation of Compendial Procedures.[1,2] In this study, the validation of the Raman spectroscopy identification method for diazepam active pharmaceutical ingredient (API) was performed on the parameters of specificity and robustness.

For testing method's specificity, Raman spectra were collected from three different positions in the same package from the same batch of diazepam API, in the original manufacturer's packaging. On the other hand, for testing the parameter robustness the effect of minor changes to the normal operating conditions was challenged, based on introduced changes in the polyethylene bag thickness. Also, the method robustness was assessed by analysis performed by different analyst using the same method parameters

The obtained results confirmed that the method is specific and robust in accordance with the validation criteria.

Keywords: validation, Diazepam, Raman spectroscopy, specificity, robustness, pharmaceutical industry

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OBPC P-3

New Esters from the Essential Oil of *Doronicum Columnae* Ten.

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The genus *Doronicum* (Asteraceae) comprises 26 different plant species, mostly distributed in Europe and southwest Asia. Although some of the monoterpenoids, sesquiterpenoids, and diterpenoids from *Doronicum* species possess significant biological activity, the genus is still poorly phytochemically and pharmacologically studied. *Doronicum columnae* Ten. is a perennial representative of this genus, and only non-volatile constituents of this taxon were previously investigated.[1]

Prompted by the lack of data on the secondary metabolites, we decided to investigate the chemical composition of *D. columnae* roots essential oil. GC-MS analysis of the oil showed the presence of 2-isopropyl-4-methylphenyl (isothymyl) and 2-isopropyl-5-methylphenyl (thymyl) isobutyrates (16.4% and 16.3%, respectively) as the main essential-oil constituents. Partial ion current (PIC) chromatograms for *m/z* 135, 150, and 220 or 234 revealed the presence of several additional esters with the same fragmentation pattern in the mass spectrum. To infer the structures of these constituents, we decided to prepare a library of esters of (iso)thymol and (iso)carvacrol (isobutyrate, butyrate, 2-methylbutyrate, 3-methylbutyrate, and valerate), 20 compounds in total, which led to the identification of three new natural products: isothymyl 2-methylbutyrate, isocarvacryl isobutyrate, and isocarvacryl 2-methylbutyrate. The synthesized esters were characterized by spectral (MS, 1D, and 2D NMR) and chromatographic (GC and GC-MS) techniques.

Keywords: *Doronicum columnae*, essential oil, esters, spectral characterization

Acknowledgment: This work was funded by the Ministry of Science, Technological Development and Innovations of Serbia [No. contract 451-03-47/2023-01/200124].

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OBPC P-4

Molecular Dynamic Simulations in Binary Liquid Mixtures

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Experimental data of liquid binary mixtures can provide the thermodynamic and transport properties[1]. Molecular dynamics simulations (MD) are preformed on the same mixtures at the same experimental conditions: at different temperatures and different mixture compositions. Molecular dynamics simulations can gain a deeper understanding of the behavior of liquid mixtures at the molecular level. It can be used for analyzing specific properties, such as the radial distribution functions (RDFs), interactions in the mixture, thermodynamic and transport properties, understanding the dynamics of the system. This information can be used to obtain insight into the molecular level, to understand the nature of the interaction and to predict the behavior under specific conditions. The right force field are essential for describing the system and using the density of the simulated systems as a represented data to compare to the experimental data. We performed experimental measurements and molecular dynamics simulations on four systems to study influence of double bonds on the properties of alcohol mixtures. The data of the molecular dynamic simulations are in an agreement with the data from experimental measurement, and at the same time we can observe interactions at the molecular level that indicate different noncovalent interactions of double bonds in comparison with single bonds.

Keywords: binary mixtures, thermodynamic properties, molecular dynamic simulations

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OBPC P-5

Synthesis, *In silico*, and *In vitro* Biological Testing of Novel 19-halogenated D-homo Lactone Steroids as Potential Antitumor Compounds

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Multiple tumors have been proven to be hormone-dependent, meaning that their development and growth are induced by endogenous human hormones. This fact was the basis for the design and development of antitumor steroidal drugs such as testolactone and exemestane. With the same goal in mind, we have performed a synthesis of C19-halogenated steroidal D-homo lactones. Previously synthesized 5α-bromo-6β-hydroxy D-homo lactone derivative[1] was used as a starting compound. It was transformed into a 19-hydroxy derivative through two synthetic steps: 6,19-epoxidation and reductive epoxide opening. Next synthetic steps led to the synthesis of two new halogenated derivatives as well as one intermediate and two side products. All novel synthesized compounds, halogenated, intermediate and side products, were tested *in silico* for their ADME properties (SwissADME Prediction), and *in vitro* for their cytotoxicity against a panel of cancer cell lines (MTT). Their relative binding affinities to the ligand-binding domains of androgen receptor and estrogen receptor α and β isoforms, were measured using a fluorescence-based assay in yeast.

Keywords: androstane, cytotoxicity, hormone derivatives

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OBPC P-6

A Systematic Study of Esterification of Ibuprofen with Common Alcoholic Excipients using LC-MS/MS

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Ibuprofen is a nonsteroidal anti-inflammatory drug with non-narcotic, analgetic and antipyretic action. It is widely used in the treatment of pain in many different pharmaceutical preparations. The usage of alcohols as excipients is known in topical preparations to increase the solubility of ibuprofen, as well as to enhance its skin permeability. Because of the chemical nature of ibuprofen, reaction of esterification in the presence of alcohols is expected to occur in such preparations and the products should be identified and their concentration monitored.[1]

In this work, a systematic study has been carried out focused on the esterification reactions between ibuprofen and simple alcoholic excipients with different structural complexity: ethanol, isopropanol and propylene glycol. The detected products have been separated with an optimized reversed-phase chromatographic method and characterized with mass spectrometry.[2] The developed LC-MS method has enabled structural characterization of the ester of ibuprofen with ethanol and with isopropanol as well as two monoesters and one diester of ibuprofen with propylene glycol obtained in the stressed binary mixtures by their MS and MS^2 spectra.

Keywords: Ibuprofen, alcohol, ester, drug, API, excipient, LC-MS/MS

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OBPC P-7

Estimation of Measurement Uncertainty for Total Chlorides Content Determination in Concentrated Solutions for Hemodialysis

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The uncertainty in measurement is a crucial segment of the estimation of experimental analytical results. Moreover, the results without an uncertainty estimation cannot be considered as complete. The aim of this work was an estimation of the combined standard and extended measurement uncertainty (MU) for three simple and rapid methods for routine determination of total chlorides content in concentrated solutions for hemodialysis. The first two methods were based on potentiometric titration, with minor differences in the sample preparation, while the third method was based on a simple volumetric titration. The approach applied for the MU estimation was according to the Guide for the expression of uncertainty in measurement[1].

The MU estimation was performed for the same sample with the three methods in order to test which one is the most precise. Based on the reproducibility data obtained from six repetitions it can be concluded that the first method was the most precise one, accompanied by lowest input of Type A uncertainty and confirmed by the MU value, as well. On the other hand, the volumetric method was found to be more precise than the second potentiometric method, based on the lower input of type A uncertainty. However, the uncertainty estimation showed that the potentiometric method was the one characterized by lower MU value, indicating that the volumetric method was associated with higher Type B uncertainty.

Furthermore, the obtained results demonstrate that MU provides additional valuable information for the method performance and point out its importance in the interpretation of the obtained analytical results.

Keywords: total chlorides content, measurement uncertainty, potentiometric titration, volumetric titration.

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OBPC P-8

Multivariate Analysis Approach in API-Excipient Compatibility Testing in the Development of Pharmaceutical Dosage Forms

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Partial least squares–discriminant analysis (PLS-DA)[1] using Simca® 17 software was applied for evaluation of the results obtained from a compatibility study designed for the active pharmaceutical ingredient (API) ibuprofen with selection of twelve excipients used in the formulation of pharmaceutical finished products. Fourier-transform infrared spectroscopy (FTIR) and X-Ray powder diffraction (XRPD) were used as techniques for solid-state characterization of the samples.

The obtained results have shown that the optimal PLS-DA model was obtained for the FTIR spectra, explaining 83.3% of the changes in the FTIR spectra and predicting new datasets quite good (R^2X=0.833, R^2Y=0.991 and Q^2=0.960), as well as the PLS-DA model built based on the XRPD diffractograms (R^2X=0.892, R^2Y=0.986 and Q^2=0.946). Moreover, the main variations in the FTIR and XRPD data were attributed with highest VIP (Variable importance for the projection) scores in the corresponding VIP plots, proving the model capability for predicting incompatibilities. The prediction power of the optimal models for FTIR and XRPD experimental data was further confirmed (Root mean squared error of prediction, RMSEP=0.10% and 0.35%, respectively).

The obtained results demonstrated the potential of multivariate statistical analysis for monitoring of API-excipients solid-state compatibility during the routine analysis in the preformulation development.

Keywords: ibuprofen, compatibility, partial least squares-discriminant analysis

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OBPC P-9

Investigating the Structural Features of Some Monocarbonyl Curcuminoids: Insights Into Their Pharmacological Profile

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To fully exploit the therapeutic potential of curcumin, overcoming its pharmacokinetic limitations is crucial. An effective strategy for addressing this challenge involves replacing the central 1,3-diketo moiety of curcumin with a single carbonyl group. Inspired by this promising approach, we synthesized a series of monocarbonyl analogs of curcumin (MACs).

The objective of this study was to investigate the effects of various structural features on the pharmacological characteristics of MACs. Hence, the analogs were systematically evaluated for drug-likeness and absorption, distribution, metabolism, and excretion (ADME) attributes using popular software packages. The satisfactory predictions obtained for their pharmacokinetic parameters and drug-like nature offer significant insights for the development of more effective molecules in terms of their metabolic behavior and overall performance. Furthermore, the stability of the analogs at physiological pH was assessed using UV-Vis spectroscopy and their toxicity against normal erythrocytes was evaluated using a hemolytic assay. While curcumin displayed a notable decrease (17 %) in maximum absorbance within 30 minutes, the active MACs

exhibited negligible changes (0.2 – 2 %), indicating improved chemical stability. The curcuminoids were also found to be non-hemolytic and non-toxic at concentrations up to 150 μM.

The results of both *in vitro* and *in silico* investigations confirmed the potential of these compounds as viable drug candidates, paving the way for further research and structural refinement in anticipation of their future clinical application.

Keywords: monocarbonyl analogs of curcumin; ADME; hemolytic activity; stability; pharmacokinetics

OBPC P-10

Design and *in Vitro* Evaluation of Monocarbonyl Curcumin Analogs Eliciting Breast Cancer Cytotoxicity

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Breast cancer is the most prevalent malignancy in women worldwide and is heterogeneous and highly complex in nature. Curcumin, owing to its pleiotropic molecular structure and recognized bioactivities, has established its role in anticancer research. Regarding curcumin's limiting factors from therapeutic applicative aspect, the monocarbonyl analogs of curcumin (MACs), possessing improved pharmacological properties, offer promising prospect for the development of new anti-breast cancer agents.

Guided by our previously built quantitative structure-activity relationship (QSAR) model[1] novel and previously reported MACs with different central cores and ring substituents were designed and synthesized. The cytotoxicity of selected compounds against the MCF-7 breast cancer cell line was evaluated using an MTT assay. The viability values obtained for the cell line under the influence of various

MACs were in the range of 2 – 76 %. This confirmed the influence of structural features on the anticancer activity of the molecules. Furthermore, the experimental results were in accordance with the QSAR trend, and both reflected the inhibitory activity of curcumin analogs on the survival and proliferation of breast cancer cells *in vitro*. In conclusion, MACs represent a promising chemical architecture with anticancer potential.

Keywords: monocarbonyl analogs of curcumin; QSAR; MTT; MCF-7; anti-breast cancer

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OBPC P-11

Inclusion Complexes of β-Cyclodextrin and Selected Phenolic Acid Derivatives

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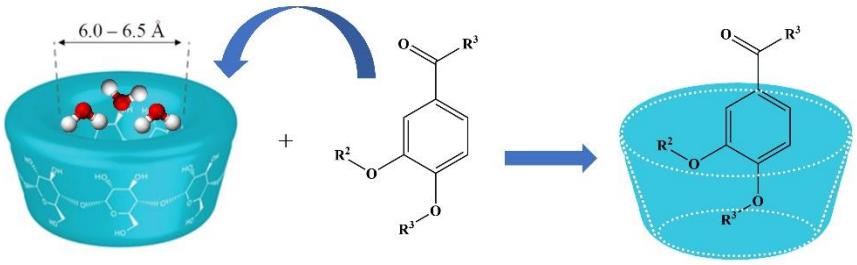
The key ability of cyclodextrins to form inclusion host-guest complexes found numerous applications in pharmacy, medicine, food, textile, and cosmetic industry, agriculture, nanotechnology, and other fields.[1] Regarding this, in this work, the synthesis of β-cyclodextrin inclusion complexes with protocatechuic and vanillic acid derivatives (esters, hydrazides, and pyrazoles) was performed in aqueous media.



After the reaction completion (24h), the obtained products were isolated by solvent evaporation in a yield of 91–94%. The formation of host-guest complexes was confirmed by ^{1}H NMR and IR spectra, and elemental analysis, whereas the stoichiometric ratio (1:1) was determined by Job's plot method. Also, inclusion complexes and starting compounds were subjected to antimicrobial investigations which exposed good activity against several bacterial strains.

Keywords: β-cyclodextrin, host-guest complexes, phenolics, antimicrobial activity

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OBPC P12

The Essential Oil of *Acmella Oleracea* (L.) R.K. Jansen: Structural Elucidation and Acute Toxicity of New Esters

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Amazon rainforest is one of the most significant biodiversity hotspots in the world and represents a phytochemical gold mine with countless plant species with immense pharmacological potential.[1] One of them is paracress (*Acmella oleracea* (L.) R.K. Jansen (Asteraceae)) with already proven pharmacological properties including, but not limited to antinociceptive, anti-inflammatory, antioxidant, immunomodulatory, antimicrobial, antiviral, and diuretic activity.[1] A detailed GC-MS analysis of the chemical composition of the essential oil of paracress revealed, among more than 120 identified constituents, the presence of 12 compounds that were, according to their mass spectral fragmentation, tentatively identified as long-chain α-keto esters of isobutyric, 2-methylbutanoic, isovaleric, angelic, tiglic, and/or

senecioic acids. To determine the exact structure of these minor essential-oil constituents, 18 (completely new) esters were prepared starting from the synthesized 2-oxoundecan-1-ol, 2-oxododecan-1-ol, and 2-oxotridecan-1-ol with the mentioned acids. All synthesized compounds were spectrally and chromatographically characterized. GC-MS, in combination with NMR analyses of the compounds, provided proof of the identity of the mentioned *A. oleracea* constituents. The acute toxicity of these compounds was tested in the *Artemia salina* model to assess the safety of these naturally occurring esters (12 out of 18 synthesized compounds). The obtained results suggest that the intake of these compounds in naturally available amounts, on their own, would probably not represent a risk to human health.

Keywords: *Acmella oleracea*, essential oil, esters, spectral characterization

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OBPC P-13

Chemical Composition of the Defensive Secretion from *Pachyiulus Varius* (Fabricius, 1781) (Diplopoda, Julida)

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Numerous millipede species produce a defensive secretion that contains a variety of volatile compounds grouped into alkaloids, quinones, phenols, and esters.[1] Chemical composition of defensive secretion is unknown for the majority of members of the genus *Pachyiulus* Berlese, 1883 and up to now analyses of secretion constituents were done only for *P. hungaricus* and *P. cattarensis*.[1,2] Herein, mass spectra (MS), gas chromatographic data (GC(RI)), synthesis, and chemical transformations of crude extracts (synthesis of dimethyl disulfide adducts and transesterification), enabled the identification of more than 90 constituents of the defensive secretion of *Pachyiulus varius* (Fabricius, 1781) from Serbia. The

analyzed samples contained, along with the ubiquitous quinones, alkanes, 1-alkenes, and long-chain *n*-esters, a homologous series of, predominantly hexyl, esters of *n*- and branched (*iso*- and *anteiso*-) long-chain (un)saturated acids. Thirty-nine identified esters represent new natural products that could be excellent chemotaxonomic markers for *Pachyiulus* species.

Keywords: *Pachyiulus varius*, defensive secretion, GC-MS, esters

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OBPC P-14
Metal salts of ascorbic acid and their stability at stress conditions

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L-Ascorbic acid, commonly referred to as Vitamin C, is a water-soluble molecule renowned for its remarkable antioxidant properties[1]. In this form it is susceptible to physico-chemical changes caused by a change in temperature, moisture, light and oxygen[2], and can often easily form metal ascorbate salts[3]. Among these salts, magnesium, sodium, and calcium ascorbate are particularly renowned and extensively employed within the cosmetic, food, and pharmaceutical industries due to their potent antioxidant characteristics[1].

The present study aims to investigate the stability of magnesium and sodium salts of ascorbic acid, along with binary mixtures of ascorbic acid and

excipients containing magnesium, calcium, and sodium. Under stress conditions (25 °C/60 % RH and 40 °C/75 % RH), noticeable visual changes manifested across all samples, characterized by darker hues. Notably, the magnesium ascorbate sample exhibited complete decomposition after 30 days. FT-IR analyses unveiled broadening of vibrational bands, as well as the emergence of new vibrational bands, potentially indicative of the decomposition of the ascorbate salts. Furthermore, DSC profiles displayed distinct deviations, such as the loss of the melting endotherm or a downward shift in the melting endotherm temperature.

Keywords: ascorbic acid, ascorbate salts, solid-state analysis, FT-IR, DSC

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OBPC P-15

Method Optimization and Validation for Particle Size Distribution for Cefixime Trihydrate Using Malvern Mastersizer 3000

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Particle size distribution refers to the quantification of particles based on their respective sizes. Maintaining precise control over the distribution of particle sizes is crucial for pharmaceutical drug development and production. The particle size distribution of powders is extensively used as a significant parameter for assessing both quality and performance.

Given the significance of particle size distribution (PSD), our study focuses on optimizing and validating the PSD method using Malvern Mastersizer 3000 for determining the particle size distribution of cefixime trihydrate, active pharmaceutical ingredient (API) . The method proposed by the API manufacturer

employs sunflower oil as a dispersant, which often exhibits inconsistent quality, thereby affecting the final results.

Hereby, additional optimization based on paraffin oil as dispersant is proposed, retaining the application of the initial instrument parameters. Consequently, the measurement of PSD using Malvern Mastersizer 3000 with paraffin oil as a dispersant affords control of the API PSD within the specification limits. The optimized method is validated by assessing the repeatability of the measurements and intermediate precision. The criteria for validation include an RSD of no more than 10% for D50, RSD of no more than 15% for D90, and for particles smaller than 10 microns, the RSD limit is doubled.

Keywords: Mastersizer 3000, particle size distribution, paraffin oil, dispersant, validation, optimization

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OBPC P-16

Zinc Complex of 3-Hydroxyflavone: Spectrophotometric Determination and their Antioxidative Profiles

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Flavonoids, widely distributed second metabolites of plants, have a large number of functions. Nowadays, with more nature-oriented lifestyle, the role in plants and potential benefits for humans and animals became more and more important.[1]

3-Hydroxyflavone (3HF) represents the backbone of all flavonols, a widespread class of flavonoids. Interestingly, this compound is not found naturally in plants. Regardless, 3HF is commonly applied as a model molecule because it possesses an excited-state intramolecular proton transfer effect and may serve as a

fluorescent probe in studies of either membranes or intermembrane proteins. It has also been shown that 3HF inhibits metastasis of human osteosarcoma cells and reduces tumor growth in vivo.

With aim to find wider application of 3HF, its complexes with metal ions attract the attention of the researchers. Beside the characterization of zinc complex with 3HF, we reported the validation of the developed simple and low-cost spectrophotometric determination of 3-hydroxyflavone based on its zinc complex. Furthermore, the antioxidant capacities of the synthesized complex and 3HF itself were tested by the DPPH method, followed by the evaluation of more positive issues of zinc 3HF complex. The results of the performed study highlighted the suitability of zinc complex 3HF both for spectrophotometric determination, as well as to explore future applications of its potent bioactivity.

Keywords: 3-hydroxyflavone; zinc complex; spectrophotometric determination; DPPH.

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OBPC P-17

Selected Phenolic Hydrazones as Potential M^{pro} Inhibitors

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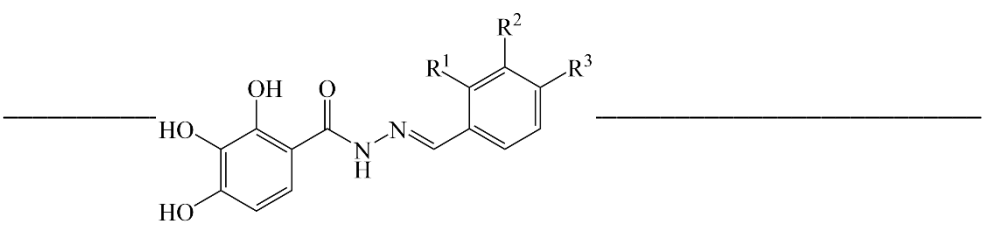
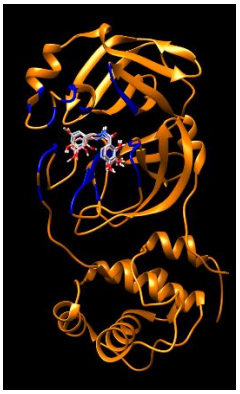
Hydrazone-type compounds are known for their versatile biological activities.[1] This encouraged us to subject six phenolic hydrazones (**1**-**6**) to *in silico* investigation of potential antiviral activity against SARS-CoV-2. For this purpose, molecular docking was performed on the protein involved in viral reproduction processes main protease (M^{pro}).[2]





The obtained results revealed that all compounds docked within the active site of M^{pro}. Binding affinities of all compounds were in the range of -7.6 to -8.1 kcal/mol. Considering that the binding energy of FDA approved drug Lopinavir amounts -7.7 kcal/mol, investigated phenolic hydrazones can be considered as promising M^{pro} inhibitors.

Keywords: phenolic hydrazones, SARS-CoV-2, molecular docking, M^{pro}

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OBPC P-18

Synthesis, Characterization, and Antioxidant Activity of the Selected Phenolic Hydrazone Derivatives

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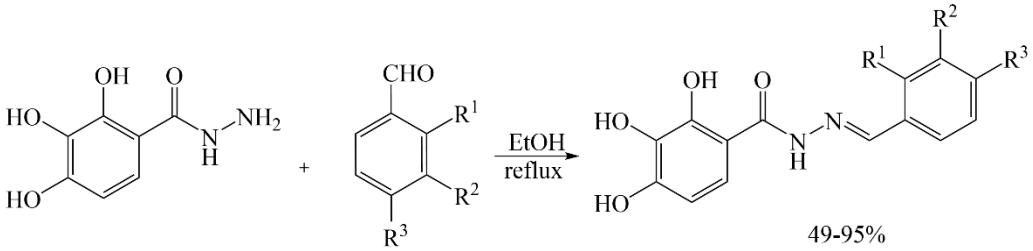
Hydrazone core represents a valuable pharmacophore in medicinal chemistry and drug design.[1] The ease of synthetic transformations and their tunability granted hydrazone-type compounds diverse activities of biological importance.[2] In this work, the synthesis of five novel phenolic hydrazones was

performed in the reactions of 2,3,4-trihydroxybenzohydrazide with various aromatic aldehydes.



The obtained solid products were filtrated, dried, and characterized by NMR, IR, and UV-Vis spectra, melting points, and elemental analysis. Also, the antioxidant capacity of the synthesized compounds was assessed using the 2,2-diphenyl-1-picrylhydrazyl (DPPH) method. All analogs exhibited excellent inhibition potency of the DPPH radical with IC_{50} values in the range of 2.5–9.8 μM. The best radical inactivation potency exhibited compound bearing vanillin moiety, whereas the highest IC_{50} value was determined for the R^3-NO_2 derivative. The obtained results highlight the importance of the design and synthesis of novel phenolic hydrazones with antioxidant properties.

Keywords: phenolics, phenolic hydrazones, antioxidant activity, DPPH

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OBPC P-19

The Role of Proteins in Cosmetic Preparations

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The use of proteins as active cosmetic substances dates back to ancient times, the reason for their use in cosmetic preparations is that they have been found to improve skin that is old (mature skin with visible signs of aging), have a positive effect on hair and nails. The use of proteins in cosmetic preparations contributes to repeated cellular division of skin cells, hydrates the epidermis, stimulates the

creation of collagen and elastin, restructures collagen and regenerates elastin, thus increasing the elasticity of the skin, these processes on the other hand however, the application of proteins in cosmetic preparations slows down the aging process of the skin. With the presence of proteins in cosmetics, it is possible for the epidermis to be constantly moisturized on the skin itself and the transepidermal water loss from the skin is reduced. In addition to being used in creams, serums and gels for old skin, proteins can also be found in a large number of cosmetic preparations such as shampoos, hair masks, hair conditioners whose purpose of the proteins present in these preparations (mostly keratin) is to regenerate the damaged hair and scalp, which are most often damaged during various chemical changes to the hair (dyeing, bleaching and cold permanent undulation). Various proteins of animal origin improve the condition of the skin, hair and nails. The most used are scleroproteins: collagen, elastin and keratin. Protein complexes are also used together with PAM (surface active substances) and fatty acids (used in preparations, they act as antimicrobial or antiseptic). Nowadays, vegetable and microbial proteins are mostly used. In this paper, the characteristics of proteins that are an integral part of the formulations of cosmetic preparations will be shown.

Materials used for the formulation of anti-aging protein cream are the following substances: active component mango extract (Mangiferin) 3% w/w, fatty phase stearic acid 10% w/w, cetyl alcohol 6% w/w, liquid paraffin 6.6 w/w. Aqueous phase – glycerine 5% w/w, methyl paraben 0.05% w/w, propylene glycol 30% w/w, distilled water made up to 100%. Mango extract is the carrier of the proteins in the formulation.

Keywords: proteins, cosmetic preparations, formulation, creams, lotions

OBPC P-20

A Boiled-Egg to Predict Gastrointestinal Absorption and Brain Penetration of Sulfonylurea Herbicides

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Sulfonylureas (SU) are group of substituted urea herbicides, primarily used for the control of weeds (annual and perennial) in early growth stages of cultivations. Structurally they consist a sulfonyl group (-$S(=O)_2$) (Fig. 1). The side

chains (R_1 and R_2) distinguish various sulfonylureas, such as pyrimidinyl-sulfonylureas and the triazinyl-sulfonylureas.

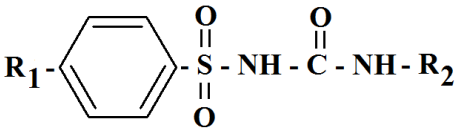

Figure 1. Structural formula of sulfonylurea compounds

SwissADME is a web tool designed for predicting pharmacokinetics parameters, which can be used for pesticides. The BOILED-Egg (Brain or Intestinal Estimated permeation) method, as part of SwissADME tool, can predict the transfer of drugs across the blood-brain barrier with high accuracy.

The BOILED-Egg graph was applied for investigated pyrimidinyl-sulfonylureas and the triazinyl-sulfonylureas. The BOILED-Egg allows for intuitive evaluation of passive gastrointestinal absorption and blood-brain penetration (BBB) in function of the position of the molecules in the WLOGP (a purely atomistic method based on Wildman and Crippen's piecewise system of the octanol-water distribution coefficient (log P) used as a measure of lipophilicity)-versus-TPSA (topological polar surface area) referential in the SwissADME a web tool. In BOILED-Egg graph, the yellow area represents the transition to the blood-brain barrier (BBB), and the white area represents the absorption in the gastrointestinal system (AGS).

Our results showed that a large proportion of studded herbicides (> 92.59%) is predicted to be low absorbed by the human gastro-intestinal tract (gray region). Only sulfometuron methyl and chlorsulfuron are high possibility of passive absorption by the gastrointestinal tract (white region).

Keywords: pesticides, SwissADME, BOILED-Egg graph, sulfonylureas

OBPC P-21

Analysis of QSAR Models Quality

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The investigation of the quantitative structure activity/property relationships (QSAR/QSPR) of organic compounds is an essential aspect of present experimental chemistry, biochemistry, medicinal chemistry, and especiallyin drug discovery. The obtained information is composed of mathematical equations relating the chemical structure of the compounds to a wide variety of their physical, chemical and biological properties. In our previous work, QSAR study of set of various substituted hydrazones was performed to estimate the quantitative effects of the selected physicochemical descriptors on experimentally determined dissociation constant. Several statistical parameters: correlation coefficients (R^2), adjusted coefficient of correlation ($R^2_{adj.}$), mean squared error (MSE), root mean square error (RMSE) and Fischer test (F-test) were used to test the quality of the developed QSAR models. All QSAR model were statistically significant: $R^2R^2_{adj}$> 0.8, MSE < 0.003, RMSE < 0.05. Advantage of this method is when a correlation between structure and activity/property is found, any number of structurally similar compounds (compounds with hydrazine moiety), can readily be screened *in silico* for selection of structures with desired properties. As a continuation of our previous work, we tested QSAR model using different type of hydrazine compound. We calculated their pK values constant, using our models and those values were compared with their literature values. The results showed that the application of models would largely depend on the structural similarities/differences of the tested compounds compared to the compounds on which the models were constructed.

Keywords: QSAR/QSPR, hydrazones, p*K* constant, descriptors

OBPC P-22

QSAR Modeling of Sulfonylurea Herbicides

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Sulfonylureas inhibit the biosynthesis of branched-chain amino acids in plants by inhibiting the enzyme ALS, and are widely used worldwide for selective

weed control in various field-crops such as wheat, cotton, oil seed rape and corn, orchards (such olive groves) and vegetables (including tomato and potato) in pre-planting and post-planting applications. Some of these herbicides are highly persistent in the soil, with a long-term residual activity that results in damage to sensitive plants even several years after application to the soil.

The pKa constant is a measure of the acidity of a molecule or compound and itsis an important parameter in many chemical and biological processes, and its value can have significant effects on the behavior of molecules and compounds. The behavior of pesticides and their metabolites in the environment are largely dependent on their physicochemical properties. In case of ionisable pesticides, their pKa, values determine the degree of ionisation in water at the pH of the soil or biological system, and this in turn determines their effective lipophilicity. Accurate pKa values are therefore necessary to model pesticide behavior.

Herbicides SMILES codes was collected online from for PubChem database. pKa values were taken from Pesticide Properties Database (PPDB) website, a comprehensive source of data on pesticide chemical, physical and biological properties.

The experimental database in this study (modeling set), was divided into: 75% training set and 25% test set herbicides. QSAR (quantitative structure–activity relationships) models where created by training set, while model's efficacy after creation were estimate by test set. To build and test the MLR models, several variable selection methods such as Stepwise (SW), Forward (FW) and Best model selection with 2, 3 and 4 descriptors (BM2, BM3 and BM4), were used.

Initial QSAR models were assess according to R^2 values: 0.464 for SW and FW; 0.532 for BM2; 0.672 for BM3 and 0.719 for BM4, which is the statistically promising model.

Keywords: Sulfonylurea herbicides, pKa values, QSAR modeling, MLR

OBPC P-23

Volatile Compounds and Cytotoxic Effects of *Lavandulae Aetheroleum*

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Lavender flowers as well as essential oil are often used as herbal remedy for nervous disturbance, anxiety, mild depression and aromatherapy[1]. GC/MS method was used for identification of volatile compounds in *Lavandula aetheroleum*. Cytotoxic activity was determined using the Brine shrimp lethality assay (BSLA)[2,3]. Meyer's and Clarkson's scales were used to categorize the essential oil cytotoxicity based on the obtained LC50 values. GC/MS analyses resulted in identification of 26 components, representing 95.35% of the essential oil. Dominant components were monoterpenes linalool acetate (18.88%), bornyl acetat (7.28%), terpinen-4-ol (6.00%), *β*-ocymene (4.27%), myrcene (3.16%), borneol (3.07%), *α*-terpineol (2.27%), geranyl acetate (2.14%), lavandulol (2.13%) and linalool (1.18%) and sesquiterpenes caryophyllene E (4.88%) and β-farnesene (1.10%). *Lavandulae aetheroleum* showed cytotoxicity after 24h with LC50 value of 58.08 μg/mL. According to the Meyer's[2] and Clarkson's scale[3], this essential oil showed toxic and highly toxic activity, respectively. Additional examinations should be done in order to established the relationship between the determined chemical composition and the cytotoxic activity.

Keywords: Lavandula officinalis, essential oil, volatile components, cytotoxicity

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OBPC P-24

Analysis Of Organic Compounds in Single-Use Gloves and Surgical Masks Using Spectroscopic and Gas Chromatographic Methods

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During the COVID-19 pandemic there was extensive use of masks and gloves in order to reduce the infection rate. The bulk of the gloves used during

pandemic were nitrile gloves, latex gloves and foil gloves, which are polymeric materials (nitrile-butadiene rubber, polyisoprene and polyethylene respectively). The most used masks were the surgical masks to many health risks composed of three fabric layers made from different materials. The outside and inner layers are made of polypropylene and the middle layer is made of cotton. Several commercially available samples of surgical masks and gloves were gathered and the integral parts were analyzed with ATR-FTIR spectroscopy to confirm/determine the composition. For preliminary analysis, a direct headspace gas chromatographic mass spectrometric HS-GC-MS method (glove/mask in 22 mL vial closed with PTFE/silicone septum) was introduced in order to check for presence of volatile and semi-volatile organic compounds. Afterwards, gas chromatographic-mass spectrometric (GC-MS) method was developed for analysis of organic compounds (residuals and additives) utilizing solvent extraction. The effects of the solvent(s) used and the extraction techniques were investigated.

This study provides starting point regarding the identity of organic compounds present in disposable protective gloves and masks, which would be beneficial for risk assessment especially for long-term use.

Keywords: single-use protective gloves, surgical masks, GC-MS, analysis, organic compounds

OBPC P-25

GC-MS Analysis of Volatile Organic Compounds in Aerosol and Integral Parts Of IQOS® E-Cigarettes

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Due to many health risks from traditional smoking, certain tobacco companies invented a new type, modern Heat-not-burn tobacco products. These products include electric devices that heat modified cigarettes to produce an aerosol

for inhalation without causing combustion. In the USA, the Food and Drug Administration (FDA) has approved "I-Quit-Ordinary-Smoking (*IQOS)® Tobacco Heating System*" as modified risk tobacco products (MRTPs). The internal studies of the manufacturer resulted in the finding that *"Heat-not-burn"* products are a way safer type of smoking than traditional one.

More detailed studies are needed to confirm these claims and also to initiate further studies in order to increase the safety of the product(s). As a starting point, qualitative analysis was performed using a GC-MS on aerosols from some of commercially available tobacco-flavored *IQOS® HeatSticks*. Head space GC vial was directly filled with the aerosol and after appropriate thermostating, it was transfered for GC-MS analysis. The main components were identified as benzyl alcohol, nicotine, triacetin and menthol, with the last one being the most abundant.

Based on these preliminary results, it can be concluded that *IQOS® Tobacco Heating System* is somewhat safer than traditional smoking due to less harmful components and nicotine control, but the risks are not fully annulled. The short and long-term toxicity and synergistic effects of the main and minor components in the aerosol should be thoroughly investigated, as well as the effects of the proper cleaning of the device.

Keywords: e-Cigarettes, GC-MS, volatile organic compounds, Heat-not-burn tobacco products, aerosol

OBPC P-26

Investigating the Interactions Between Active Pharmaceutical Ingredients and Lubricants Using FTIR and DSC

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Examination and understanding of interactions between active pharmaceutical ingredients (APIs) and other constituents of solid dosage forms, including lubricants, is one of the crucial steps in pharmaceutical formulation and manufacturing process. Lubricants are additives used in small quantities whose role

is to reduce friction between the contact surface of the manufacturing equipment and powder during pharmaceutical operations such as roller compaction, tableting and capsule-filling[1]. The aim of this study was to explore the thermal properties as a potential indicator for interactions between active pharmaceutical ingredients and lubricants.

For that purpose, the thermal behavior of binary mixtures between APIs and lubricants was investigated using differential scanning calorimetry (DSC) as well as Fourier-Transform infrared spectroscopy (FTIR). Several APIs with diverse structures were selected and binary mixtures (1:1 and 9:1) were prepared with three commonly used lubricants: sodium stearyl fumarate, magnesium stearate and sodium lauryl sulfate. The FTIR spectra and DSC thermograms of the individual compounds and binary mixtures were compared and discussed. Significant changes in the FTIR spectra were not detected suggesting that chemical changes have not occurred during the mixing processeswhereas some shifts in the DSC curves implied physical interactions between certain APIs and lubricants likely due to adsorption phenomena. The obtained results demonstrate that this methodology could be used as an additional tool for monitoring the API-lubricant interactions, which can significantly affect the stability and efficacy of the final product.

Keywords: active pharmaceutical ingredients, APIs, lubricants, differential scanning
calorimetry, DSC, Fourier-Transform infrared spectroscopy, FTIR

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OBPC P-27

Determination of Trace Metals in Salbutamole Sulfate with ICP-OES

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The accurate determination of trace metals in pharmaceutical products is of great importance for their safety and efficacy. Salbutamol sulfate is a commonly

used bronchodilator drug and it is often manufactured using palladium as a catalyst. However, trace amounts of it can remain in the final product, and this can have implications for patients sensitive to the metal. Therefore, determination of palladium content is of crucial importance when assessing the quality of the product.

In this study, inductively coupled plasma - optical emission spectroscopy (ICP-OES) was applied for data collection[1-3]. The method was optimized by adjusting various parameters in order to be suitable for our instrument type: RF power 1.2 kW, reading time 5 s, stabilization time 25 s, viewing mode - axial, viewing height - 8 mm, nebulizer flow 0.7 L/min, plasma flow 12.0 L/min, aux flow 1.5 L/min, make up flow 0.00 L/min. Three replicates of each measurement were performed with pump speed 12 rpm, uptake delay 30 s and rinse time 35 s. Calibration was performed using five standards (0.08; 0.2; 0.4; 0.6 and 0.8 ppm) at wavelength 340.458 nm, and 1% HCl as blank solution (zero standard concentration).

Salbutamol sulfate is known to be highly hygroscopic drug and can absorb moisture from the atmosphere rapidly. The presence of moisture can cause the substance to decompose, which can generate heat, so the samples were first dissolved in a suitable solvent (1% HCl) and then injected into the instrument. The measured palladium content in the samples is expressed in ppm with correlation coefficient of 0.9997. The obtained result is 0.0019 ppm (limit - NMT 1 ppm).

Overall, this modified method is cost-effective and rapid and can be used successfully for quality control purposes, pharmacological and pharmaceutical research where Salbutamol sulfate palladium content determination is required.

Keywords: bronchodilator drug, catalyst, ICP-OES, ppm, hygroscopic

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OBPC P-28

Resolving a Long-Standing Discrepancy: Investigating the Configuration and Occurrence of 2,6-cyclocuparan-3-ols

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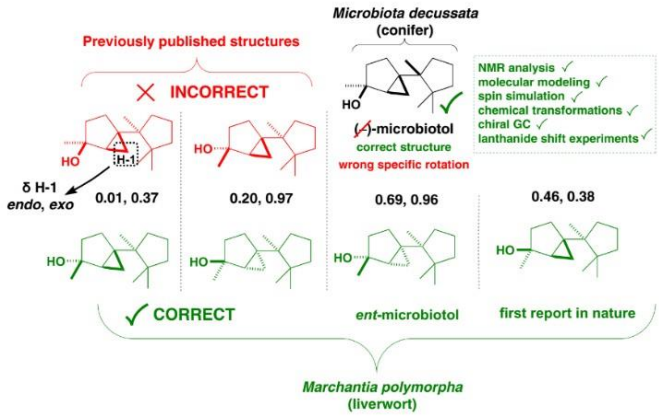
2,6-Cyclocuparan-3-ols are chemical markers and major volatiles of several liverwort species. Conflicting reports on the structures of these cyclocuparanols can be found in the literature–different research groups assigned the same spectral data to different structures, yet these inconsistencies were never addressed, let alone satisfactorily explained. Following the isolation of all four diastereoisomeric cyclocuparanols from *Marchantia polymorpha*, their relative and absolute configurations were extensively studied by chemical and spectroscopic methods and definite stereostructures were proposed.[1]



Keywords: *Marchantia polymorpha*, Marchantiaceae, liverwort, essential oil, cyclocuparanols, structural revision, microbiotol

Acknowledgement: This work was supported by the Ministry of Science, Technological Development and Innovations of the Republic of Serbia (Contract Number 451-03-47/2023-01/ 200124).

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OBPC P-29

Chemical Analysis of the Diethyl-Ether Extract of *Microbiota Decussata*

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The GC, GC-MS, and NMR techniques were utilized to examine the phytochemical composition of *Microbiota decussata*. A comparative analysis was performed with a previously published study conducted by Raldugin et al. in 1981.[1] In contrast to the findings of the Russian group, our sample did not contain hedycaryol, which was identified as the major alcohol component. Instead, thujopsan-2α-ol dominated most of the sesquiterpenol-containing chromatographic fractions, comprising approximately one-third of the total extract mass. Furthermore, whereas Raldugin and colleagues could not detect any diterpenoids, we isolated totarol, constituting 10% of the extract, along with minor quantities of ferruginol. The most polar compound, microbiotol, accounting for 5% of the extract, was thoroughly examined using NMR and chiral GC to determine its relative and absolute configurations.

Keywords: *Microbiota decussata*, thujopsan-2α-ol, totarol, NMR, GC-MS

Acknowledgement: This work was supported by the Ministry of Science, Technological Development and Innovations of the Republic of Serbia (Contract Number 451-03-47/2023-01/ 200124).

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AEC O-1

Innovative Approaches in Monitoring and Removal of Contaminants of Emerging Concern from Water

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Due to the numerous chemicals in daily use, there are many compounds that reach the environment unintentionally and/or uncontrolled, which presence is not subjected to regular monitoring or control measures. Hence, there are many different classes of these so-called compounds of emerging concern (CECs) such as pharmaceutically active compounds, personal care products, polar pesticides, poly- and perfluoroalkyl substances, microplastics, industrial chemicals, etc. Some evidence has shown that "cocktail" of CECs in the environment may adversely affect human health and ecosystems, although many of them are generally present in traces (e.g., from ng/L to μg/L in water samples). Among them, there are many persistent and mobilriverbankss passing natural and artificial barriers (e.g., riverbanks, filtration in water treatment plants) and accumulating for a long period in the environment. If the degradation occurs, the formed products are also regarded as CECs, additionally affecting the chemical safety of the environment. Having different physical and chemical properties, the simultaneous selective and sensitive detection of CECs is an important analytical challenge.

The intention of this presentation is to give an overview of the work conducted so far on the CECs monitoring in water resources from Western Balkan countries, and to discuss selected new analytical approaches and technologies for removal of CECs in water. These are the main research topics within the Horizon Europe project TwiNSol-CECs (101059867), important for harmonizing the relevant research efforts across the region and beyond as an important link in transition foreseen by European Green Deal towards zero pollution, toxic-free environment.

Keywords: CECs, analysis, screening, UHPLC-MS, membrane processes, biosorbents

AEC O-2

Detection of Organic Compounds in Outdoor Urban Air in Kosova and Macedonia Using a Passive Sampling Technique and Gas Chromatography Coupled with Mass Spectrometry

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Urban organic pollutants have a significant direct and indirect impact on air quality, human health, and climate.[1,2] Herein organic emissions in outdoor urban air were monitored in selected cities in the Republic of N. Macedonia and Kosova in 2022. For that purpose, Radiello® passive/diffusive samplers were used.[3] After appropriate desorption the samples were subjected to analysis using gas chromatography coupled with mass spectrometry (GC/MS). The most abundant detected in the urban air were BTEX (benzene, toluene, ethylbenzene, and xylenes), C_9-C_{11} alkyl aromatics (1,2,4-trimethylbenzene, 1-ethyl-3-methylbenzene, 1,3,5-trimethylbenzene, 1-methyl-4-propylbenzene), linear alkanes (*n*-undecane, *n*-dodecane, *n*-tridecane and *n*-tetradecane) and monoterpenes (α-pinene and limonene). Furthermore, BTEX compound ratios and correlations have been employed as a marker for finding VOC emission sources in the atmosphere.[4] Long-term objectives include developing quantitative assessments of volatile organic compounds in outdoor air and regularly monitoring their amounts throughout the year. The above-mentioned method is simple and in the future, comparative studies can be carried out with active sampling.

Keywords: VOC, air pollution, gas chromatography, Radiello® passive sampling.

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AEC O-3

Peptide-Molecular Wires as Conductive Supports in Electrochemical Bioassays

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We report a study on the electrochemical properties of a peptide molecular wire used as both conductive support for immobilizing ligands in affinity-based bioassays and as signal amplifier for the ultrasensitive detection of H_2O_2 in biological samples. A short helical peptide sequence with alternating polar and ionizable side chains was synthesized to modify the surface of the biosensor. The peptide was functionalized on-site with Methylene Blue (MB) at one end and anchored to the gold surface through the gold/thiol chemistry[1]. Thus, the modified peptide acted as a molecular wire, facilitating a two-step electron transfer (ET) process from MB to the gold surface[2]. To assess the kinetics of the electrode reaction, we analyzed the forward and backward components of the square wave voltammetric (SWV) signals obtained in the presence of the peptide wire. The experimental data were compared with simulated results, revealing a good fit for the surface EE mechanism[3].Two high-molecular-weight (HMW) targets (the anti-tumour-associated carbohydrate antigen-antibody, and the growth hormone secretagogue receptor) were detected via affinity interaction with their small ligands grafted onto the peptide wire. Another significant advancement is the ultrasensitive detection of H_2O_2, by leveraging the electrocatalytic properties of MB within the peptide/thiol mixed layer.

Keywords: biosensor, molecular wire, electron transfer

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AEC O-4

Starch-Based Adsorbents for Environmental Applications

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The textile industry effluents containing various types of synthetic dyes is one of the significant cause of water contamination and pose a serious threat to the natural ecosystem. More than one hundred different types of dyes are commercially available that are used in the annual production of over 80 million tons of textile fabrics globally, and the annual cumulative consumption of dyes exceeds 7×10^5 tonnes[1]. Dyes are also widely applied in other industries like printing, pharmaceuticals, paper, and rubber products. It is reported that around 10–15 % of total dyes produced are discharged into water bodies and become toxic due to their mutagenic and carcinogenic nature[2].

The adsorption technique has numerous advantages over the other methods of dyes removal such as low operational cost, ease of operation, high efficiency, environment friendliness, wide adaptability, lower generation of secondary pollutants, etc. Due to their biodegradable and non-toxic nature, various starch-based adsorbents have been developed and have shown remarkable success in heavy metals and dyes removal from wastewater.

The aim of this study was to applied polymeric microspheres based on modified starch, dimethacrylate ethylene glycol, and vinyl acetate for basic dye removal from dyeing baths. The impacts of phase contact time, adsorbate initial concentration, and auxiliaries' presence (electrolytes and surfactants) were evaluated on dye sorption effectiveness on starch based adsorbents. Kinetic and equilibrium parameters, as well as desorption and reuse possibility were also discussed.

Keywords: dyes removal, starch-based adsorbent, textile wastewaters

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AEC O-5

Fabrication of a Novel Colorimetric Paraoxon Ethyl Biosensor Using CUPRAC Reagent as a Chromogenic Reagent

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Copper(II)-bis-neocuproin complex ($[Cu(Nc)_2]^{2+}$), which was first developed by Apak et al. in 2004 and known as CUPRAC reagent, has been used as a useful chromogenic reagent in many colorimetric sensor studies.[1-3] However, according to our literature search, a paraoxon ethyl (POE) biosensor using the CUPRAC reagent based on acetylcholine esterase (AcHE) inhibition has not yet been reported. First, an enzymatic reaction takes place between AcHE and its substrate, acetylthiocholine (ATCh), followed by a colorimetric reaction between the enzymatically produced thiocholine (TCh) and the CUPRAC reagent. While $[Cu(Nc)_2]^{2+}$ reduces to a yellow-orange cuprous complex ($[Cu(Nc)_2]^{+}$) which gives maximum absorbance at 450 nm, TCh oxidizes to its disulfide form. However, the absorbance of $[Cu(Nc)_2]^{+}$ is proportionally decreased depending on the increase in the concentration of POE due to the inhibition of AChE by POE. Based on this strategy, the linear response range of a colorimetric biosensor was found to be between 0.15 and 1.25 µM POE with a detection limit of 0.045 µM. The fabricated biosensor enabled the selective determination of POE in the presence of some other pesticides and metal ions. Acceptable recovery results were obtained from water samples spiked with POE.

Keywords: Acetylcholine esterase; Paraoxon ethyl; Colorimetric biosensor; CUPRAC

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AEC O-6

Filtering Efficiency of Pollutants in Heavy-Duty Vehicle Cabins

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Quality of air in the cabin of transportation vehicle is of high importance due to increase in globalization that hinders rise of transportation of goods worldwide. The largest source of street pollution in urban areas is vehicular combustion, constituted mainly of gaseous pollutants such as CO_2, CO, oxides of nitrogen (NO_x), ozone (O_3), and particles comprising ultrafine particulate matter (UFP). Drivers of heavy-duty vehicles (HDV) are spending both their working and free time in vehicle cabins, rendering them highly exposed to toxic gases and hazardous aerosols. Intensive industrial development is more concentrated in metropolitan areas, and since it still relies on fossil fuel energy for goods transportation, it results in high pollution of air with traffic-related air pollutants (TRAPs). Primary sources of UFPs in the urban environment near road sites are thus strongly related toHDVs, and they enter cabin air through windows, accumulating in the cabin air and on the surfaces, resulting in up to three times higher concentration of TRAPs in the cabin than outdoor air. Exposures to high CO_2, $NO_x$and UFP can significantly reduce decision-making performance and is considered a contributory cause of premature deaths of HDV drivers. Development focus is to improve use of human-machine interactions. However, sedimentation and/or collection of UFP onto filter surfaces, long filter exposure times, and high temperatures within cabins in turn cause decrease of air-flow within the filter and drastically decrease filtering efficiency. By combining experimental results obtained from in-field measurements performed in the city of Belgrade, during peak traffic hours, for air filtration systems (AFS) placed at different positions within the cabins, we obtained master data representing the functional role of air filtration systems. Following analytical study of experimental results, we propose a mathematical model to describe AFS efficiency in cabin pollution mitigation. Predicted results are in close agreement with the experimental data showing that knowing the levels of outdoor to cabin pollutant concentrations itis possible to estimate the efficiency, depending on design and local terrain, filtration exposure time and thermodynamic parameters within the cabin. We hope that this research raises organizational attention to the health and welfare of HDV drivers and will result in reduced levels of human exposure to harmful vehicle pollutants.

Keywords: heavy-duty vehicle, HDV, air filtration system, AFS, HDV cabins

AEC O-7

Rapid GC-MS/MS Analysis of Multiple Pesticide Residues in Cereal-Based Products

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For the simultaneous detection of 95 pesticides in cereal-based products, a quick GC-MS/MS method was validated in order to determine the safety and compliance with the legal maximum residue levels.[1,2] The samples, fortified with triphenyl phosphate as an internal standard, were first extracted with acetonitrile, followed by a salting out process using the QuEChERS extraction kit, and a dispersive SPE cleanup. Analysis of spiked samples, prepared by adding standard pesticide solution mixture to one representative sample consisting of five pesticide-free grains was conducted at three different levels (2.5, 5 and 10 μg kg^{-1}). Mean recoveries from six replicates ranged from 70.78 to 115.05%, with RSD lower than 20. The limit of quantification for all pesticides was 5 μg kg^{-1}. The correlation coefficient was ≥ 0.990 for all pesticides. Evaluation was performed using a matrix-matched calibration curve for each pesticide in a concentration range of 2.5 to 50 ng mL^{-1}. This method with a 21-min run time demonstrated the ability to quantify pesticides at concentrations below the LOQ, suggesting that it may have a useful application for the safety control of residues in cereal-based food, even when other components are present in the samples. Such method that could determine residues at lower levels than legal limits is needed to ensure a high degree of consumer protection, since a specific pesticide/product combination may exceed health-based recommendation levels and pose a risk to health.

Keywords: cereal-based products, pesticide residues, GC-MS/MS.

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AEC P-1

Pinpointing the Origin of Volatile Organic Compounds in Urban Air Using Passive Sampling and Gas Chromatographic Methods

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Air pollution is one of the major environmental risk factors affecting human health, resulting in more than nine million deaths worldwide yearly.[1,2] The studies for volatile organic compounds (VOC) in urban areas in the southern Balkans are scarce and our objective was to monitor the organic emissions in outdoor air in seven cities in Kosova for several months. Radiello® diffusive passive samplers were placed in appropriate locations and applied for sampling organic analytes from urban air.[3] In parallel, the profile of VOC from commercially available gasoline and diesel fuels in the respective cities was determined using static headspace gas chromatography/mass spectrometry (SHS-GC-MS). In the analyzed gasolines, the most abundant organic compound is toluene and in the diesel fuels *n*-tetradecane and *n*-hexadecane are the most abundant. Based on the results of the GC-MS analyses, the most common VOC identified in monitoring sites are aromatic compounds, normal alkanes, and oxygenated compounds. The BTEX and alkyl aromatics originated from unleaded gasoline, whereas the linear alkanes come most likely from diesel fuel. The detected limonene and alpha-pinene are most likely from plant origin, but they also may be present in cleaning products. The long-term goal is to carry out a quantitative analysis of volatile organic compounds in outdoor air throughout the year.

Keywords: VOC, air monitoring, urban atmosphere, Radiello®, passive sampling.

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AEC P-2

Solar Photocatalysis as a Method For Passive Air Purification Using Modified Recycled Rubber Tiles

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Air quality is one of the key factors that determine human health and longevity. The air that we breathe can be contaminated with various impurities such as; sulfur oxides (SO_X), carbon monoxide (CO), ozone (O_3) and the volatile organic compounds (VOCs).[1] The primary idea of this work was to achieve the synergistic action between immobilized photocatalyst titanium dioxide, TiO_2, on the surface of recycled rubber tiles and solar radiation. The synergistic action triggers redox reactions on the photocatalysts surface to degrade various impurities previously mentioned.[1] TiO_2 irradiated with UV light, can decompose many organic compounds to water, carbon dioxide, and mineral acids or their salts.[2]

Immobilization was validated by SEM-EDS and FTIR analysis. The stability and environmental impact were investigated by leaching test, AAS and TOC analyses. Photocatalytic tests were done in a custom-made wind tunnel reactor with a simulated polluted atmosphere to confirm the activity. Successful immobilization of TiO_2 on the reference rubber tile was achieved, and the photocatalytic activity of the immobilized layer was confirmed by successful degradation of ammonia.

Keywords: titanium dioxide; photocatalysis; recycled rubber; air purification

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AEC P-3

Determining the Chemical Quality of Drinking Water in Central Serbia

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Healthy drinking water is a basic prerequisite for good health, as it is necessary for maintaining life and personal and general hygiene. The World Health Organization (WHO) classified the quality of drinking water into twelve basic indicators of the health status of a country's population. The quality of drinking water is a constant task for the employees of anywater factory. Quality drinking water implies the satisfaction of high quality criteria that can only be achieved with a good knowledge of the basic processes of eutrophication and proper management of the accumulation. Management, among other things, implies the implementation of necessary protection measures in the watershed and adequate monitoring.

This study based on the spectrophotometric determination of the chemical parameters of water, i.e. content: manganese, ammonia, nitrate, nitrite, iron and aluminum in raw and final water plants. Mn for the raw water ranged from 0.024 mgMn/l to 0.061 mgMn/l, while for the final water it was 0.000 mgMn/l. Fe for the raw water ranged from 0.000 mgFe/l to 0.043 mgFe/l, and for the final water it was 0.000 mgFe/l. The concentration of NH_4^+ for the raw water ranged from 0.026 mg(NH_4^+)/l to 0.122 mg(NH_4^+)/l, and for the final water it was 0.000 mg(NH_4^+)/l. According to the measurements, NO_3^- concentration for the raw water ranged from 0.986 mg(NO_3^-)/l to 1.548 mg(NO_3^-)/l, and for the final water from 1.158 mg(NO_3^-)/l to 1.594 mg (NO_3^-)/l. While NO_2^- concentration for the raw water ranged from 0.002 mg(NO_2^-)/l to 0.004 mg(NO_2^-)/l, and for the final water it was 0.000 mg(NO_2^-)/l.

The obtained results for drinking water are in accordance with Drinking Water Quality Standards of the Republic of Serbia.

Keywords: raw water, final water, the spectrophotometric

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AEC P-4

RP-HPLC Method for Simultaneous Determination of Some Food Additives in Beverages

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The use of food additives has been practiced a long time ago, in order to perform a specific function. So, for example, food preservatives are added to extend the shelf life of food products, artificial sweeteners are added to replace sugars, while stimulants are added to increase consumer alertness.

This study presents a developed and validated reversed-phase high-performance liquid chromatography (RP-HPLC) method with ultraviolet-diode array detection (UV-DAD) for simultaneous determination of the commonly used food preservatives (sodium benzoate and potassium sorbate), artificial sweeteners (acesulfame-K, sodium saccharin and aspartame) and caffeine in various beverages. Separation and quantitative determination of the analytes were carried out on the reversed-phase octyldecylsilane column as stationary phase, and methanol and diluted phosphoric acid as mobile phase, applying isocratic elution with the flow rate of 1 mL/min. The chromatographic analysis was performed at 210, 230 and 260 nm, and under constant column temperature at 25ºC. The developed method was validated testing linearity, precision, accuracy, the limits of detection (LOD) and quantification (LOQ). All the validation parameters were within the acceptance range. The method was successfully applied for determination of target analytes in various beverages, that were taken randomly from local markets.

Keywords: artificial sweeteners, beverages, caffeine, food preservatives, RP-HPLC method.

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AEC P-5

RP-HPLC Method for the Determination of Malathion in Pesticide Formulation

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Malathion is one of the most commonly used organophosphorus insecticides both in our country and world-wide. Its use is also approved in the countries of the European Union[1]. It is an active substance of the pesticide formulations.

The development of new analytical methods for the determination of active substances in plant protection products is of great importance and need for the control of their quality.

This study presents a simple, precise and accurate reversed-phase high-performance liquid chromatography (RP-HPLC) method for the determination of malathion in the pesticide formulation “Etiol tečni” in form of emulsion concentrate. The analysis was performed on a C-8 stationary phase using isocratic elution with mobile phase composed of acetonitrile and water, flow rate of 1 mL/min, constant column temperature at 25°C and ultraviolet-diode array detection (UV-DAD) at 220 nm. The specificity, selectivity, linearity, precision, accuracy, limit of detection (LOD) and quantification (LOQ) were tested for the method validation according to the CIPAC (Collaborative International Pesticides Analytical Council) guidelines. The calculated values for the recovery ranged from 100.68 to 102.00 %, while the relative standard deviation (RSD) from 0.15 to 1.36 %. The obtained results showed that the proposed method can be used for routine

analysis of the active substance malathion in the pesticide formulation “Etiol tečni” following the CIPAC rules.

Keywords: malathion, plant protection product, RP-HPLC method.

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AEC P-6

Application of the Kinetic-Spectrophotometric Method for Co(II) Ion Determination in Baby Tea Samples

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The aim of this work was application of the kinetic-spectrophotometric method for the Co(II) ion determination in baby tea samples. Cobalt is an essential element and it is important for the function of many vital processes, such as the production of erythrocytes, i.e. red blood cells, as well as in the production of antibacterial and antiviral compounds that prevent the occurrence of infections. The method is based on the indicatory reaction of oxidation of para-nitrophenol by hydrogen peroxide which is catalyzed by Co(II) ion in alkaline mediaat wavelength of 386 nm. The calibration curves were constructed in the interval from 0.059 to 0.59μg/ml and from 0.59 to 59 μg/ml. Ten commercially available tea samples were used for the optimization and validation of the new kinetic method. Samples prepared by the microwave digestion described by Yeneman and Ikem[1,2]. The kinetic method was successfully applied for Co(II) ion determination with recovery of 94.31 to 105.0%. The results are presented in Table 1. Statistical comparation of the results with ICP AES method showed good agreement.

Table 1. Determination of Co(II) ions determination in babytea samples

Sample	Found by kinetc method (μg/ml)	RSD	(%)	Found by ICP AES (μg/ml)	Recovery (%)	F-test	t-test
T1	5.92±0.5	8.44	3.71	5.70±0.012	96.30	2.85	0.84
T2	0.21±0.005	2.40	4.54	0.22±0.004	95.45	1.43	1.36

T3	3.40±0.3	3.53	1.19	3.36±0.05	99.00	3.28	2.05
T4	4.57±0.06	1.31	6.02	4.31±0.102	94.31	2.16	1.74
T5	1.92±0.1	5.20	1.58	1.89±0.01	98.40	2.36	0.63
T6	3.51±0.01	4.00	0.28	3.52±0.05	99.71	1.58	1.95
T7	5.72±0.03	5.24	4.95	5.45 ±0.06	105.0	1.32	2.16
T8	0.092±0.002	2.17	6.12	0.098±0.003	93.87	3.56	1.07
T9	1.18±0.02	1.69	3.28	1.22±0.01	96.72	2.12	1.54
T10	1.94±0.02	1.03	1.57	1.91±0.05	101.57	1.74	1.87

Keywords: Co(II), kinetic method, baby tea samples

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AEC P-7

Fly Ash/Chitosan Composites as Adsorbent of Heavy Metal Ions

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Water contamination is a serious problem which increases concern because of its effects on living organisms as well as the surrounding environment. Microorganisms, organics, and inorganics are the three primary types of pollutants found in water. Because of their toxicity to ecological and biological processes, heavy metals ions (HMI), which make up the majority of inorganic contaminants, have increased a lot of concern. As a result, scientists, water regulatory agencies, and government agencies are concerned about maintaining and improving water quality. Due to the problems created by the inclusion of HMs in wastewater, traditional wastewater treatment techniques such as adsorption, coagulation, flocculation, precipitation, reverse osmosis, biological process, gamma radiations, and photocatalysis were used to remove them.

The subject of this work was to obtain and to test the Fly ash/chitosan composites aimed for HMI adsorption in polluted waters. Three different types of fly ash waste particles were used, two types supplied from EURONICKEL company, and one supplied from OSLOMEJ thermal power plant, Macedonia. The surface of the fly ash (FA) particles was modified by treated with nitric acid. Several types of composite adsorbents were prepared using the chitosan as a polymer matrix. The characterization of the FA waste particles was performed by XRF, XRD, TGA, SEM and FTIR analysis, while the obtained composites were

tested by TGA, SEM and FTIR analysis. It was found that the structure, morphology, and thermal properties of FA particles have been significantly changed and it is expected that it will improve their adsorption capacity towards HMI. FA/chitosan composites were tested as an adsorbent for Cu (II), and Pb (II) from aqueous solutions. The effect of contact time, solution pH, and initial metal concentration was studied in batch experiments at room temperature. Maximum metal sorption was found to occur at pH 6.0. The equilibrium adsorption data for Cu (II) and Pb (II) ions were fitted to Langmuir isotherm model. The obtained Q_{max} values for the removal of Cu^{2+} and Pb^{2+} by FA/chitosan composites were (1.068, 1.00, 1.042, 1.369 mg/g), and (2.532, 2.063, 1.036, 2.146, 2.482 mg/g), respectively. The efficiency trend was Pb (II) > Cu (II). The results indicated that the removal efficiency for Cu (II) and Pb (II) ions was 91.1% and 99.7% respectively.

Keywords: fly ash, chitosan, composite, adsorbent.

AEC P-8

Opportunities and Challenges in Wastewater Treatment with Membrane Pressure Processes

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Compared to alternative wastewater treatment methods such as adsorption, coagulation/flocculation, usage of aerated/aerobic lagoons, and many others that enable the removal of certain types of contaminants and the creation of a large amount of waste at the end of the process, membrane pressure processes enable the removal of a wide range of contaminants and the generation of very small amounts of waste at the end of the process.[1] In this way, the wastewater can be brought to a high quality that enables further use, for example, in the production process. Membrane pressure processes such as microfiltration, ultrafiltration, nanofiltration, and reverse osmosis are gaining more and more popularity in wastewater treatment processes.[2] Apart from creating a small amount of waste, this technology does not require the use of chemicals during processing, which makes it an environmentally friendly technology.[3] Despite the mentioned advantages, membrane separation processes suffer from certain problems, e.g. membrane fouling, which can be reduced by the use of hybrid coupling. Thus, conventional processes can be combined with a membrane system or it can be a combination of several membrane processes.[4] Also, choosing membranes with a specific material can increase selectivity and permeability. Usually they are membranes made of polymer but by

use sustainable natural (Zeolite, Clays, lignin) and waste-based materials (recycled polystyrene) can improved previously mentioned features. [5]

Keywords: membrane pressure processes, waste, ultrafiltration, microfiltration, nanofiltration, reverse osmosis, fouling

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AEC P-9

Edible Plants and Aquatic Systems in Serpentine Region in Bulgaria

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The serpentine soils are formed due to the weathering of ultramafic rock types (peridotites (dunite, wehrlite, harzburgite, lherzolite) and the secondary alteration products formed by their hydration including serpentinite. These soils are generally deficient in plant essential nutrients, have a calcium-to-magnesium (Ca:Mg) molar ratio of less than 1 and have elevated levels of toxic elements such as nickel, cobalt, and chromium. Ecosystems with serpentine soils are generally less productive, however these type of soils might be also used for edible plants growing and the question arising is –what will be the content of essential and toxic content in the plants as well as what will be the influence on the local aquatic systems frequently used for the irrigation of agriculture field. In the present study the

concentration of chemical elements (Ca, Mg, Fe, Mn, Zn, Cr, Cd, Pb, As) was determined in aqueous phase and biota in rivers from serpentine region in Bulgaria, situated also in the vicinity of abandon chromium mines. The content of essential and toxic elements (Ca, Mg, Fe, Mn, Zn, Cr, Cd, Pb, As) was determined in edible plants (*P. vulgaris*, *Cucumis sativa*, *Capsicum annuum*, *N. tabacum*, *Lycopersicon esculeutum*, *Solanum tuberosum*) grown in the same region. Samples are collected in one season, chemical elements in all samples (river water, plant and biota) were determined by ICP-MS/ICP-OES. Results obtained will be discussed from the view point:

- Correlation between bioavailable concentration of chemical elements in soil and their content in edible plants.
- Correlation between bioavailable concentration of chemical elements in soil and in aquatic systems –aqueous phase used for plant weathering and biota.

Conclusions will be directed to hazard assessment of toxic elements content in edible plants and in biota used for human consumption.

Keywords: serpentine soil, chemical element, river water, biota.

AEC P-10

Carbonized Jute Sorbent for Oil Cleanup

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Over 90 million tons of textile waste is produced every year. A large share of waste comes from the goods made of cellulose fibers. Recently, special attention has been directed towards the use of textile cellulose waste for clean-up of oil spills[1]. The major problem relies on their relatively small oil capacity and complex separation of individual cellulose fibers from the treated spills. In an attempt to overcome this drawback, a non-woven sorbent based on recycled jute fibers obtained from the carpet industry was manufactured. Improvement of porosity and hydrophobicity/oleophilicity of the sorbent was achieved by carbonization process in an inert atmosphere. FESEM analysis revealed the fiber reduction of almost 40% induced by fiber degradation while EDX analysis confirmed the increase in the

carbon content by 75% after carbonization. Oil capacity in water medium, buoyancy, oil retention and reusability of non-carbonized and carbonized sorbents were evaluated by testing four different oils (crude oil, diesel oil, two motor oils). After carbonization process, the oil sorption capacity was doubled in comparison with non-carbonized sorbent independent of oil viscosity. Carbonized sorbent not only remained afloat after 24 h of staying in water, but it sorbed a negligible amount of water unlike non-carbonized sorbent. in addition to good buoyancy, oil retention on carbonized sorbents ranged from 64-80% after 30 min of draining. Larger uptake was achieved with oils of higher viscosity, but their retention was worse. Oil sorption capacity after 5 repeated sorption/desorption trials was significantly larger in the case of carbonized sorbent since it retained 80-88% of its initial oil sorption capacity depending on tested oil.

Keywords: Oil cleanup, Jute, Sorption, Carbonization

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AEC P-11

Comparison of different approaches for quantification of volatile organic compounds in ambient air

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Emission of volatile organic compounds (VOCs) leads to a significant decrease in air quality in many regions around the world and has a negative impact on climate change, human health and the biosphere. Quantitative analysis of these substances by gas chromatography coupled to mass spectrometry (GC-MS) is especially challenging since VOCs are usually present in ambient air at low levels (pg/L to μg/L) and it is often impractical, expensive or even impossible to provide standard substances for all compounds identified in the real samples. Thus, in this paper we compare two methods for quantification of fourteen VOCs belonging to different chemical classes: one based on external calibration and one based on anisole as an internal standard. Then, both methods were used for determination of the concentrations of the detected VOCs in ambient air samples taken on Radiello

adsorbents at two locations in Skopje: Institute of Chemistry and Macedonian Academy of Sciences and Arts.

Both methods gave comparable results and the calculated concentrations for each VOC was within ±30% of the theoretical concentration. Calibration curves were linear in the range from 100 to 4000 μg/L and the RSD of the average RRF met the acceptance criteria and was ≤ 30% for each target VOC[1]. Toluene, chlorobenzene, C_6-C_2 and C_6-C_3 substituted benzenes gave similar values for the average RRFs in the range from 1,260 to 1,601 and RSD of 8,533%. It can be concluded that quantification based on anisole as an internal standard is a simple and reliable method for determination of concentrations of VOCs as a convenient alternative to external standard calibration.

Keywords: volatile organic compounds, internal standard, external calibration, GC-MS

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AEC P-12
Volumetric Properties of Solutions of 1-Ethyl-3-Methylimidazolium Chloride Ionic Liquid in Tetraethylene Glycol at Different Temperatures

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The densities of moderately dilute solutions of 1-ethyl-3-methylimidazolium chloride ionic liquid (EMImCl-IL) in tetraethylene glycol were measured using Anton-Paar DMA 4500M densimeter at different temperatures, Θ = 10, 15, 20, 25, 30 and 35 °C. From the obtained density data, volumetric properties (apparent molar volumes and partial molar volumes) have been evaluated.[1] The volumetric data have been analyzed using Masson's equation.[2] The limiting apparent molar volume or partial molar volume at infinite dilution, and the slope of Masson's equation at different temperatures for EMImCl-IL in tetraethylene glycol have been interpreted in terms of ion-ion and ion-solvent interactions, respectively.[3]

Keywords: 1-ethyl-3-methylimidazolium chloride; tetraethylene glycol; Masson's equation; volumetric properties.

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AEC P-13

The Potential Ecological Risk Assessment of Heavy Metals in an Urban Shallow Lake

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Urban lakes sediments unfortunately have received a large amount of wastewater containing various contaminants such as heavy metals (HMs). Heavy metals in urban lake sediments mainly originate from industrial discharge, heating sources, traffic emissions and waste from municipal activities. The human health and the whole ecosystems are threatened with potential harmful effects of following metal pollutants As, Cd, Cr, Cu, Hg, Ni, Pb and Zn, due to their persistence, non-degradability, inherent toxicity, and bioaccumulation[1]. Therefore, the analysis of lake sediments is a useful and important approach to characterize environmental

pollution in aquatic ecosystems. Due to the diverse environmental conditions and sources of HMs, different pollution indices are used to assess the anthropogenic impact of PTEs in sediment samples[2,3]. In this study, ecological risk assessment of the urban shallow lake sediments in Central Serbia by HMs was analyzed by calculating single and multi- pollution indices and using multivariate techniques to reveal the associated adverse effects of the investigated contaminants.

Keywords: risk indices; anthropogenic pollution; sediment quality; multivariate analysis; positive matrix factorization.

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AEC P-14

Polycyclic Aromatic Hydrocarbons in Dry Herbs: Source Identification, Quantification, and Health Risk Assessment

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Polycyclic aromatic hydrocarbons (PAHs) are amongst the most toxic compounds known to man. Several PAHs are proven to be carcinogenic, mutagenic, and teratogenic. Due to their wide distribution in the environment and their toxicity, it is considered important to monitor the levels of these compounds in foodstuffs.

PAHs have been detected in many food products including plant-based such as vegetable oils, cereal grains, herbs, spices, teas, and supplements[1,2]. As the awareness of the healthy lifestyle has increased globally, the intake of medicinal herbs such as teas and spices has also grown immensely. Therefore, an even bigger emphasis must be made to monitor the toxic levels of PAHs in herbs. The maximum concentrations of certain contaminants in food in the Republic of Serbia included PAHs values in dry herbs only by the end of 2019 ("Official Gazette / RS", No. 81/2019)[3]. Herein, were investigated the sources of PAHs contamination in dry herbs collected from the different parts of Serbia, its quantification and the potential health risk posed by their toxicity.

Keywords: analytical chemistry, PAH, processing, pollution

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AEC P-15

Kinetic and equilibrium studies about sorption removal of textile dye from water

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Dyes are comprehensively used in food, textile, plastic, metal, pharmaceutical and many other industries. Currently, more than 700 000 tons of dyes are required each year, of which at least 10–15% are discarded into the wastewater and responsible for water pollution. These dyes alter the color of water, and inhibit light penetration, reducing the rate of photosynthesis and the oxygen level, causing damage to aquatic ecosystem. Often, these dyes are carcinogenic and initiate various diseases in humans.[1] Therefore, it is essential to remove dyes from wastewater.

Numerous processes have been used for removal of dyes, but the sorption process is one of the progressive and highly effective treatments. Sorbents synthesized using wood sawdust and chemically modified using inorganic oxides, such as alumina, are highly efficient, low-cost, renewable, ubiquitous, and environmentally friendly.[2]

The main aim of this research was modification of oak sawdust using alumina. The application of the sorbents was evaluated using textile dye Reactive blue 19 and the kinetics and equilibrium study of sorption process was studied in detail. The sorption mechanism was best described by Langmuir isotherm followed pseudo-second order kinetics and the maximal sorption capacity was 324.8 mg/g.

Keywords: wood sawdust; modification; alumina; kinetics; isotherms

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AEC P-16

A comparative study on the degradation of textile dyes with UV-activated peroxide and peroxydisulfate

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The development of industry and technology has led to the increasing water pollution, causing many hidden dangers to human health and lives. [1] Wastewater from the textile industry is classified as the most polluting of all industrial sectors in terms of effluent volume and chemical content. Advanced oxidation processes (AOPs), based on the generation of highly active species, such as hydroxyl radicals ($HO^{\bullet}$), sulfate radicals ($SO_4^{\bullet-}$), and superoxide anion radicals ($O_2^{\bullet-}$), have been identified as efficient technologies for the degradation of wide range of organic pollutants in aqueous matrices.

The aim of this study was to compare the degradation behaviours of two textile dyes from different classes, azo dye Reactive Orange 4 (RO 4) and anthraquinone dye Reactive Blue 19 (RB 19), with UV/H_2O_2 and UV/$S_2O_8^{2-}$ process. Both processes are suitable for complete decolorisation of the investigated dyes under optimal operational conditions. The removal of textile dye RO 4 was faster with the UV-activated peroxide compared toUV/$S_2O_8^{2-}$ process, while on the contrary faster decolorisation of textile dye RB 19 was achieved with UV/$S_2O_8^{2-}$ process. The obtained results are probably related to different pathways of the oxidation of the investigated dyes by hydroxyl and sulfate radicals.[2]

Keywords: sulfate radicals, hydroxyl radicals, azo dye, anthraquinone dye

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AEC P-17

Investigating the Possibility of Using a Cheap Adsorbent Based on Fly Ash to Remove Neonicotinoid Insecticides from Water

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This research aims to solve several problems in the environment imposed on us by modern society. The first is the removal of the systematic insecticide imidacloprid from the group of neonicotinoids, whose mass use in agriculture leads to elevated concentrations in water, which manifests negative effects on the environment. Also, huge amounts of waste products in the form of fly ash and boiler ash are generated in thermal power plants for the purpose of obtaining

electricity. Its disposal uses large areas of land and a huge amount of water and energy and presents a major health, ecological and economic problem.

In this paper, the possibilities of fly ash as a cheap adsorbent for removing the insecticide imidacloprid from water were examined. This study recognizes that fly ash (FA) is a promising adsorbent for the removal of various pollutants. Fly ash from the Morava thermal power plant was simply chemically treated with CaO and water to give modified fly ash (MFA), which proved to be an effective adsorbent for the removal of imidacloprid from water. The content of lime (CaO and water) in the fly ash in relation to the adsorption capacity of imidacloprid and the adsorption conditions (pH value of the system, mass of adsorbent, temperature and time) were optimized by applying D Optimal design of the response surface method (RSM). For this purpose, the commercial software "Design expert 9" was used. The results showed that the pseudo-first-order rate equation effectively describes the adsorption kinetics, and that the adsorption equilibrium was established after 90 minutes. The Langmuir model exhibited a better fit to the adsorption isotherm than the Freundlich model. The maximum Langmuir adsorbent capacity for imidacloprid was 73.25 mg g^{-1} at 25 °C at a solution pH of 7.

Keywords: fly ash, adsorbent, imidacloprid, water, adsorption capacity, optimization.

AEC P-18

The Impact of Deltamethrine on Copper and Zinc Content in Oriental Tobacco and Soil

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Pyrethroid pesticides are substances of intense interest for use in tobacco protection because of their desirable environmental properties of short persistence and nontoxicity to mammals. These features combined with their broad spectrum of pesticidal activity have made the pyrethroids alternatives to the older

organochlorine compounds and the natural pyrethrins. The main aim of this investigation is to study the impact of different deltamethrine concentrations on Cu and Zn content in different organs of oriental tobacco and soil. Filed experiment was caried out with one untreated control, with recommended dose and 30%, 50%, 70%, 100% increased dose. According to our findings we can conclude that content of Cu and Zn in the plant material is higher in the samples with recommended dosage of deltamethrine compared to the untreated variant. Except for recommended dosage, almost all investigated samples differ in the content of both tested elements and are uneven regarding the treated variants.

Keywords: Deltamethrine, oriental tobacco, soil, copper, zinc

AEC P-19

Evaluation of the ICP-AES Method for Element Determination in Samples of Rosa Dumalis Bechst.

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An inductively coupled plasma - atomic emission spectrometry (ICP-AES) method for the determination of 21 elements (Al, As, B, Ba, Ca, Cd, Cr, Co, Cu, Fe, K, Mg, Mn, Na, Ni, P, Pb, Si, Se, V and Zn) in samples of Rosa dumalis Bechst was optimized and validated. Robust plasma conditions were achieved at a radiofrequency power of 1150 W and an argon nebulizer flow of 0.5 L min^{-1}. All

experiments in axial and radial view modes were performed under these analytical conditions. Standard addition curves obtained from Rosa dumalis Bechst samples spiked with different concentrations were then compared with external calibration lines established from multi-element standards to select analytical lines free from spectral interferences. The validation process included accuracy, precision, and linearity. The standard addition method was used to assess the accuracy and precision of the method. The recoveries obtained ranged from 89% to 107%. The correlation coefficient for the calibration curves was higher than 0.999. Among the macroelements, K is the most abundantelement, followed by Ca, P, Mg and Na. Among microelements, Mn is the most abundant element, followed by Si, Fe, Ba, Zn and Al. The maximum allowed limits recommended by the World Health Organization (WHO) for Pb and Cd are 10 mg kg^{-1} and 0.3 mg kg^{-1}, respectively. The concentrations of Pb and Cd in all samples studied were lower than the maximum levels allowed by WHO.

Keywords: elements, Rosa dumalis Bechst., ICP AES, optimization, validation

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AEC P-20
Pretreatment of Burley Tobacco Stalks as Raw Material for Bioethanol Production

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Tobacco stalks, as agricultural waste, due to the lignocellulosic composition can be evaluated as a potential raw material in bioethanol production. Pretreatment of lignocellulosic materials is the first step in the bioconversion process utilized to break down the lignin, open up the crystalline structure of cellulose, and its hydrolysis to sugars by application of acids or enzymes.[1]

The effect of the pretreatment time on the concentration of reductive sugars, lignin, and insoluble lignin in burley tobacco stalks was investigated. The pretreatment procedure involved immersingthe stalks in 4% H_2SO_4 at 80°C and ultrasound sonication for 30, 45, and 60 minutes. The tobacco stalks before and after pretreatment were characterized by the determination of the contents of reductive sugars using the dinitrosalicylic acid (DNS) method, insoluble lignin by the Klason lignin extraction method, and acid-soluble lignin by measuring the hydrolysate absorbance at 205 nm.[2]

Increasing the pretreatment time resulted in higher concentrations of reductive sugars, from 7.3 mg/L at 30 minutes to 11.2 mg/L at 60 minutes. The pretreatment time insignificantly affected the content of soluble and insoluble lignin. The insoluble lignin content decreased from 22.7% to 21.3% at pretreatment for 60 minutes. In the studied pretreatment conditions, the reductive sugar content increased, while the lignin was insignificantly degraded.

Keywords: Tobacco stalks, pretreatment, lignin, reductive sugars.

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AEC P-21

Design of Cobalt Oxide Functionalized Carbon Paste Electrode for the Detection of Levofloxacin

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This study prepared a modified cobalt oxide (Co_3O_4) carbon paste electrode to detect Levofloxacin (LEV). Co_3O_4 nanoparticles were synthesized by the chemical coprecipitation method. The electrochemical properties of LEV at this electrode were investigated by cyclic voltammetry (CV) and square wave voltammetry (SWV). In addition, electrochemical impedance spectroscopy (EIS), inductively coupled plasma–optical emission spectrometry (ICP-OES), transmission and scanning electron microscopy (TEM and SEM), and X-ray diffraction (XRD) were used to characterize the synthesized materials. The prepared electrode showed a better electrocatalytic response than the bare carbon paste electrode. After optimization of square wave voltammetry (SWV), the electrode showed a wide linear working range from 1 to 85 μM at pH 5 of Britton–Robinson buffer solution (BRBS) as the supporting electrolyte. The satisfactory selectivity of the proposed method, with good repeatability and reproducibility, strongly suggests a potential application of the method for determining LEV in real samples, especially in pharmaceutical formulations.

Keywords: fluoroquinolone alkaloid; electrochemical sensor; modified electrode; pharmaceutical formulations

Acknowledgement: This research has been financially supported by the Ministry of Science, Technological Development and Innovation of Republic of Serbia (Contract No: 451-03-47/2023-01/200026 and 451-03-47/2023-01/200168) and Ministry of Science and Higher Education of the Russian Federation (agreement No. 075-15-2022-1135) and South Ural State University.

AEC P-22

Boron-Doped Diamond Electrode as an Environmental-Friendly Electrochemical Tool for the Detection and Monitoring of Mesotrione in Food Samples

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Various types of pesticides are used to improve agricultural productivity and maintain the freshness of agricultural products. However, due to increasing and uncontrolled application, pesticides and their derivatives represent a major threat to entire ecosystems. Therefore, development of new methods for their detection and monitoring is of primary matter. In present work, the unmodified boron-doped diamond (BDD) electrode was utilized for quick, simple, efficient, and sensitive electrochemical detection of mesotrione (MST), a hazardous herbicide used primarily in maize culture. This is the first efficient application of BDD electrode for MST detection. MST undergoes an oxidation process, on the surface of the BDD electrode, at a high potential value of +1.4 V. The detection limit of 75 μM and remarkable selectivity among the common interfering molecules were achieved. Furthermore, a straightforward practical application of the method in real samples (corn-origin food products) analysis was demonstrated.

Keywords: boron doped diamond electrode; triketone herbicide; corn products; green sensing

Acknowledgement: This research has been financially supported by the Ministry of Science, Technological Development and Innovation of Republic of Serbia (Contract No: 451-03-47/2023-01/200026 and 451-03-47/2023-01/200168) and Ministry of Science and Higher Education of the Russian Federation (agreement No. 075-15-2022-1135) and South Ural State University.

AEC P-23

Development and Validation of RP-HPLC-UV Method for Determination of Related and Degradation Products of Active Pharmaceutical Ingredient in Tablet Formulation

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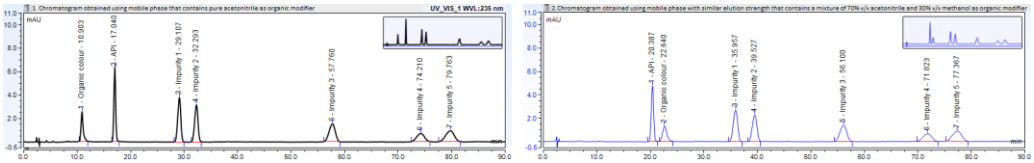
The aim of this work was to develop and validate a stability-indicating reversed phase high performance liquid chromatography (RP-HPLC) method with UV-detection for quantitative determination of related and degradation products of active pharmaceutical ingredient (API) in tablet formulation. Phosphate buffer at pH

7.0, at which the active compound is stable and exists in its molecular, un-ionized form was chosen as aqueous part of the mobile phase, whereas octadecylsilyl silica was selected as stationary phase. As organic modifier, initially acetonitrile was chosen, but in order to solve a problem with separation and retention stabilization of an excipient in the formulation – organic colour erythrosine, using a mixture of acetonitrile and methanol was necessary. The addition of methanol in the organic modifiers mixture causes change in selectivity,[1] that affects several components present in the formulation through different mechanisms (hydrogen bonding, overcoming steric restrictions).



After optimization, which includes creating a gradient elution program, the method was successfully validated according to ICH guideline Q2(R1). The robustness of the method has been evaluated using Plackett-Burman experimental design and the results showed fulfilment of the selected system suitability criteria inside the created design space.

Keywords: related and degradation products, HPLC-UV, selectivity, organic modifier

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AEC P-24

Development of Analytical Method for Quantitative Determination of Propyphenazone Residues on Manufacturing Equipment

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The analytical method is one of the deciding factors in establishing the cleanliness of pharmaceutical manufacturing equipment.[1] The purpose of this research is to develop and validate a sensitive and accurate HPLC method, suitable for quantitative determination of propyphenazone residues on manufacturing equipment.

The method has been validated to show specificity, linearity and range, accuracy, precision, the limit of quantification (LOQ) and limit of detection (LOD),

as per ICH guideline Validation of analytical procedures: Text and Methodology Q2(R1).[2,3] Accuracy is measured through the recovery of samples from the equipment surface and extraction of the recovered samples into a testing solution. It is reported as % recovery of the amount of analyte in the recovered samples measured against the amount of analyte spiked onto the sample recovery surface. In our case, the recovery for propyphenazone was 98.59%. The precision of the method was evaluated using six samples and the result for RSD was 0.6%. Using diluent, blank, standard and spiked samples it was determined that the method was specific. It exhibited good linearity between the responses of propyphenazone related to the concentrations of standard with correlation coefficient r=1.00. The LOD and LOQ were determined at a signal-to-noise ratio of 3:1 and 10:1, respectively. The limit of detection was 0.03 µg/mL and the limit of quantification was 0.10 µg/mL.

From the obtained results, it was concluded that the method is appropriate for determining the amount of propyphenazone residues on manufacturing equipment. In view of the obtained data, the developed method can be applied for routine control of pharmaceutical equipment cleanliness.

Keywords: method validation, method development, equipment cleanliness, recovery

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AEC P-25

Modified Fly Ash for Adsorption of Pharmaceuticals from Water: Chemometric Approach to the Optimization of Adsorption Method

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The immense quantity of industrial waste is a global problem that requires new solutions in accordance with the principles of circular economy and sustainable

development. Therefore, in this work, fly ash obtained as waste from thermal power plants was used as an adsorbent for the removal of pharmaceutical residues from water. To improve the adsorption efficiency of fly ash, different modification methods were applied. Obtained adsorbents were characterized by SEM and FTIR. In order to improve the adsorption characteristics, the adsorption parameters were optimized (volume, initial concentration, and pH value of adsorbate solution, adsorbent mass, and contact time between adsorbent and adsorbate). Artificial neural networks were applied to establish the correlation between the examined adsorption parameters and to define the parameters having the greatest influence on the adsorption efficiency. The chemometric approach enabled the reduction of variables, i.e., the number of experiments necessary for the optimization of pharmaceutical residue adsorption onto modified fly ash, giving a good basis for the commercial application of fly ash in the field of wastewater treatment.

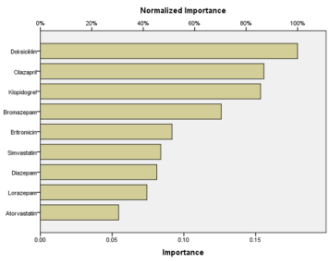

Figure 1. Prediction of drug adsorption efficiency using artificial neural network

Keywords: fly ash, pharmaceuticals, adsorption, optimization, chemometric tools, ANN

Acknowledgment: This work was supported by the Science Fund of the Republic of Serbia within the project SIW4SE (Contracts No. 7743343)

AEC P-26

Removal Of Cadmium(II) Ions from Water by Polyethylenimine Modified Fly Ash

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Accumulation of waste represents one of the biggest problems of modern civilization, from the energy, construction, urban, ecological and technological point of view. In this work, fly ash, as waste material from the power plant Nikola

Tesla, was activated with sodium hydroxide at elevated temperature and then chemically modified with different amounts of polyethylenimine (PEI). The successfulness of modification was confirmed by scanning electron microscopy and Fourier transform infrared spectroscopy. Prepared materials were then used to remove cadmium from wastewater and an increase in adsorption efficiency was observed for the fly ash sample modified with a smaller amount of PEI, with respect tothe unmodified sample.The results of the adsorption experiments were processed using Langmuir and Freundlich adsorption isotherms and pseudo-first and pseudo-second order kinetic models. Also, the possibility of reusing the material in several cycles was examined. It was found that fly ash, modified with an optimal amount of polyethyleneimine, could be an effective adsorbent.

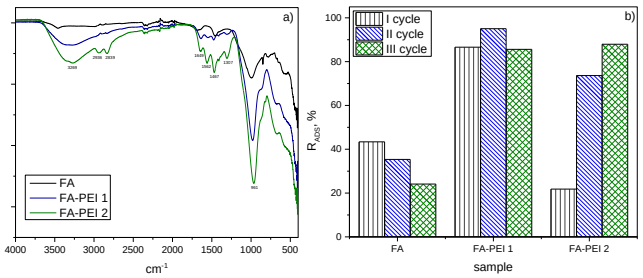

Fig. 1. FTIR spectra (a) and adsorption efficiency (b) of unmodified and modified fly ash

Keywords*:* fly ash, polyethylenimine, modification, adsorption, heavy metals

Acknowledgment: This work was supported by the Science Fund of the Republic of Serbia within project „Serbian Industrial Waste towards Sustainable Environment: Resource of Strategic Elements and Removal Agent for Pollutants - SIW4SE“(Contracts No. 7743343).

AEC P-27

Modification of Waste Hemp and Flax Fibers for Removal of Selected Sedative Residues from Polluted Water

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The possibility of utilizing waste lignocellulosic fibers for the removal of selected sedative residues from polluted water was investigated as an attempt to reuse textile waste and reduce its disposal costs. To increase the adsorption efficiency, waste hemp (H) and flax (F) fibers were modified with a benzoyl

peroxide solution. Unmodified and modified fibers (H_{BP} and F_{BP}) were characterized by scanning electron microscopy and Fourier transform infrared spectroscopy, and it was found that applied modification caused the differences in morphology and surface chemistry, as the consequence of changes in the distribution of hemicelluloses in the structure of examined fibers. Adsorption properties were examined in the means of adsorption kinetics, isotherms, and the influence of the initial pH of the adsorption solution. The applied modification increases the adsorption capacities of examined fibers, especially for bromazepam removal. Also, modification increases the adsorption rate and changes its order, while adsorption equilibrium data fits better the Langmuir isotherm model. Obtained results showed that waste hemp and flax fibers can be applied as low-cost adsorbents to efficiently remove sedative residues from water.

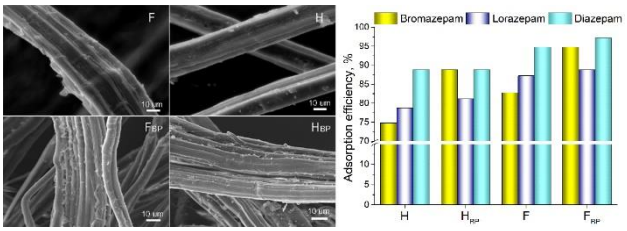

Fig. 1. SEM photographs and adsorption efficiency of examined fibers

Keywords*:* waste materials, lignocellulosic fibers, modification, adsorption, sedatives.

Acknowledgment: This work was supported by the Science Fund of the Republic of Serbia within project „Serbian Industrial Waste towards Sustainable Environment: Resource of Strategic Elements and Removal Agent for Pollutants - SIW4SE“ (Contracts No. 7743343).

AEC P-28

Use of spectrometric techniques in the identification of mechanical impurities in solid pharmaceutical dosage forms

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The manufacturer of the medicinal product must manufacture medicinal products to ensure that they are fit for their intended purpose; they comply with the

requirements of the Marketing Authorization or Clinical Trial Protocol and do not place patients at risk due to inadequate safety, quality or efficiency.

In the study, a case of identification of mechanical impurities incorporated on the surface of the tablets was considered, which with the use of spectrometric techniques was proven to originate from microcrystalline cellulose (Avicel PH 102 /Microcrystalline cellulose), which is used as an excipient in the formulation of solid pharmaceutical dosage forms. Impurities are manifested in the stage of the production process - tableting, as faintly visible black dots incorporated on the surface of the tablets.

The aim of the research in this study is the benefits of using an infrared (FTIR) spectrometric technique in the quick and precise identification of mechanical impurities in a product, which originate from incoming raw materials, and which have been proven by previous research to be a technologically unavoidable phenomenon as a consequence from the production process and the chemical composition of the raw material.

Keywords: solid pharmaceutical dosage forms, mechanical impurities, FT-IR, spectroscopic methods, microcrystalline cellulose.

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AEC P-29

Cleaning Validation of Primary Packaging Equipment Line in Pharmaceutical Industry

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Cleaning validation is documented evidence that an approved cleaning procedure will consistently remove previous product or other residues on product contact equipment surfaces below scientifically set acceptable

levels. The cleaning validation consequently ensures that the quality of the next product manufactured shall not be compromised by cross-contamination.[1,2]

The aim of this study was to validate the cleaning procedures of primary packaging equipment line IMA C80HS. Automated washing and drying machine DeLama were used for effectively washing and drying of disassembled packaging equipment parts. By performing a risk assessment considering solubility, toxicological effect and cleanability it was concluded that Alprazolam tablets 1mg is a worst-case product for primary packaging equipment line IMA C80 HS. Three consecutive cycles of cleaning and testing were executed after packaging of Alprazolam tablets 1mg. After each cleaning validation cycle swab and rinse samples were collected for physico-chemical analysis. The samples were analyzed with specific and validated HPLC method for quantification of residues from previous product. The column used was Zorbax Eclipse XDB C18, 150mm x 4.6mm i.d; 3.5μm; column temperature of 25
ºC; at a 1.0 mL/min flow rate and 254 nm detection. Mobile phase: mixture of ammonium acetate buffer solution pH=4.2 and methanol in ratio 35:65 %(*V*/*V*). The injection volume was 20μL.

The obtained data provide evidence that all results are within the acceptance criteria. The cleaning validation study confirms that the standard operating procedure for cleaning of primary packaging equipment parts is effective and reproducible and therefore approved as validated.

Keywords: cleaning validation, cross-contamination, risk assessment, HPLC method

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PSSE O-1

Optimization of Biochemical Sensitivity of Screen-Printed Electrodes for Monitoring Traces of Anticancer Drugs

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Anticancer drugs can cause serious health hazards such as organ toxicity and drug resistance because of their high potency if not properly dosed. Have a reliable method for concentration monitoring and detection of trace amounts of anticancer drugs in biological samples is of great importance for narrowing the gap between the therapeutical and toxic doses. The need for rapid and sensitive in-situ detection of biochemical entities finds a promising solution in the application of screen-printed electrode (SPE) based electrochemical nanosensors.

SPE-based electrochemical nanosensors modified with various techniques (gamma irradiation, polymer and composite drop casting etc.) for screening of pharmaceutical ingredients and products in biological matrices are presented in this work. Three commercial electrodes are used as a modification substrate – one polymer (polyaniline, PANI) and two carbon systems (graphene, G and carbon nanotubes, CNT). All obtained electrodes are tested in 0.1 M phosphate buffer saline of Doxorubicin Hydrochloride (DOX) with pH 6.8. The electrochemical activity of the commercial and modified electrodes is followed by cyclic voltammetry, as an electrochemical characterization technique. Fourier-transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM) are used for electrode's physical characterization, whereas ultraviolet-visible spectroscopy (UV-Vis) is used for structural changes following of the used buffer solution before and after current exposure. The modified electrodes show excellent response in terms of lower electrical resistance and higher electrical conductivity, compared to the commercial electrodes. The best performance is shown by PANI modified electrodes, especially by the polyaniline/carbon nanotubes-polyacrylic acid (PANI/CNT-PAA) modification.

Keywords: nanomaterials, electrochemical nanosensor, screen-printed electrode, anticancer drugs, Doxorubicin hydrochloride

PSSE O-2

IR Investigation of Some Organotin(IV) Compounds Immobilized on Mesoporous Silica

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The IR-ATR and IR transmittance spectra of (4-*O*-acetyl ferulato)triphenyltin(IV) and (fenoprofenato)tributyltin(IV)[1] were recorded and analyzed. It was possible using the splitting of the ν(COO) band in the IR spectrum of the compounds to prove amonodentate binding mode of the carboxylate group to the Sn atom. Also, the IR-ATR spectrum of theMCM-41 and SBA-15 mesoporous silica nanoparticles (MSNs)[2] were recorded and analyzed in order to check the mesoporous structure of the synthesized materials. The changes of the band profile, assigned to the Si-OH (H_2O) stretching vibration of the non-bridging oxygen atoms on heating the samples, prove that the two MSNs are mesoporous. Finally, the organotin (IV) compounds immobilized in both MSNs were analyzed using IR-ATR and IR transmittance spectroscopy, in order to assess the loading intothe MSNs and the changes in their spectra connected to the interaction with the silica matrix.

Keywords: Infrared spectroscopy; Organotin(IV) compound; Mesoporous silica

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PSSE O-3

Synergistic Effects of the Supporting Material and Annealing Temperature on the Performance of Pt Thin Film Catalysts

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The electrocatalytic oxidation of small organic molecules, such as methanol, ethanol and formic acid has been extensively studied due to their properties that make them suitable for use in fuel cells. Particularly, the electrochemical oxidation of formic acid has been comprehensively examined as the anodic reaction in direct formic acid fuel cell. The main goal in the development of the catalysts for formic acid oxidation (FAO) is to find the optimal balance between catalytic performance (activity/stability) and the catalyst cost, i.e. quantity of the noble metal used.

In the work presented herein, we explored the synergistic effects of the supporting material and annealing temperature on the performance of Pt thin film catalysts for FAO in acidic media. Our results show that compared to the as-prepared Pt films, the annealed (500 ^{o}C) films show exceptional activity for FAO reaction on both Pt/Ni and Pt/Cr catalysts, with 5-fold and 15-fold improvement, respectively.

The 500 ^{o}C annealed Pt/Cr catalyst was found to be the most active, the most selective and the most stable catalyst in our study. A catalyst with the best marks for all three characteristics is a very rare find in electrocatalysis in general.

Keywords: platinum thin film catalysts; formic acid oxidation; chromium; nickel

Acknowledgement: This work was financially supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (contract No 451-03-47/2023- 01/200026) and by the Science Fund of the Republic of Serbia under grant No 7739802

PSSE O-4

Computational Modeling of Solvent Effects on Electronic Spectra of Carbonyl Chromophores

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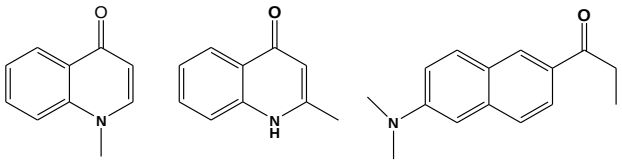
Interpretations of observed solvent effects on light absorption and emission by dye molecules have traditionally been associated during recent decades with time dependent density functional theory.[1] More sophisticated theoretical approaches have been applied to small molecular examples only. Here we compare some ways of accounting for the solvent effect using model specific solvent-solute interactions in continuum in the ground S_0 and the fluorescent first excited state singlet (S_1), considering specifically registered and predicted electronic spectra of hydrogen-bonded complexes. Comparisons of TD DFT predictions with more recent DLPNO-STEOM-CCSD[2] computational results are presented.



Keywords: electronic spectra, general and specific solvent effect, TD-DFT and STEOM-CCSD computing

Acknowledgement: This research has been financially supported by Grant KP-06-N59/1, 15.11.2021 of the Bulgarian NSF. The allotted computer facilities of the e-infrastructure of the NCHDC under Grant D01-168/28.07.2022 are gratefully acknowledged

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PSSE O-5
Sensitive Voltammetric Determination of Salbutamol at Nafion and *f*-MWCNT Modified Disposable Pencil Graphite Electrode

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Salbutamol (SLBT) is a phenylethanolamine with potent pharmacological activity used to treat chronic obstructive pulmonary disease as well as allergic or exercise-induced asthma[1]. Therefore, many analytical methods have been developed to detect SLBT and other β-agonist residues in both drugs and animal tissues. Today, electroanalytical techniques are of great interest to researchers due to several advantages such as low detection limit, high analyte selectivity, compact structure, simple sample preparation procedure, low cost, adaptability to field use, and minimal use of toxic organic solvents[2]. In this context, the successful electrochemical determination of SLBT has been reported by the use of nanomaterial, or composite material-modified carbon-based electrodes such as GCE[3], CPE[4], and surface-printed carbon electrodes (SPCE)[5]. In this study, a nafion and acid-functionalized multi-walled nano-carbon modified pencil graphite electrode (Nf@*f*-MWCNT@PGE) was used for the first time for the electrochemical determination of SBLT. From the differential pulse voltammograms recorded under the optimized conditions, the linear range were found to be between 0.10 and 10 μM with a detection limit of 0.04 μM. The proposed disposable electrode has been successfully used to determine SBLT in commercial pharmaceuticals and human serum samples with good accuracy and satisfactory recoveries.

Keywords: Salbutamol; Pencil Graphite Electrode; Modified Electrode; Voltammetry.

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PSSE O-6

Quantitative Evaluation of IR and Corresponding VCD Spectra

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Contemporary literature does not explain the infrared and vibrational circular dichroism (VCD) spectra of chiral molecules from a classical perspective.[1,2] As a result, the primary usage of VCD spectra is to determine the absolute configuration of a chiral molecule through comparison of experimental data and quantum mechanical calculations. Classical treatments of IR and VCD spectra can provide insight into the spectra. E.g., dispersion analysis based on wave optics and dispersion theory can be applied, which was extended by Born and Kuhn to include chiral substances. VCD dispersion analysis, as we devised it,[3] uses pairs of coupled oscillators to quantitatively describe the dielectric function and the chiral admittance functions that make up IR and VCD spectra. Oscillator strength, damping, oscillator position, vertical distance between coupled oscillators, and the coupling constant are the five parameters used to model the dielectric functions and chiral admittance functions of α-Pinene and Propylene oxide. In most cases, this model is sufficient to achieve a good correspondence between experimental and simulated data. The coupling can also impact the conventional IR spectra of chiral compounds by shifting peaks and transferring oscillator strengths.

Keywords: Vibrational circular dichroism; Infrared spectroscopy; Dispersion Analysis.

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PSSE O-7

One Century of the Debye-Hückel Equation: A Simple Explanation of its Thermodynamical Background

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In 1923, Peter Debye and Erich Hückel published a paper in which they derived a simple equation that could be used to quantitatively predict mean activity coefficients of electrolytes in dilute aqueous solutions.[1] The equation soon became one of the most widely used equations in analytical and physical chemistry and was soon adapted also for calculation of many other thermodynamical and transport properties in electrolyte solutions.

Despite its widespread use, the Debye-Hückel equation is still not well understood, as evidenced not only by physically incorrect derivations of the Debye-Hückel equation in numerous respected textbooks of physical chemistry and electrochemistry,[2] but also in the classic treatise on the thermodynamics of polyelectrolyte solutions.[3]

Here we show that the activity coefficient of a single ion in the Debye-Hückel equation can be easily determined from the electric potential in the solution, while the energy involved in attractive and repulsive interactions within the model ionic solution can be determined simultaneously. The change in Gibbs free energy can be evaluated by summing up the attractive and repulsive electrostatic interactions in the solution determined through the two-step process. With this new insight into the Debye-Hückel equation, it is possible to better understand the thermodynamics of electrolyte solutions.

Keywords: activity coefficient, electric potential, Debye length

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PSSE P-1

Comprehensive Structural Analysis of Gamma Irradiated Carbon Nanomaterials

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Gamma irradiation as a valuable technique enables structural modification such as introduction of desired functional groups and surface properties enhancement, expanding the potential applications of carbon nanomaterials in various fields. A study on gamma irradiation interaction with carbon nanostructures was conducted to investigate and unlock their full application potential. Three carbon samples (multiwalled carbon nanotubes – MWCNTs, graphene – G, and hybrid – MWCNTs/G*)* irradiated with gamma rays in different doses (50, 100, 250 and 500 kGy) in argon atmosphere were characterized and compared. In order to acquire a thorough understanding of the samples' structure, the following physical characterization techniques were employed: differential scanning calorimetry (DSC), thermogravimetric analysis/derivative thermogravimetry (TGA/DTA), elemental analysis, and scanning electron microscopy (SEM). Selected techniques were utilized to gather detailed information about the samples' composition, thermal behavior, and surface morphology, facilitating a comprehensive analysis of their structural properties and changes owing to the gamma irradiation treatment.

Keywords: carbon nanomaterials, multiwalled carbon nanotubes, graphene, gamma rays, irradiation, ionization

PSSE P-2

The First Electrochemical Studies of Metallocarbonyl Complexes with Imides

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Metallocarbonyl complexes, also known as carbon monoxide releasing molecules (CORMs), containing imides can serve as novel compounds to overcome antibiotic resistance. CORM interfere with cell wall biosynthesis, target cytoplasmic membrane, depolarize membranes, and induce oxidative stress. They are characterized by anti-inflammatory, anti-apoptotic, anti-atherosclerotic, anti-proliferative and cytoprotective agents. One of the ways of pharmacological action of this type of compounds is oxidation and reduction reactions.

The aim of the presented studies was to determine the electrochemical activity and properties of metallocarbonyl complexes (Fe, Ru) with maleimide and succinimide ligands (Fpm, Rpm and Fps).

The synthesis of metallocarbonyl complexes (Fe, Ru) with maleimide and succinimide ligands (Fpm, Rpm and Fps) was carried out based on the photochemical reaction (η^5-C_5H_5) $M(CO)_2I$ (M = Fe, Ru) in the presence of diisopropylamine. Electrochemical studies of the synthesized metallocarbonyl complexes Fpm, Rpm and Fps were carried out in Britton-Robinson buffer solutions at different pH 5, 7 and 10 at the glassy carbon electrode using cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS). In addition, the working glassy carbon electrode was characterized in a solution of the Fe(III)/Fe(II) standard redox system using CV and EIS and the topographic properties of the electrode surface were determined using an atomic force microscope (AFM).

Keywords: Metallocarbonyl complexes, cyclic voltammetry, electrochemical impedance spectroscopy

PSSE P-3

Cyclic Voltammetry Study of $DMAPbI_3$ Perovskite Material

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In the last decade, the most investigated perovskite materials are the hybrid organic-inorganic perovskites (HOIPs) due to their optoelectronic properties and possible application in production of photovoltaics. As a result, there is a continuous ongoing search for new ones, but also a thorough investigation of the properties of already known HOIPs. Here we present the cyclic voltammetry study of dimethylammonium lead iodide ($DMAPbI_3$).

A slightly modified synthesis of $DMAPbI_3$ than the one described in the literature was performed. Stoichiometric amounts of lead iodide (PbI_2) and dimethylammonium iodide (DMAI) were dissolved in acetonitrile, followed by temperature-controlled evaporation at 60 °C. This lead to the formation of $DMAPbI_3$ yellow crystalline powder. The identification and purity of the obtained compound was confirmed by PXRD, vibrational spectroscopy, and SEM/EDX analysis.

Cyclic voltammetry studies of $DMAPbI_3$ were conducted in dichloromethane (DCM) and tetrabutylammonium chloride (TBAC) as the electrolyte. A paraffin-impregnated graphite electrode (PIGE) was utilized as the working electrode, on which the perovskite microparticles were immobilized. The electrochemical activity of $DMAPbI_3$ is evident through an intense, wide, and irreversible anodic peak that initiates at -0.153 V. The voltammograms recorded with lower scan rates revealed that this peak is complex consisting the oxidation of $DMAPbI_3$constituents. The organic cation (DMA+) exhibits oxidation to various oxidation states, including the possibility of being oxidized to CO_2. The lead ion can undergo oxidation to form leadoxide, while the iodide ion can undergo oxidation to different oxidation numbers, but most probably to elemental iodine. However, the quantity of elemental iodine produced is minimal, making it difficult to detect. The observed vague and small reduction peak may be attributed to some of these by-products, rather than originating from the perovskite itself.

Keywords: dimethylammonium lead iodide, cyclic voltammetry, PXRD, vibrational spectroscopy, SEM/EDX

PSSE P-4

Structural, Spectroscopic and Thermal Analysis of Hydrogenphosphate Salts $Ca_2MH_7(PO_4)_4 \cdot 2H_2O$ ($M = K^+$, NH_4^+)

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New knowledge about various aspects of little-known acid salts is of great scientific and practical importance in view of their potential application in different areas such as proton conductors. A study of the salts $Ca_2MH_7(PO_4)_4 \cdot 2H_2O$ ($M = K^+$, NH_4^+) was conducted in terms of spectral, structural, and thermal means in order to obtain useful data on these salts and further discuss their potential for exhibiting proton conductivity properties.

The two isostructural compounds $Ca_2KH_7(PO_4)_4 \cdot 2H_2O$ and $Ca_2(NH_4)H_7(PO_4)_4 \cdot 2H_2O$ are stable up to 90–95 °C and then undergo multiple-steps thermal decomposition process owing to dehydration of the crystallization water and dehydration-condensation[1]. Furthermore, the structural data[2] for such compounds was used to obtain essential information regarding their infrared and Raman spectra in terms of different modes of vibration, the intensity, and the number of bands in the corresponding spectra. As expected, the infrared spectra of these compounds are fairly similar, especially in the region of stretching HOH vibrations. Since the systems of interest exhibit strong hydrogen bonding, a set of specific bands (*ABC* trio) appear in both of the salt's spectra. In the ammonium salt $Ca_2(NH_4)H_7(PO_4)_4 \cdot 2H_2O$ a few additional bands due to N–H vibrations are observed, of which particularly important is the band at 1450 cm^{-1} due to $\nu_4(NH_4)$. In addition to this, the recorded Raman spectra were compared with the obtained infrared spectra which further assisted in interpretation of some bands present in the corresponding infrared spectra.

Keywords: Infrared spectra, Raman spectra, proton-conductivity, thermal analysis.

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PSSE P-5

Oxidation Mechanism of Dopamine and Serotonin Using Cyclic and Square-Wave Voltammetry

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Dopamine and serotonin are main neurotransmitters that maintain excellent mental wellbeing and regulate physiological functions in human tissues. Oxidation of both neurotransmitters is of great importance in understanding their mechanisms of actions in the human body. This scientific study reveals the most probable oxidation mechanisms of these neurotransmitters in simulated physiological conditions (phosphate buffer with *p*H = 7.4) using voltammetric techniques (cyclic and square-wave voltammetry).

Results were obtained using several commercial unmodified electrodes, glassy carbon electrode (GC), platinum electrode (Pt), basal plane pyrolytic graphite electrode (BPPG) and gold electrode (Au) and compared with the literature[1,2]. Different electrodes gave distinctive voltammetric signals, with slightly better results on both carbon electrodes. Using both techniques and scan rate (frequency in SWV) analysis, both oxidation mechanisms were discussed and explained in terms of the recently proposed ECE mechanism (dopamine)[2] and ECEC mechanism (serotonin)[3]. Furthermore, fitting the experiments with theoretical simulations, we were able to find several values for key parameters of the proposed mechanisms.

Keywords: dopamine, serotonin, cyclic voltammetry, square wave voltammetry, electrodes.

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Introduction and Application to Exploring the Oxidation Mechanism of Serotonin, *The Journal of Physical Chemistry C.***2009**,113 (32), 14285-14289. DOI: 10.1021/jp904083e.

PSSE P-6

Micro-Dendritic Electrodeposited Bismuth and Food Coloring Sensing

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The kinetics and mechanism of cathodic electrodeposition of bismuth on a glassy carbon (GC) electrode were studied using cyclic voltammetry and chronoamperometry. The initial phase of bismuth electrodeposition was studied using the potentiostatic pulse technique in different electrolytes (nitric acid and acetate buffer solution) with and without the addition of EDTA as a complexing agent. A bismuth film (Bi-film) electrode was formed using the optimum bath parameters, deposition time and potential. The Bi(III)complexes reduction is inhibited by the specific structure of the formed Bi-film. Scanning Electron Microscopy (SEM) and cyclic voltammetry (CV) were employed to characterize the formed Bi-film. We proposed a facile electrochemical method for the determination of Artificial Food Colors (AFCs), in food samples, using Bi-film electrode.

The controversies concerning use of AFCs date back to the 1920s, when they were related with hyperactivity, hypersensitivities, learning problems, impulsive and negligent behavior and negative effects on cellular immune responses in children corresponding to the behavior pattern diagnosed with ADHD. Thus, monitoring of AFCs in foods is important.

The Bi-film exhibited an excellent recognition capacity toward SY. Finally, a procedure for quantifying SY in several food products and drinks is proposed.

Keywords: cathodic electrodeposition, bismuth film electrode, Artificial Food Colours, voltammetric methods, food analysis

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PSSE P-7

Design of PtSnZn Nanocatalysts for Anodic Reactions in Fuel Cells

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In order to achieve widespread application of fuel cell technology, the development of an efficient and economical catalyst is a crucial step. Reducing the diameter of catalyst particles, producing particles with a specific orientation surface, and alloying noble metals with less expensive metals are possible approaches to improve catalyst performance. This study will be focused on novel ways for creating PtSnZn catalysts that are more effective for the anodic reactions in fuel cell such are methanol, ethanol and formic acid oxidation reactions. PtZn and PtSnZn nanoparticles were produced using the microwave assisted polyol method and were supported on high surface area carbon Vulcan XC-72R material. The electrochemical behavior of synthesized catalysts was investigated utilizing the cyclic voltammetry, chronoamperometric technique, and electro-oxidation of adsorbed CO. To determine the catalyst's physicochemical characteristics, X-ray diffraction (XRD), transmission electron microscopy analysis (TEM), and thermogravimetric analysis (TGA) were used. High catalytic activity of the PtSnZn/C catalysts was achieved thanks to the benefits of microwave synthesis and carefully adjusted metal alloying.

Keywords: platinum catalysts; methanol oxidation; ethanol oxidation, formic acid oxidation;

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PSSE P-8

Correlation of H-bonding Distances and Strengths in API Solvates Case Study on Nitrofurantoin and Pyridoxine

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Hydrogen bond solvation affects molecular properties and functions both in solution and solid-state formation of solvates. Many of Active Pharmaceutical Ingredients (APIs) exist as solvates with different solvents that, depend on the nature and polarity, co-crystallize with their appropriate molecular structures in wide range of polarity, either non-ionizable or deprotonated acids and bases and their protonated forms, respectively. Despite H-bonding networking that occurs in a highly competitive solvent in biological systems, synthetic chemists have been facing difficulties to control and predict the H-bonding motifs from de novo in competitive solvents media. The concept of crystal engineering, based on molecular noncovalent recognitions and formation of self-assembled supramolecular clusters opens the opportunities for designing the solvate type of crystals with desirable properties.[1]

The crystallographic parameters of the determined crystal structure of two types of API solvates are presented. The N, N dimethylformamide solvate of the chemotherapeutic class of API for treatment of urinary infection, nitrofurantoin, and hydrated form of molecular salt that pyridoxine (vit B6) form with ferulic acid (derivate of hydroxybenzoic acid) .[2,3] The correlation of the H-bond distances with the bond strength are depicted on Hirshfeld surface's 2D fingerprint plots.

Though many of solvents are not with pharmaceutical relevance in terms of their high risk for toxicity, their co-crystallization with API molecules in crystalline systems offer opportunities to analyze the H-bond patterns and study the propensity

of occurring the motifs i.e., synthons among solvated crystals that are deposited in Cambridge Crystal Crystallography Database (CCCD).

Keywords: Crystal engineering, solvates, Hydrogen bonding, molecular recognition

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PSSE P-9

Phosphate-Based Mixed Polyanion Compounds as Promising Electrode Materials for Post-Lithium Ion Batteries

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The investigations on next generation of electrode materials that should meet the increasing requirements for high power, safety, low cost and environmental compatibility are a hot research topic in the field of energy storage. Iron containing phosphate-based electrode materials offer a great promise for large scale application due to high structural and thermal stability, good cycling stability and low cost.

One effective way to achieve high energy density is to increase the $M^{(n+1)+}/M^{n+}$ redox potentials though introducing more anion units with different electronegativity in the chemical composition (cooperative inductive effect). In this regard, we have focused on compounds which composition contains two kinds of anionic units: $NaFeV(PO_4)(SO_4)_2$ and $Na_4Fe_3(PO_4)_2P_2O_7$ (labeled NFVPS and NFPP, respectively). They are prepared by a precursor method using freeze-drying of solutions containing the needed components. To overcome the low electronic conductivities of NFPP and NFVPS two types of carbon-based composites have been prepared as cathode materials *via* ball-milling: with rGO (reduced graphene oxide) and carbon black (15 % each). The composites have been characterized by different methods. Their electrochemical performance have been studied in Lihalf-

cells using $LiPF_6$ in EC:DMC as electrolyte in galvanostatic and potentiostatic regimes at 20 and 40 °C. It is established that rGO is more effective additive than carbon black in the achievement of higher specific capacity for the two compounds. After 100 cycles at C/2 rate very good values for the discharged capacities have been obtained: 115 mAh/g and 82 mAh/g for NFVPS/rGO at 40 and 20 °C, respectively, and 105 mAh/g for NFPP/rGO (20 °C). The presence of rGO additive promotes the capacitive behavior in addition to the intercalation reactions owing to Fe^{3+}/Fe^{2+} and V^{3+}/V^{4+} redox reactions which results in higher specific capacities. The present study demonstrates the effectiveness of carbon-based composites with tunnel-type mixed polyanion compounds for achievement of promising electrochemical performance in hybrid metal-ion batteries.

Keywords: Li/Na-ion batteries, Electrode materials, Mixed polyanion compounds

PSSE P-10

Pinus Nigra Essential Oil and Its Main Active Components as Sustainable Compounds for Mitigation of Carbon Steel Corrosion

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The use of compounds for corrosion protection such as chromates and some synthetic organic substances is prohibited or restricted due to their hazardous and carcinogenic nature. Recently, research has been focused on green corrosion inhibitors, whose name is mostly associated with plant essential oils and extracts that are environmentally friendly, non-toxic, inexpensive, not harmful to human health, and with high corrosion inhibition efficiency. Many plant oils and extracts have been used as effective corrosion inhibitors for steel in hydrochloric acid (HCl) solution, and they are a rich source of bioactive components.

The inhibitory properties of *Pinus nigra* needle essential oil (PN), as well as its active ingredients, were analyzed on a carbon steel sample in a 1M HCl solution. The dominant components of this essential oil are α-pinene (66,529 %), germacrene

D (14,054 %), (E)-caryophyllene (5,671 %), and β-pinene (2,105 %). The effectiveness of the inhibition was investigated using electrochemical methods such as electrochemical impedance spectroscopy and potentiodynamic polarization measurements. It has been shown that the effectiveness of all inhibitors increases with time. The most abundant substance in the essential oil, α-pinene, showed a lower corrosion inhibition efficiency compared to β-caryophyllene at the same concentration of 80 ppm. Based on the recorded polarization curves, it was concluded that black pine essential oil, as well as its components, act as mixed-type corrosion inhibitors, reducing the rate of both anodic and cathodic reactions. The inhibition capacity of PN could be ascribed to the adsorption of its organic constituents on the surface of carbon steel.

Keywords: corrosion, carbon steel, green inhibitors, EIS, polarization measurements.

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PSSE P-11

Correlation Between Morphology and Structure of Galvanostatically Electrodeposited Tin Dendrites

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Tin dendrites found wide application in various industries.[1] They can be obtained by both non-electrochemical and electrochemical methods of synthesis. In this study, they were produced by a galvanostatic regime of electrolysis from alkaline hydroxide solution at a current density of –3 mA cm^{-2}, 1.5 times larger than the limiting diffusion current density, with an amount of the electricity of 200 and 400 mC. In the dependence of an amount of the passed electricity, Sn dendrites of various morphology and crystal orientation were obtained: the fern-like dendrites predominantly oriented in (220), (440) crystal planes are obtained with 200 mC and the spear-like and the dendrites with prismatic branches showing the strong (200),(400) preferred orientationwere obtained with 400 mC.

The strong correlation between morphology and structure of Sn dendrites is established and it can be explained by analysis of chronopotentiometry response obtained at the given current density and by morphological and structural analyses

of Sn dendrites obtained by a potentiostatic regime at cathodic potentials corresponding to values attained after the passed amount of the electricity of 200 and 400 mC. The chronopotentiometry response after spent 200 mC was dominantly in the (–1600 ÷–1740) mV vs. Ag/AgCl range, and the fern-like dendrites with the strong (220), (440) preferred orientation were obtained in this potential range. After spent 400 mC, the chronopotentiometry response was about –1200 mV vs. Ag/AgCl, and the spear-like and the dendrites with prismatic branches with the strong (200),(400) preferred orientationwere obtained at this cathodic potential.

Keywords: tin; electrolysis; morphology; structure; dendrite.

Acknowledgment: This work was financially supported by MSTDI of RS (Grant No. 451-03-47/2023-01/200026) and Science Fund of RS (Grant No. AdCatFC: 7739802).

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PSSE P-12

Facile synthesis of Sn-Pd catalysts with high performances for ethanol electro-oxidation in alkaline medium

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Nanostructured materials present unique properties as electrocatalysts for various industrial needs such as electrochemical energy conversion and storage. Aiming to enhance the electrocatalytic properties of Pd towards the electrochemical oxidation of ethanol, we used the electrodeposited Sn dendrites as a sub-layer for Pd. We tested the resulting Sn-Pd electrocatalysts for ethanol oxidation reaction (EOR). It was obtained that different morphological characteristics of Sn contribute to and determine Pd electrochemical behavior in EOR. By varying the amount of Sn loading prepared in the potentiostatic regime and keeping constant Pd loading, a series of Sn-Pd electrocatalysts with various ratios of Sn and Pd were synthesized and among them, Sn0.6-Pd0.4 showed to be the most active and poisoning tolerant

catalyst in EOR. It was pointed out that optimization of composition and morphology assures well synergy of Sn with Pd towards EOR and at the same time demonstrates the guide for the design of novel materials with specific properties. Therefore Sn-Pd catalysts have emerged as a suitable and promising anode material for direct alcohol fuel cells.

Keywords: tin; palladium; morphology; composition; electrooxidation.

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PSSE P-13

Greenhouse gas emission from the rare earth metals electrolysis

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Rare earth metals, mainly related to neodymium, praseodymium or dysprosium are usually produced by molten salt electrolysis in which oxy-fluoride or chloride molten salt systems are used as the electrolytic bath. Minimizing the perfluorocarbon compounds (PFC) emission in rare earth electrolysis should be the primary goal owing to their high global warming potential[1]. There is growing interest in the oxygen and fluoride ions oxidation reactions on the graphite anode, particularly in the mechanism of C-F in the PFC formation. In the present work, we investigated the off-gas emission during the Nd and Pr electrodeposition from oxy-fluoride melts by the in-situ FTIR-spectrometry to understand the nature of the reactions taking place on the anode and the mechanisms behind them. During the electrolytic reduction of rare earth metals in the oxy-fluoride system with tungsten or molybdenum used as cathode, tungsten as a reference electrode and a GC electrode used as an anode, the produced oxygen species subsequently react with carbon and generate CO and CO_2. With F^- ions present, PFC compound emission,

such as CF_4 and C_2F_6 gases also can be evolved from the GC anode as well. During the electrolysis, carbon monoxide was evolved in variable quantities, but always below 1000 ppm. Evolved quantity of CO_2 was around 200 ppm during the potentiostatic deposition. The quantity of recorded CF_4 was well below 10 ppm. At the same time C_2F_6 was not detected under the applied potentiostatic regime of the electrolysis. To suppress greenhouse gas emissions and to achieve high-purity Nd and Pr metal production on the working substrate we chose low-deposition overpotential.

Keywords: rare earth metals, electrodeposition, greenhouse gas emission
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PSSE P-14
Copper Electrodeposition onto Palladium from a Deep Eutectic System Based on Choline Chloride

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Recently, there has been an increasing interest in developing non-aqueous electrolytes which have been widely employed as an alternative media for a range of metals and metal alloys electrodepositions. A promising and new class of electrolytes among ionic liquids (ILs) are deep eutectic solvents (DESs)[1]. The purpose of the copper deposition study from DESs is the application of copper coating and copper alloys in both, industry and fundamental research. In this work, the electrochemical deposition of copper onto palladium working substrate from ChCl/EG (1:2 ratio) DES electrolyte at 50°C was investigated. Additionally, the Cu(II) electroreduction process was studied by potentiodynamic measurements, cyclic voltammetry, chronoamperometry, in the electrolytes with different concentrations of Cu(II) ions ranging from 0.1 M to 0.5 M.

The cyclic voltammetry results indicated that the bulk deposition of Cu(II) begins to occur at around –0.080 V vs. Cu. It was found that copper deposition onto the Pd cathode from ChCl:EG electrolyte under potentiostatic conditions is achievable.

Data collected from X-ray diffraction (XRD) analysis proved that the cathodic deposits are composed of Cu and CuPd intermetallic. CuPd alloys with different Pd-Cu ratios were prepared by constant potential of –0.100 V vs. Cu from ChCl/EG containing 0.1 M and 0.5 M Cu(II). It is worth noting that the X-ray data indicated that the composition of the produced Pd-Cu films could be varied by changing the concentration of Cu(II) ions in the electrolyte or changing the deposition mode.

Keywords: deep eutectic solvents(DESs), Cu-Pd alloys, electrodeposition

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PSSE P-15

Formic Acid Electrooxidation on Cr-Supported Platinum Thin Film Catalyst

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In this study, the formic acid electrooxidation reaction was studied on a platinum thin film catalyst obtained by deposition on chromium support (Pt/Cr). In an attempt to reduce the proneness of Pt to poisoning species i.e. CO and improve the catalytic performance of Pt/Cr at low potentials in the formic oxidation reaction, the as- prepared catalyst was modified using controlled thermal treatment. The influence of thermal treatment on the electrode surface morphology was monitored using an atomic force microscope (AFM). Thus obtained catalyst was electrochemically characterized with cyclic voltammetry and oxidation of CO monolayer, while the performance of the catalyst was tested in a formic acid oxidation reaction. The improved activity on annealed Pt/Cr system is a consequence of the surface reconstruction of Pt film with

predominant (111) orientation. Compared to other facets, the (111) facet selectively favors direct HCOOH oxidation, avoiding CO_{ad} poisoning at low potentials. Moreover, the Pt (111) facets offer improved stability of the catalyst compared to the as-prepared polycrystalline film. Finally, the Cr substrate also experiences improved stability after annealing, presumably due to the formation of a protective oxide layer. Thus, with the successful choice of the supporting material and annealing temperature, we were able to create a thin film catalyst with improved activity, selectivity and stability, in contrast with commonly observed activity-stability tradeoff in catalysis.

Keywords: Pt thin films; Cr support; thermal treatment; electrooxidation; formic acid

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BFT O-1

The Changes in Bioactive Compounds During the Fermentation of Spirulina

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Biotreatment with lactic acid bacteria (LAB) is a popular solution to degrade cyanobacterial cell walls, to produce molecules with enhanced properties. The aim of this study was to investigate the changes in L-glutamic acid (L-Glu), gamma-aminobutyric acid (GABA) and biogenic amines (BA) during the fermentation of Spirulina with *Lacticaseibacillus paracasei*; *Levilactobacillus* brevis; *Leuconostoc mesenteroides*; and *Liquorilactobacillus uvarum*. It was established, that the ratios of BA/GABA and BA/L-Glu ranged from 0.5 to 62 and from 0.31 to 10.7, respectively, as well as, the GABA content was correlated with putrescine, cadaverine, histamine, tyramine, spermidine, and spermine contents. Finally, while high concentrations of desirable compounds are formed during fermentation, the formation of non-desirable compounds must also be considered due to the similar mechanism of their synthesis.

Keywords: lactic acid bacteria; Spirulina; fermentation; gamma-aminobutyric acid; biogenic amines

BFT O-2

Shaping the Future of the Food Production by CRISP/Cas9 Gene Editing

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In previous decades advanced biotechnological techniques, including transgenesis, enables the precise and efficient targeted modification of an organism's genome. However, when it comes to food production, very few topics in science raised so much controversy as that of genetically modified organisms, or GMOs. As GMOs are generated through the transgenic introduction of foreign DNA sequences, a hazard that may arise from GMPs is uncontrolled integration of recombinant DNA into the genome[1]. The recent discovery of gene-editing tool CRISPR/Cas9, gives a promise for a completely new approach to the production of crops with desirable genetic traits. CRISPR/Cas9 tool, with the ability to cut out genes and splice in new ones, generates 'genome-edited crops' (GECs) through

precise editing of an organism's native genome[2]. Thus, genomic alterations through the use of genome-editing technology are quite similar to those found throughout naturally occurring populations. Even more, gene editing by CRISPR/Cas9 is doable in an in vivo system, opening a completely new door in the crops and food production[3]. First CRISPR'd food reached the consumer market in September 2021, by Japanese startup Sanatech Seed. It was a variety of tomatoes containing high amounts of gamma aminobutyric acid (GABA) that may replace GABA supplements conventionally used to treat high blood pressure, insomnia, and other health problems. It is fully clear that CRISPR/Cas9 technology has a tremendous potential to shape the future of food production.

Keywords: CISPR/Cas9, Gene editing, Food production

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BFT O-3

Fate of Deoxynivalenol During the Production Process of Bakery Products

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Producing safe food is a goal and an obligation for each producer. Mycotoxins by representing the most significant contaminants of grain are considered to be the main risk in the production of safe bakery products.[1]

Conditions during the production process defined by temperature regime, duration of the temperature regime, moisture content, pH value, as well as the type and level of mycotoxin concentration in the matrix are the most important factors influencing the reduction of mycotoxin content.[2]

The aim of this study was to examine the influence of production process of different types of bread, rusk, bread crumbs and biscuits on the content of

deoxynivalenol in bakery products. Samples of naturally contaminated whole grain wheat flour (conc. 700 μg/kg), wheat flour type T-1100 (conc. 500 μg/kg) and whole kernel corn flour (conc. 2420 μg/kg) were used to examine the influence of the production process on the content of deoxynivalenol in bakery products. Experimental production of different types of bread, rusk, bread crumbs and biscuits was conducted in a bakery pilot plant. Ridascreen® ELISA-assay was used to analyze the content of deoxynivalenol.

Based on the results it was concluded that the process of production of bread, rusk, bread crumbs and biscuits significantly reduces the content of deoxynivalenol in final products ($p<0,05$). However, in some cases (rusk and bread crumbs) results raised a question if the % of reduction is high enough to make the final product compliant to European legislation (Reg. 1881/2006)[3].

Keywords: deoxinivalenol, bakery products, ELISA

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BFT P-1

Effect of Coffee Roasting Temperature on Nutritive and Sensory Profile of Traditionally Prepared Black Coffee Beverage

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The aim of this research was to determine the effect of coffee roasting temperature in industrial conditions on: (i) the nutritive quality of coffee (Arabica 1st class, Arabica 2nd class, Robusta); (ii) the sensory quality of traditionally prepared black coffee beverage; (iii) correlation between roasting temperature and beverages sensory quality. The basic chemical composition, titratable acidity, pH, content of caffeine, chlorogenic acid, and free fatty acids were determined for each of three coffee samples and four treatments: green coffee; light roasted (167°C);

medium roasted (171°C); dark roasted (175°C). The sensory quality of black coffee beverage traditionally prepared from roasted coffee was determined and compared.

It was found that relatively small changes in coffee roasting temperature in industrial conditions affect numerous, mainly statistically significant changes in its nutritive and sensory quality. These changes are also related to the coffee type and class. Black coffee beverage traditionally prepared from medium roasted (171°C) Arabica 1st class coffee had the highest sensory quality of all analyzed samples, with markedly expressed pleasant coffee-like and roasted coffee aromas and moderately expressed pleasant bitterness, acidity, and body.

Keywords: coffee, roasting, nutritive quality, sensory analysis.

BFT P-2

Physicochemical Characteristics of Scotta from Different Whey Cheese Types

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Whey is the yellow liquid byproduct obtained at cheese production. It is characterized by several commercial applications, mainly for whey cheese. In the dairy industry, the term „Scotta“ is used for the whey separated after whey cheese production. Because of its high availability and high-value compoundssuch as proteins, peptides, and lactose, scotta could be used in the food and pharmaceutical industry, cosmetics, or as a raw material for biofuel and biodegradable polymers.[1]

This study aimed to determine the physicochemical parameters of the scotta obtained as a byproduct from the production of Macedonian whey cheese-Urda. The Urda was obtained from the whey of white brined cheese and Kashkaval production processes. The whey was treated with lactase enzyme before being processed into whey cheese. The physicochemical parameters: dry matter, fats, proteins, lactose, and pH were determined according to the AOAC methods.[2]

In the scotta samples, depending on the whey type, pH values ranged between 5.19 to 5.34, whilethe contents of dry matter, fats, proteins, and lactose from 4.52÷4.84%, 0.01÷0.12%, 0.39÷0.48%, and 0÷3.93%, respectively.The determined values of the physicochemical parameters highlight the possibility to use scotta in fermented beverages production or concentrated with membrane processes, it can be used as a raw material for spreads, yogurts, or other dairy products.

Keywords: Whey, whey cheese, scotta, physicochemical parameters.

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BFT P-3

Effect of The Heat Treatment Time On the Whey Cheese Yield

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Cheese produced by thermal denaturation, followed by aggregation and precipitation of the whey proteins is known as whey cheese. Lactic acid bacteria are not included in the production, therefore, whey cheese does not require a ripening period. The whey cheese shelf-life is notably shorter compared to other cheese types due to the higher moisture quantity and high water activity value. Urda is

Macedonian whey cheese with a long tradition usually obtained from whey that is a byproduct of the production of semi-hard yellow cheese such as Kashkaval or „Beaten“ cheese from sheep and cow milk.[1]

The study aimed to investigate the impact of the duration of thermal treatment of the whey on the Urda yield. Whey was obtained as a byproduct of the standardized industrial production process of white brined cheese and Kashkaval from cow's milk. The yield was calculated as Urda quantity obtained from 1L whey.[2]

The formation of the first whey cheese aggregates was observed after reaching a temperature of 70°C. The dependence of yield from the thermal treatment time had a sigmoid shape. In the period from 50 to 130 min, maximal values for whey cheese yield were achieved at 100 min or after holding for 20 min at 90°C temperature. The yields of whey cheese decreased linearly in the period between 100 and 130 min, which is related to the losses as a result of the whey foaming during the process and also, an increase of whey cheese dry matter with prolonged thermal treatment.

Keywords: Whey, thermal treatment time, whey cheese, yield.

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BFT P-4

Assessment of Silymarin Content in Plant Material and Extracts Using HPLC and Raman spectroscopy

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Silymarin is a mixture of flavonolignans from the plant *Silybum marianum* (L.) Gaerth., which derives mainly from its fruits. *S. marianum* has been found to exhibit antioxidant, lipid-lowering, antihypertensive, antidiabetic,

antiatherosclerotic, anti-obesity, and hepatoprotective effects. In modern therapy, standardized silymarin products are used. According to the European Pharmacopoeia (Ph. Eur. 11.0), the nominal silymarin content in the dried seeds is not less than 1.5% w/w, while in the refined and quantified milk thistle dry extract, it is within the range of 30-65%.

Therefore, this research work aimed to estimate the silymarin content in wild and cultivated milk thistle fruits as well as in commercially available dry extracts according to the monograph in Ph. Eur. 11.0 and to speed up the analysis by applying rapid quantification methods such as Raman spectroscopy. The Ph. Eur. 11.0 method involves very long and complex sample preparation followed by extensive HPLC analysis.

The obtained HPLC results of the samples of cultivated milk thistle fruits collected throughout several years showed that silymarin content varied within 0.3–1.8% w/w. The same extracts were analyzed using a portable Raman spectrometer, and the collected spectra were assigned and used for building a partial least-squares (PLS) model for quantification, where HPLC was used as a reference technique. The extracts from the wild-growing plants were quantified with the developed model, and the content in all samples was found to be above 1.5% w/w. Furthermore, the dietary supplements containing silymarin-rich dry extract (35% w/w) were quantified both with HPLC and the Raman method, and the obtained results were complementary and met the Pharmacopoeial requirements for silymarin content.

Keywords: *Silybum marianum*, quantification, PLS model, chromatography, spectrometry.

BFT P-5

Testing The Quality of White and Green Leaf Proteins Using Mixolab^{tm} for Applications in Bakery Products Formulations

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Incorporation of alternative plant protein concentrates or isolates into cereal-based matrices can lead to the production of nutritionally improved products such as bread with high protein content and an improved essential amino acid

profile, especially lysine. Green leaves, as the richest protein source containing soluble – *white* and insoluble – *green* proteins, seem to be an attractive and sustainable source for obtaining alternative proteins in line with the concept of green biorefinery, compared to the cultivation of soybeans for protein production. Thus, the overall objective of this study was to evaluate the quality of white and green proteins from various leaf sources for inclusion in a library of alternative proteins and for use in the development of plant protein-based products.

A food-grade, sustainable three-step process was used to produce the protein concentrate from the pumpkin and spinach leaves, including mechanical pressing of the leaves with screw presses, thermal coagulation, and acid precipitation. The functional properties of the white and green protein concentrates, such as solubility, emulsifying activity/stability, and water/oil holding capacity, were investigated. The rheological behaviour of wheat flour enriched with leaf protein was studied using the Mixolab Chopin. The functional properties of the leaf protein concentrates, as well as, the rheological properties of the leaf protein-enriched flour were compared with a soy protein concentrate that served as a reference.

The leaf protein concentrates showed comparable or better functional properties than the currently used soy protein concentrates. The changes in the rheological behaviour were observed in terms of water absorption, development and stability time, mechanical resistance during mixing, and behaviour of the protein-enriched flour during heating. This study has shown that leaf protein has the potential for the production of leaf protein-rich baked goods.

Keywords: Pumpkin leaves, spinach leaves, white and green leaf protein, functional properties, rheological properties of protein-enriched flour, Mixolab^{TM}

Acknowledgment: This research was supported by the Science Fund of the Republic of Serbia, #GRANT No 7751519, Multifunctional leaf protein and assembled nanocarrier structures delivered by enzyme technology - MultiPromis.

BFT P-6

Pumpkin leaf-isolated RuBisCO as a protein source for bioactive peptides

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RuBisCO (ribulose-1,5-bisphosphate carboxylase/oxygenase) is a non-allergenic, easily digestible protein found in the leaves of C3 plants, accounting for up to 50% of the total. It is similar to the FAO's ideal protein and is offered as a

valuable alternative for meeting nutritional requirements. Plant-based proteins provide amino acids for human cell development and act as precursors of bioactive peptides. Protein sources and proteolytic enzymes are crucial for producing bioactive peptides effectively.

This research aimed to optimize the hydrolysis of pumpkin leaf-isolated protein in terms of time and type of process, one or two-step process, by using endo- and exo-peptidases. The efficiency was assessed using SDS-PAGE electrophoresis, quantitative hydrolysis analysis, and peptides' capacity to chelate Fe^{2+} ions and scavenge $ABTS^{\bullet+}$ radical cations. The peptide molecular weight was determined by implementing the size-exclusion UFLC method.

The highest degree of hydrolysis, which is correlated with higher antioxidant activity was shown by Alcalase and Everlase (19.5%), and Neutrase (21.5%) with a tendency to favor Neutrase due to more favorable process conditions and a more sensory-acceptable product. Hydrolysis with Neutrase-Flavourzyme during 225 min yielded hydrolyzates with a 43.5% degree of hydrolysis, and antioxidant activities of 0.74 μmol TEAA/mg (*i.e.* 48%) and 0.30 μmol EEAA/mg (*i.e.* 44%). Five peptide fractions were identified as follows: F1 (> 27 kDa), F2 (20-27 kDa), F3 (10-20 kDa), F4 (3-10 kDa), and F5 (< 3 kDa). By establishing a correlation with antioxidant activity, it has been confirmed that a large proportion of peptide fractions F3, F4, and F5 were accountable for Neutrase-Flavourzyme hydrolyzate's good antioxidant activity. Examined enzymatic approaches contributed to generating the antioxidant peptides from pumpkin-leaf proteins with diverse peptide profiles.

Keywords: Plant-based proteins; RuBisCO; Protease; Bioactive peptides; Size-exclusion UFLC

Acknowledgment: This research was supported by the Science Fund of the Republic of Serbia, #GRANT No 7751519, Multifunctional leaf protein and assembled nanocarrier structures delivered by enzyme technology–MultiPromis.

BFT P-7

Evaluation of Anthocyanins Extracted from Black Rice, Acai and Purple Cabbage Using Uv-Vis Spectroscopy

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Anthocyanins are bioactive compounds that are present in various fruits and vegetables. They can enhance the visual appeal of food products, as they are responsible for their vibrant purple, blue and red hues. Anthocyanin-rich extracts obtained from plants can change colour in response to pH, temperature, light, and oxygen variations. By changing their colour accordingly to the pH of the food product, the anthocyanins have a potential to be used in active and intelligent food packaging as they can be incorporated in polymer/biopolymer films[1-3]. In this research, a quantitative measurement of anthocyanin content is provided. Anthocyanins were obtained by solvent extraction from black rice, acai, and purple cabbage using different concentrations of ethanol/water and citric acid. The absorbance of the extracted solution was determined using a spectrophotometer. The pH of the extracted solution was adjusted using 1M NaOH or 1M HCl for achieving basic or acidic state, respectively. The color spectrum was immediately measured at a pH range of 2–12 at a wavelength range of 400–700 nm. The colour changes of the extracted solutions were also photographed and monitored using colorimeter[4].

Keywords: Anthocyanins, Uv-Vis spectroscopy

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BFT P-8

Effect of Orange-Carbon Dots on Plants' Antioxidative Response in Green Beans Cultivated in the Soil

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Orange-carbon dots (o-CDs) have the potential to enhance photosynthesis and productivity in plants playing an important role in agroindustry[1]. Therefore, it is of interest to estimate regarding possible oxidative stress they may initiate in plants. This study reports the impact of o-CDs on the parameters of secondary metabolism - total antioxidative activity (TAA) and total phenolic content (TPC) measured in the extract of green bean leaves after foliar o-CDs' application at 1 and 5 mg/L. The plants were cultivated in the soil in outdoor conditions and the leaves were collected for analysis after three cycles of o-CDs treatments. Both tested parameters are indicators of antioxidative disorder in plants. TAA is related to the contribution of different low-molecular-weight antioxidants including phenolic acids, vitamins, sugars, etc.,[2,3] while TPC includes phenolic secondary metabolites and participates in the regulation of plant defense responses.[3,4] The results revealed an increased TAA in green beans only at 5 mg/L of o-CDs. At the same time, the TPC did not change after any of the two applied o-CD concentrations. The results may be evidence of the oxidative stress increase in green bean leaves with enhanced o-CDs concentrations, indicating that the 1 mg/L is more appropriate for use.

Keywords: green beans, orange-carbon dots, total antioxidative activity, total phenolic content

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BFT P-9

Stability of Cyaniding-Derivatives in Homemade Raspberry Jams

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High-performance liquid chromatography with diode array detection (HPLC-DAD) was used to study the stability of individual anthocyanins during preparation of homemade raspberry sugar jam and sugar-low jam at high temperatures (90, 95, 100 and 105 °C).

Acidified methanol was used for anthocyanin extraction. Several derivatives of cyanidin, were identified: cyanidin-3-sophoroside (cy-3-soph), cyanidin-3-glucoside (cy-3-glu) and cyanidin-3-rutinoside (cy-3-ru). Cy-3-soph was the most abundant, followed by cy-3-glu and cy-3-ru. The lowest loss of cy-3-soph, cy-3-glu and cy-3-ru was measured after 5 minutes of cooking at 90°C, yielding 35.6%, 38.4% and 29.6% in sugar jam and 13.4%, 24.6% and 11.7% in sugar-low jam. The greatest loss of cy-3-soph, cy-3-glu and cy-3-ru was observed after 30 minutes of cooking at 105 °C, yielding 74.5%, 81.1% and 71.7% in sugar jam and 44.2%, 55.1% and 42.6% in sugar-low jam. Apparently, the presence of larger amount of sugar had negative effect on stability of anthocyanins in raspberry jam. Anthocyanins exibited greater stability towards thermal degradation in sugar-low jam. Cy-3-soph and cy-3-ru have shown relatively equable stability in sugar-low jam. Cy-3-glu was the least stable in both jam types.

Obtained results are in accordance with literature data where cy-3-soph has been identified as the most stable pigment in raspberry juice and wine, while cy-3-glu was the least stable and the most reactive pigment, which undergoes polymerization faster than all other anthocyanins[1].

Keywords: cyanidin, raspberry, HPLC, jam.

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BFT P-10

Sensory Analysis of Meat Analogues – Veggie Burgers

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The surging trend of plant-based food regimens has stimulated the innovation and improvement of alternative meat products. In this regard, meat analogues such as veggie burgers have emerged as a notable choice for consumers that are perpetually seeking healthier and more environmentally sustainable dietary choices[1-4].

In order to successfully incorporate these analogues into the mainstream portions, an understanding of their sensory characteristics is crucial. Therefore, a comprehensive sensory analysis of veggie burgers has been conducted, including the perceptions and preferences of individuals from different age ranges. Four types of veggie burgers were prepared, using rice, rye, wheat and oats as a basis for the burger. The processing of the veggie burgers included baking at 200^{o}C. After the burgers were cooled down, the sensory analysis was performed. It included a structured questionnaire in which subjective perceptions of taste, texture, colour, aroma and overall palatability on a hedonic scale were evaluated.

The results disclosed some interesting observations about the sensory characteristics of the meat analogues. Furthermore, it included a discussion about the preference of the analogues over the original meat burgers. The results from the questionnaire showed that the majority of the participants preferred the original meat burgers over the veggie burgers and were not likely to purchase plant-based meat. This way, through comprehension of individuals' preferences, the food manufacturers can modify their products to satisfy the shifting demands of the consumers[5].

Keywords: veggie burger, meat analogues, sensory analysis

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BFT P-11

Volatile Profile of Grašac Wines Produced with Different Commercial Inactivated Yeast Derivatives

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The aim of this study was to investigate the influence of different commercial inactivated yeast derivatives (IYDs) on the volatile profile of wine during aging. The study was performed with Grašac grapes from Srem wine region (Serbia). After fermentation was complete, wine samples were treated with different IYDs in two doses. After the six-month aging period, the volatile profile of wine samples was analyzed using HS-SPME-GC-MS method.

The results showed that esters were the major volatile compounds, with ethyl acetate and 2-phenyl ethyl acetate being the most abundant among all samples, followed by ethyl dodecaonate, ethyl decanoate and 3-methyl-butyl-octanoate, all of them contributing to different fruity and floral aromas. The major higher alcohol phenyl-ethyl alcohol was notably above its odor threshold level in most samples at both time marks. As the concentration of IYDs applied increases, we observe a corresponding rise in the levels of certain volatiles. In addition, most of the IYDs applied helped to preserve or, even more, increase the amounts of specific volatiles during the aging period. PCA analysis showed clear separation among the Grašac wine samples, while it was found that samples treated by the same IYDs, regardless of the concentration, were relatively similar and distributed closer to each other in the PCA plot.

The findings indicated that wine can be influenced differently by various types of IYDs, each serving a specific purpose. This information equips winemakers with the means to precisely control and attain the intended sensory characteristics of the wine.

Keywords: yeast derivatives, wine aging, Grašac, volatile composition

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BFT P-12
Organoleptic Characteristics of Laboratory Brewed Herbal Beers

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Throughout the centuries, various botanicals have been utilized as additives in beer for different purposes, including their preservative properties, perceived medical benefits, desired psychotropic effects or simply for enjoyable flavors[1]. A study was conducted to determine the taste and appearance of laboratory prepared beers infused with nettle (*Urtica dioica* L.), sage (*Salvia officinalis* L.) and chamomile (*Matricaria recutita* L.). The beers were prepared by adjusting the beer wort to 12% extractive matter and infusing it with herbs or hops, followed by a seven-day fermentation process. Throughout fermentation, the pH value and extractive substances were measured. After clarification, an untrained panel of tasters evaluated the beers' appearance, taste, and mouthfeel using a survey questionnaire. Hedonic tests and the check-all-that-apply (CATA) method were used to assess acceptability and appearance.[2,3] The research findings indicate that bitterness has a detrimental impact on the overall preference for a particular beverage, while flavors of sweetness, citrus, and wheat hold a greater appeal. It is noteworthy that participants' level of interest and familiarity with beer significantly influence their taste preferences. Regarding herbal beers, the infusion of sage was identified as yielding the least desirable outcome. Through the implementation of the CATA test and principal components analysis, the sensory descriptions of each herbal beer were carefully evaluated and classified.

Keywords: herbal beer, organoleptic properties, check-all-that-apply.

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BFT P-13

Enhancing Strawberry Shelf Life with Essential Oil-Infused Edible Coating

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The objective of this study was to enhance the shelf life of strawberries using natural antimicrobial components applied to edible biofilms. To achieve this, a thin edible film composed of chitosan infused with essential oils from basil and clove was applied to the strawberries. The strawberries' shelf life was assessed through measurements of color change, weight loss, hardness using a texturometer, and visual inspection for mold presence.

Results showed that the coated strawberries exhibited a significant reduction in the number of infections compared to the uncoated strawberries, which began to deteriorate upon storage initiation. The incorporation of essential oils into the chitosan matrix improved the water barrier properties of the coatings, resulting in reduced respiration rates, preserved fruit color, and extended shelf life of the products. Notably, the basil and clove coatings demonstrated excellent mechanical and antimicrobial properties, effectively preventing the growth of mold on the strawberries and prolonging their preservation period.

Keywords: Strawberries shelf life, edible biofilm, antimicrobial components.

BFT P-14

Improving lycopene extraction from tomato skins through enzymatic treatment

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Lycopene, a potent antioxidant associated with remarkable health benefits, found in high concentrations in tomato skins, holds immense importance when extracted from waste materials. Utilizing tomato skins as a source of lycopene offers several benefits. Firstly, it helps reduce food waste and supports sustainable practices by utilizing a byproduct that would otherwise be discarded. Improving the extraction process contributes to minimizing environmental impact due to lowering the quantity of extraction solvents.

The research aimed to extract lycopene from tomato skins using *n*-hexane and compare three different methods: extraction with simple mixing, enzymatic treatment prior to extraction, and extraction with ultrasound. Skins from fresh tomatoes were piled, dried to constant mass at room temperature in the absence of light, and powdered using a food processor. In all three extraction methods, *n*-hexane was added in the ratio of 1:50 and the extraction was done at 25^{o}C. For the enzymatic treatment prior to extraction, which was carried out for 1 hour, commercial cellulolytic enzymes in concentration according to the specification were used. The extracts were obtained in triplicate. The lycopene was determined by measuring absorbance at 502 nm using a UV-VIS spectrophotometer and calculating the concentration from the extinction coefficient.

Enzymatic treatment of tomato skins was found to significantly improve the extraction of lycopene compared to the method with simple mixing and to the ultrasound-assisted method. This utilization of waste material showcases the potential of innovative approaches in maximizing the value of natural resources while promoting human well-being.

Keywords: Lycopene extraction, tomato skin, enzymatic pretreatment.

POL O-1

Evaluation of Overall Properties and Cytotoxicity of PEO/rGO Scaffolds for Potential Use in Tissue Engineering

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Electrospinning provides an attractive means of producing micro/nanoscale polymeric fibers because of its simplicity, reproducibility, and scale-up possibilities. Electrospun polymeric scaffolds mimic natural three-dimensional extracellular matrix (ECM), which is composed of complex fibrous structures with porous architectures, and thus, can be used to promote cell, tissue, and/or organ growth. The incorporation of 2D graphene/reduced graphene oxide (rGO) nanofillers into polymeric nanofibrous composites increase mechanical strength and electrical and thermal conductivities. In this study, polyethylene oxide (PEO) based scaffolds containing from 0.1 to 20 wt% rGO were obtained by electrospinning. Morphological, thermal, and electrical properties of the scaffolds were characterized by SEM, Raman spectroscopy, XRD, DSC and electrical measurements. The obtained results show a good dispersion of rGO at lower concentrations, and a drastic reduction in the fiber diameter with increasing nanofiller concentration up to 20 wt%. The morphology of the scaffolds was significantly affected by the presence of nanofiller. XRD and Raman analysis revealed delamination of the graphene layers, and exfoliation of rGO was detected for the samples with rGO concentration lower than 1 wt%. Significantly reduced electrical resistivity of the scaffolds was detected above the percolation threshold of nanofiller (7.4 wt% rGO). The biocompatibility of the scaffolds was tested by determination of the viability of epithelial colon cancer cells, and the results have shown an evident trend of increasing cell viability as rGO concentration increases.

Keywords: Nanofibrous scaffolds, Reduced graphene oxide, Polyethylene oxide, Electrospinning, Cytotoxicity

POL O-2

Synthesis, Spectroscopic and Thermal Characterization of New Polymeric Microspheres Based On Starch and Acrylic Monomers

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Starch belongs to the group of polysaccharides of plant origin. It is composed of glucose mers linked by α-glycosidic bonds and acts as an energy store in plants. Starch is a very interesting biopolymer, the possibilities for its use in sorption processes being created by its very interesting structure resulting from the presence of hydroxyl groups. The undoubted advantages of using starch are its very wide availability, low price and hydrophilic nature. What limits the use of starch is its poor mechanical resistance and partial solubility in hot water. The use of starch as an additive in the synthesis of polymeric microspheres can significantly improve the aforementioned properties and broaden the range of potential applications of this interesting biopolymer considerably.

The aim of this study was to synthesize polymeric microspheres based on dimethacrylate ethylene glycol, vinyl acetate and modified starch. Suspension polymerization was used to obtain the materials in spherical form. The reaction was carried out in an aqueous medium using poly(vinyl alcohol) as a suspension stabilizer. As a result of the polymerization, materials differing in starch functionality were obtained. A reference material without any chemical modification of starch was also obtained. The biosorbents were tested for their use as potential adsorbents of organic compounds.

Keywords: starch, suspension polymerization, polymeric microspheres, thermal properties, adsorption

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POL O-3

Protective Waterborne Coating Based on G/CNT Hybrid Filler

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The focus of this research work was to evaluate the potential of G/CNT based polymer composites to be used as protective coatings for outdoor application. In order to perform that, graphene/carbon nanotubes (G/CNT) based polymer composite was synthetized via miniemulsion polymerization. The weight ratio of G and CNT was 10:1, while the concentration of the G/CNT hybrid filler with respect to the monomers was 1 wt.%. The polymer composite was subjected to UV irradiation at accelerated aging conditions for 400 hours. The chemical and morphological changes were followed using Infrared spectroscopy with Furrier transformation and Scanning electron microscopy. The obtained results suggested that the composite filled with G/CNT hybrid did not suffer significant chemical or morphological changes after 400 h UV irradiation. After the irradiation, minor changes of the water contact angle and surface energy were observed in the case of the G/CNT/polymer composite. The water uptake of the composite was examined by immersion of the free-standing film in distillated water at ambient conditions. The mass change of the composite and the neat polymer was followed. After 300 hours of immersion the composite presented approximately 60% reduced water uptake compared to the neat polymer. The obtained results are demonstrating that G/CNT/polymer composite is promising material for application as protective coating for outdoor use.

Keywords: coatings, G/CNT hybrid, UV degradation, waterborne composites

POL O-4

Influence of The Type of Soft Segment on Selected Properties of Polyurethane Materials for Biomedical Applications

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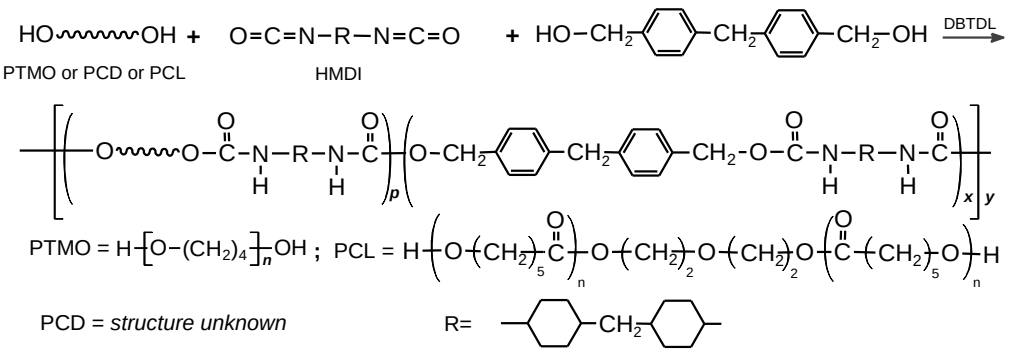
The purpose of this work was to study the effect of used (polyether, polyester and polycarbonate) soft segment on structure, morphology, crystallinity and some physicochemical, thermal as well as antibacterial activity of new type TPUs. These polymers were synthesized from poly(oxytetramethylene) diols (PTMO)s of $\overline{M}_n$ = 1000Da and $\overline{M}_n$ = 2000Da, poly(ε-caprolactone) diol (PCL) of $\overline{M}_n$ = 2000Da and polycarbonate diols (PCD)s of $\overline{M}_n$ = 1000Da and $\overline{M}_n$ = 2000Da as soft segments (SS), HMDI and unconventional chain extender [methylenedi(4,1-phenylene)]dimethanol (DMD).TPUs with hard-segment contents of 50 wt% were prepared by a one-step melt polymerization from DMD, HMDI and PTMO, PCD or PCL at the NCO/OH molar ratio of 1.05.



The resulting TPUs were high-molecular-mass materials with tensile strength in the range of 9.1–54.5 MPa and elongation at break in the range of 75–462%. Their glass-transition temperatures (T_gs) ranged from –73°C to 42°C.

Keywords: polyurethane; biomaterials; antimicrobial activity

POL O-5

The Effects of Component Changes Within Pultruded Epoxy Resin-Based Products

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The aim of this research paper is to determine the changes in mechanical properties of products when certain changes are made within the resin system that they are produced with.

With this goal in mind, the polymer composite materials[1] which were used in this research effort were obtained via pultrusion[2]. The products are cylindrical in shape and are mainly composed of epoxy resin[3] and glass fibers of 4800 tex. The fibers were initially threaded through a preform, followed by a wetting process by submerging them in a resin bath. Once the fibers were fully submerged and coated with resin, they were then pulled through a pultrusion die, heated at specific temperatures, in order to set the resin around the glass fibers, forming what is known as a polymer composite material.

The main aspects which were analyzed and taken note of during this research effort were changes that happened in the production process itself, more specifically the pultrusion of the product, keeping track of potential defects in the product, and the changes that were noticed within the mechanical properties of the products, more specifically, whether there was any improvement or loss in properties, compared to our current norm.

Keywords: epoxy resin, glass fibers, polymer composite, pultrusion, mechanical properties.

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POL P-1

Determination of Antimicrobial Activity Of Copper Activated Macroporous GMA Based Copolymer

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Macroporous (glycidyl methacrylate) GMA-based composite was synthesized via suspension polymerization in the presence of 2 wt. % magnetic nanoparticles and functionalized with triethylenetetramine. Copper was immobilized on composite by contacting modified copolymer with 0.1 M solution of CuCl2, at pH 5, and 25℃. The obtained composite was characterized by mercury porosimetry, Fourier transform infrared spectroscopy (FTIR) analysis and atomic force microscopy (AFM). GMA-based composites, due to their properties (size, porosity, etc.), and the presence of reactive epoxy group, have found a variety of applications as sorbents, enzyme supports, in biomedical applications, for metal and organic compounds sorption.1

The antimicrobial activity of the synthesized GMA/Cu copolymer against Staphylococcus aureus, Escherichia coli, Candida albicans and Aspergillus niger as representatives for Gram-positive bacteria, Gram-negative bacteria, yeast and fungi were investigated in this study.2 The copolymer displayed good antimicrobial activity against all analyzed microbes, which makes it a material that can be potentially used for biomedical (antibacterial and antifungal) applications.

Keywords: antimicrobial activity, copolymer, GMA, copper

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POL P-2

Optimizing Precipitation Conditions of BNC/Fe_3O_4 Composites

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Advancements in technology often rely on the development or enhancement of materials. Bacterial nanocellulose (BNC) has found diverse applications in fields such as biomedicine, ecology, and electronics, leading to increased interest in BNC-based composites[1,2]. Understanding the synthesis parameters that affect the crystal structure and morphology of these composites is crucial, as it directly impacts their functional properties. In this study, a composite material based on bacterial nanocellulose (BNC) and ferromagnetic particles Fe_3O_4 was investigated. BNC was obtained through the activity of bacteria during vinegar fermentation for 7 days in a suitable medium[3,4]. The research aimed to optimize the conditions for Fe_3O_4 precipitation by varying the standing time interval of BNC films in a neutral medium of distilled water after biosynthesis. Samples were allowed to stand for 7 days and 14 days before precipitation. The results showed that the samples standing for 14 days were not adequate, i.e., Fe_3O_4 precipitation was not achievable. The impact of different synthesis conditions was analyzed using SEM-EDS and FTIR methods.

Keywords: precipitation, bacterial nanocellulose, optimization

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POL P-3

Production of Thermochromic Poly(Methylmetacrylate/Butyl Acrylate) Based Coatings Via Miniemulsion Polymerization

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Energy consumption and its effects on the environment is a popular topic nowadays and it has triggered many experts to work hard on possible solutions. Probably the best and most cost-efficient outcomes are passive and energy-free technologies, such as smart windows with thermochromic properties.

A key material for the production of thermochromic varnishes is believed to be W-doped vanadium (IV) oxide (VO_2), due to its ability to undergo a phase transformation on a relatively low temperature. At this point VO_2 modulates from a fully transparent to reflective material[1]. Nonetheless, for the production of the thermochromic coatings, it was necessary to incorporate the VO_2 nanoparticles we synthesized, in acrylic latexes. In our research we used copolymer poly(methyl metacrylate/butyl acrylate), to ensure stabilization of the VO_2 nanoparticles and therefore prevent agglomeration, environmental protection, as well as, fabrication of transparent final products.[2] The glazing was then obtained via miniemulsion polymerization[3], which is well-known as an eco-friendly technique for the fabrication of the thermochromic smart coatings. The obtained glazing has several potential applications, such as building or car coatings.

Keywords: W-doped vanadium (IV) oxide, poly(methyl metacrylate/butyl acrylate), thermochromic, miniemulsion polymerization

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POL P-4

Determination of Parameters for Obtaining Resin Film for Production of Prepreg by Hotmelt Procedure

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Pre-impregnated material is used for high performance composite parts where control of resin content and the greatest versatility of material placement is required. The two main methods used for producing thermosetting prepregs are hot-melt and solvent-based impregnations. In solvent-based prepreg processing, the most important processing parameters are the temperature in the impregnation bath, the speed of the prepreg producing line and the tension on the fabric/fibers. In hot melt prepreg processing, prepreg properties depend on roller temperature, roller gap, rotation speed of the rollers in the coating unit, prepreg producing line speed and fabric/fibers tension.

The major benefit for this paper is the determination of parameters for obtaining resin film for production of prepreg by hotmelt procedure. A model has been developed to describe the resin content in thermoset prepreg as a function of the RAW film from Coating unit. Mathematical design experiments are used for the accurate selection of process parameters, providing precise control over the amount and thickness of the produced film.

The purpose of the study is to assess the applicability of full factorial experimental design in manufacturing of prepreg.

The production of the prepreg was conducted by applying 2^4 full factorial experimental design. Based on the obtained experimental data a regression equation was created which best describes the process. More from input variables have influence at RAW in hot melt prepreg processing.

Keywords: prepreg, experimental design, RAW, films.

POL P-5

Characterization of the Thermal Behaviour of a Paraffin-based Phase Change Material

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Phase change materials (PCMs) have attracted considerable attention in the field of heat storage due to their ability to absorb and release large amounts of latent heat during phase transitions. The integration of PCMs into building materials offers promising opportunities for improving the thermal performance and energy efficiency of buildings.[1]

This paper focuses on the PCM material as an advanced additive material to other building materials in energy efficient buildings. It consists of a polyurethane coating and paraffin wax filler. Thermal properties were measured by monitoring the mass change, evolved gas analysis, and the changes in heat flux (endothermic and exothermic effects) during several consecutive heating and cooling cycles. Knowing the measured thermal properties of the material is very important also from a fire safety point of view. The obtained results will help us to understand the behaviour of these materials when exposed to repetitive temperature changes or extreme temperature conditions.

Knowledge of the thermal behaviour of PCM contributes to performance optimization, material selection, system design and control, predictive modelling, and material development. This knowledge enables the effective use of PCMs in a wide range of applications that promote energy efficiency and sustainability with focus on use of fire safe materials.

Keywords: phase change materials, thermal properties, composite, building materials

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POL P-6

An Electrochemical Dopamine Sensor Based an a Cobalt(II) Coordination Polymer, $\{[Co(1,2\text{-}Bpe)_2(H_2O)_2]^{2+}\}_N$-Modified Electrode

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Dopamine (DA) is an important neurotransmitter for the function of the central nervous, renal, endocrine and cardiovascular systems. The development of a simple, selective and sensitive method to detect DA is necessary to monitor the level of DA in the human body. Many approaches have been developed for the detection of DA. The electrochemical analysis technique has received much attention as a reliable technique due to its simplicity and cost-effectiveness. Challenges to be overcome include the sensitivity and selectivity of modified electrodes for electrochemical detection of biological molecules in the presence of other interfering species. Various classes of materials have been used to construct electrochemical sensors, of which electrodes modified with porous coordination polymers have undergone explosive development. Cobalt-based coordination polymers are a promising electrochemical sensing material due to the superior electrocatalytic properties and variable valence of Co.

In this study, the electrochemical performance of the cobalt(II) coordination polymer, $\{[Co(1,2\text{-}bpe)_2(H_2O)_2]^{2+}\}_n$-modified glassy carbon (GC) electrode was analysed for the detection of DA using voltammetry techniques. It was shown that $\{[Co(1,2\text{-}bpe)_2(H_2O)_2]^{2+}\}_n$-modified GC electrode can be successfully used for the detection of dopamine.

Keywords: dopamine, cobalt(II) coordination polymer, modified glassy carbon electrode, electrochemical sensor

POL P-7

Interfacial Polarization and Dielectric Properties of Epoxy/Graphite Flakes Composites

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Dielectric properties of composites based on bisphenol-A-epoxy resin loaded with various content of graphite flakes (GF) have been studied. The dielectric permeability, tangent loss and ac conductivity have been examined in wide temperature (170 – 370 K) and frequency (20 Hz – 200 kHz) range. In composites loaded with GF flakes up to 10 wt.%, the dominant conduction mechanism is tunneling of electrons, while loading of 15 wt.% gives rise to electron conduction through direct contacts between fillers. Dielectric properties of composites are largely determined by the nature of the filler/matrix interface, the filler surface area and the inherent conductivity of the fillers. At low electric field frequencies, dominates so-called *interfacial* (or space charge) polarization due to accumulation of free charges at the interfaces between two phases (filler and matrix), which differ in electrical conductivity.Influence of the filler surface chemistry have been studied for composites loaded with 5 wt.% graphite flakes obtained: (i) under wet milling, without (GF) or with (GF-Tr100x) adding Triton-100x as a surfactant, or (ii) under dry milling in the presence of KOH (GF-KOH). The surface treatment with KOH notable increased dielectric constant of the epoxy/GF-KOH5 composite, keeping low tangent loss, comparable to the counterpart, the epoxy/GF5 composite.

Keywords: dielectric properties, composites, graphite nanosheets

POL P-8

The Synthesis and Photostability of Some New 1,8-Naphthalimide Derivative for Fluorescent Polymers

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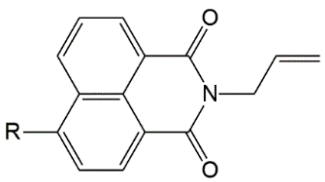
Fluorescent polymers are functional macromolecules with very important applications[1].One of the traditional methods for their synthesis is by copolymerization of traditional monomers with fluorescent monomers (unsaturated fluorescent dyes). Among them, naphthalimide derivatives are attracting much attention due to their excellent stability, photophysical, thermal, electrochemical and electroluminescence properties[2].

Three new polymerizable 1,8-naphthalimide fluorophores containing residue of an amino acid in the fourth position of the naphthalimide ring (Figure 1) have been synthesized. Their copolymers with methyl methacrylate were obtained.



R = -NHCH$_2$COOH (Dye 1)

-NHCH$_2$CH$_2$COOH (Dye 2)

-NHCHCOOH (Dye 3)
CH$_3$

Figure 1. Chemical structure of the investigated naphthalimide dyes

The optical properties of the prepared polymer films from the CIE Lab colour space have been examined. The photostability of the dyes and copolymers in solution of dimethylformamide have been investigated and an increase of the photostability of dyes included in polymer with 15-25 wt.% was observed.

Keywords: 1,8-naphthalimide dyes, fluorescent polymers, photostability

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POL P-9

Study of the Structure and Antimicrobial Properties of Composites based on (met)acrylates

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There has been a steady increase in demand for functional materials for applications not only in public buildings, but also in households. The common use of antibiotics has contributed to antibiotic resistance among many strains of bacteria and fungi. A solution to this problem may be the synthesis of composites with antimicrobial properties. The materials produced will be able to be used as coatings for cabinets, countertops, handles, handrails, or housings for medical equipment. The use of these innovative materials, due to their properties, will save time associated with systematic disinfection. It will also significantly reduce the spread and multiplication of fungi and bacteria on such protected surfaces.

The main objective of the study was to synthesize new composites based on bisphenol A dimethacrylate with the addition of active diluents such as 2-ethylhexyl acrylate, methyl methacrylate, 2-hydroxyethyl methacrylate and an additive in the form of benzethonium chloride as a filler, which has antimicrobial properties confirmed in the literature[1,2]. In order to confirm the chemical structure, ATR-FT/IR analysis of the obtained composites was performed. DSC studies were also carried out which made it possible to evaluate the thermodynamic effects occurring in the samples during heating. Modifying the diffusion-circulation and successive dilution methods, the antimicrobial properties of the composites were determined. The possibility of biofilm formation on the surface of the obtained materials was also analyzed.

Keywords: cross-linked polymer composites, methacrylates, biofilm formation, antimicrobial properties

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POL P-10

Synthesis of Lignin-Based Polymer Coatings by Miniemulsion Polymerization

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Lignin is natural polymer characteristic for its antioxidative and fire-retardant properties. In this research work lignin was used as filler for synthesis of polymer composites via in-situ miniemulsion polymerization. As monomer system were used methyl methacrylate and butyl acrylate in 50:50 weight ration. Lignin was added in 1wt%, 2 wt% and 3 wt% relative to monomers. The incorporation of lignin within the polymer matrix was confirmed by Infrared spectroscopy with Furrier transformation. The obtained composites were coated on commercial poly(urethane) – PU foam by dip coating in order to evaluate their fire-retardant ability. The successful coating of the PU foam with composite was investigated by determining the density, contact angle and surface energy of the neat PU, and PU coated with neat copolymer and with the different composites. From the obtained results was concluded that the density of the coated PU increased for approximately seven unitsand the contact angle decreased with an increase in the amount of lignin, i.e., the composite with 3 wt% lignin shows the lowest values for the contact angle (90.39°). The surface energy significantly increased by increasing the percentage of lignin in the samples, that is, compared to neat PU, the sample with 3 wt% lignin had three times higher surface energy. The flammability of the samples was investigated using UL-94 standard. The results suggested that the addition of lignin leads to decrement of the burning time of the PU foam, from 14.27s needed for burning the neat foam to 12s needed for the reinforcements with lignin.

Keywords: lignin, waterborne composites, flame-retardancy

POL P-11

Determination of the Optical Band Gap Energies of rGO/Metal Phthalocyanine/Polymer Nanocomposites

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Reduced graphene oxide/metal phthalocyanines (rGO/MPcs) are known for their outstanding optical properties. However, their synthesis is quite complicated and expensive with low material yields. Therefore, the aim of this research work was to investigate the option of placing this expensive material within polymer film and to study the optical properties of such polymer composites, in which low concentration of rGO/MPcs of 3wt.%. was added. rGO/MPcs hybrids were incorporated within polymer matrix by emulsion mixing technique. The optical properties of the obtained composite films were analyzed using ultraviolet – visible (UV-Vis) spectroscopy. It was observed that the absorbance of the composites was significantly increased compared to the neat polymer. From the UV-Vis spectra, the allowed and forbidden direct and indirect optical band gap energies were calculated. Compared to the neat polymer, the composites based on rGO/MPcs filler presented lower optical band gap energies. Specifically, the values of direct and indirect allowed band gap energies were reduced for 11.09% and 34.92%, respectively. The values of the direct and indirect forbidden band gap energies decreased for 25.81% and 39.80%, respectively. These results demonstrate the potential of the rGO/MPc/polymer composites to be used for development of optoelectronic devices.

Keywords: reduced graphene oxide, metal phthalocyanine, optical properties

POL P-12

Prediction of the Refractive Index of Polymers Using QSAR

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Polymers are a wide group of materials that have quite a wide range of applications due to their diverse properties. Their properties depend on their chemical structure, morphology, method of synthesis and processing. Since there are many variables that affect their characteristics, the characterization of these materials can be lengthy process.

In order to overcome this problem, quantitative structure–activity relationships (QSAR) modeling is a convenient tool for predicting the properties of polymeric materials.

Within this research, QSAR models were prepared for prediction of the refractive index of 100 polymers using theoretical descriptors. Descriptors were generated based on the monomer units of an appropriate number of polymers.

XLSTAT software packaging and several variable selection methods: stepwise, forward and best model with 2, 3 and 4 descriptors were used for model development. Several statistical parameters were used to test the quality of the developed QSAR models.

The correlation coefficients (R^2) and adjusted coefficient of correlation ($R^2_{adj.}$) for all QSAR models are > 0.9; mean squared error (MSE) < 0.0007; root mean square error (RMSE) < 0,003 and Fischer test (F-test)> 400, indicating that all models are statistically significant.

Keywords: QSAR, polymers, refractive index, descriptors

POL P-13

Nanocomposite PVDF/ZnO Piezoelectric Foams

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Poly(vinylidene difluoride), PVDF as a semi-crystalline polymer was widely investigated due to its ferro-, pyro- and piezoelectric behavior, combined with its excellent flexibility and mechanical properties[1]. The piezoelectric activity of this polymer is primarily dependent on the development of a specific crystal β-phase. Various procedures and post-treatments have been proposed for achieving a high β-phase content in the corresponding PVDF materials, such as spin coating, electrospinning and mechanical stretching[2]. The addition of various nanofillers in appropriate amounts in PVDF matrix, was found to act as nucleators promoting the crystallization into the desired β-phase[3].

In this work, PVDF/ZnO nanocomposites with ZnO nanoparticles content of 0.5, 1, 2, and 5 wt.%, were produced using a thermally induced phase separation method (TIPS), resulting in highly porous materials. The content of the developed beta crystal phase and the thermal properties of the produced foams were analyzed using FTIR, XRD, DSC and TGA analyses.

The results showed that the addition of ZnO nanoparticles induced high content of desired β-phase, enhancing the overall degree of crystallinity of the PVDF matrix.

Keywords: PVDF, ZnO, nanocomposites, piezoelectric foams

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POL P-14

Viscoelastic Properties of Polycaprolactone Based Polyurethane Networks

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Polyurethane networks (PUNs) based on hyperbranched polyesters (HBP), polycaprolactone (PCL), and isophorone diisocyanate were prepared.[1,2] PUNs consist of different content of hard (HS) and soft segments (SS). The impact of the HBP and the content of the SS on the structure and viscoelastic properties of the prepared PUNs were investigated. XRD analysis confirmed that PUNs with lower SS content were amorphous, while samples with the highest SS content had a certain degree of crystallinity. Viscoelastic properties of PUNs depend on the SS content and used HBP. These PUNs have potential application as coatings.

Keywords: polyurethane networks, polycaprolactone, viscoelastic properties

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POL P-15

Kinetic and Isotherm Non-Linear Study of Cr(VI) Sorption onto Amino-Modified Macroporous GMA Based Copolymer

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Hexavalent chromium, Cr(VI), is one of the most notorious pollutants with health and environmental impacts due to carcinogenic, teratogenic, and mutagenic effects on the human organism.[1] Therefore, treating wastewater containing Cr(VI) before discharge into the aquatic system is extremely necessary. In this study, the nonlinear regression method was used to determine the kinetic and isotherm parameters for Cr(VI) sorption from aqueous solution on hexamethylene diamine-modified macroporous copolymer based on glycidyl methacrylate (PGE-HMD).[2] The Avrami kinetic model provides the best correlation of the experimental data with R^2 = 0.994 and χ^2 = 0.004, while the Freundlich isotherm model best described the Cr(VI) sorption onto PGE-HMD copolymer indicating a heterogenous sorption process.

Keywords: glycidyl methacrylate, hexamethylene diamine, Cr(VI), kinetics, isotherms.

Acknowledgement: This research was financially supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Contract No. 451-03-47/2023-01/200026 and 451-03-47/2023-01/200135).

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POL P-16

Synthesis and Characterization of Magnetic Molecularly Imprinted Polymer for Aniline Recognition

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Aniline, the main representative of aromatic amines, occurs in a large number of industries, such as the production of textiles, plastics, medicines, pesticides, rubber, and varnishes.[1] Due to practicality and efficiency, a molecularly imprinted polymers (MIPs) can be used as sorbents for removing aniline.[2] In this study, magnetic molecularly imprinted polymer was synthesized via suspension copolymerization while characterization was performed by various methods in order to obtain an efficient sorbent for the aniline removal from an aqueous solution. Fourier transform infrared spectroscopy (FT-IR) confirmed characteristic vibrational bands which suggested successful synthesis of MIP, nitrogen gas adsorption-desorption measurements as well as mercury porosimetry have shown that the most dominant pores were mesopores, while scanning electron microscopy with energy dispersive X-ray spectroscopy (SEM-EDX) confirmed a 3D spherical porous structure with all the expected elements.

Keywords: molecularly imprinted polymers; MIPs; aniline; aromatic amine; characterization

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POL P-17

Investigation of the Effect of Introducing Siloxane Groups into the Polymer Chain on Selected Properties of Polyurethane Materials

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The aim of this work was the synthesis and characterization of new poly(thiourethane-urethanes) containing siloxane groups in their structure. The aliphatic diisocyanate, i.e. 4,4'-dicyclohexylmethane diisocyanate (HMDI), was used as raw materials, the soft segment was poly(ε-caprolactone) diol (PCL), while the chain extender was (methanediyl-dibenzene-1,4-diyl)dimethanethiol (DMT), synthesized at the Department of Polymer Chemistry of UMCS. Poly(dimethylsiloxane) (PDMS, Carbinol DMS-C16) was used as a modifier. Using the above substrates and the method of catalyzed polyaddition in the melt, a series of PURs with 50wt% of hard segments were obtained, in which 1, 2, 5, 10, 15 and 20wt% of PCL was replaced by PDMS.

For the synthesized PURs, the structure (by Fourier transform infrared spectroscopy) and some physicochemical properties (reduced viscosity, chemical resistance, density, contact angle values), thermal properties (by thermogravimetric

analysis (TG) and differential scanning calorimetry (DSC)), thermomechanical properties (DMA method) as well as Shore A/D hardness and mechanical properties were examined.

Keywords: polyurethane, siloxane groups, mechanical properties, thermal properties, physico-chemical properties

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CE O-1

Application of nuclear measurement technologies as tools to characterize mineral processing operations

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This work presents the application of radiation measurement technologies in the characterization of mineral processing operations. Two examples are showcased: the detection of feed flow rate imbalances in industrial flotation circuits[1], and the characterization of particle size distribution in automatic mineral-cutting devices. The feed pulp distribution was determined from mean residence time and residence time distribution data. Particle size distribution was measured by sampling the cutting devices (25 grams' samples) using coarse, intermediate, and fine-sized radiotracer particles. Radiotracer were injected into the feed and process streams and measured at various points of the circuit using nuclear instruments, allowing for non-invasive and real time detection.

Results show that in the rougher flotation stage, the feed flow is distributed evenly in lines 2 and 3 (approximately 38% of the flow goes to each line) and to a lesser extend towards line 4 (approximately 24%). In lines 1 and 2 of the scavenger stage, a greater percentage of the flow goes towards line 1 (approximately 59%) and a lesser percentage towards line 2 (41%). Line 6 of the rougher flotation is the fastest of the circuit (shortest residence time). In addition, the inlet mineral-cutting device of the rougher stage segregates particles with a bias for fine sizes (11.4% more fine sized particles than coarse ones).

This work is an example of how radiation measurement technologies can be applied to improve metal production and processes. Nuclear tools provide reliable information that can be used in combination with other metallurgical data to properly characterize industrial flotation circuits.

Keywords: radiotracers, nuclear measurements, metallurgical balance

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CE P-1

Glyceline as a Safe Purification Agent of Crude Biodiesel Produced from Inedible Oil Under Mild Conditions

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Natural deep eutectic solvent glyceline, constituted of choline chloride and glycerol in a 1:2 molar ratio, was tested for the purification of crude biodiesel. Low-acid value expired sunflower oil (0.61 mg KOH/g) was used as a feedstock for biodiesel production, prepared by the CaO-catalyzed oil methanolysis carried out at the methanol-to-oil molar ratio of 6:1, CaO amount 2.5% to oil, reaction temperature of 60 °C, stirring rate 900 min^{-1}, and reaction time of 4 h. The phases of the final reaction mixture were separated by centrifugation at 3500 rpm for 10 min. The upper layer was decanted into a flask and evaporated to constant mass under a vacuum at 40 °C using a rotary evaporator to remove unreacted methanol and other volatile impurities. Glyceline was mixed with the crude biodiesel at a 1:1 mass ratio in a two-necked glass flask equipped with a magnetic stirrer, thermometer, and

reflux condenser. The purification was conducted at 25 °C and a stirring rate of 700 rpm. The samples were taken after 60, 90, and 120 min, centrifuged, and cooled in a refrigerator at 4 °C to allow separation of glyceline and biodiesel phases. The purest biodiesel was obtained after 120 min and constituted 98.9% fatty acid methyl esters, 0.1% monoacylglycerols, 0.05% diacylglycerols, and 0.15% triacylglycerols. This study suggests glyceline as a safe, natural, and efficient solvent for purifying impure crude biodiesel under moderate conditions.

Keywords: biodiesel, deep eutectic solvent, glyceline, purification

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CE P-2

State of the Art Process and Process Controls for Production of Concentrates for Haemodialysis

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As the industrial requirements change at a rapid pace due to the drastic evolution of technology, the necessity of a more efficient manufacturing system arises more intensely than ever.

The concentrates for haemodialysis are alkaline and acidic solutions of inorganic salts with or without glucose and are used to treat patients with kidney insufficiency or failure (acute and chronic). The concentrates for haemodialysis in Alkaloid AD Skopje are manufactured in a closed system for production of concentrates for haemodialysis.[1] The system is operated automatically using PLC control system with SCADA application. This research work presents the performance qualification of the system for production of concentrates for haemodialysis at the defined ranges for the critical process parameters: temperature of solution, mixing time and dosed quantities of raw materials.[2,3]

According to the results from the performed tests on the production of the first validation batch on the system for production of concentrates for haemodialysis

it can be concluded that the process of production is capable of producing a product with reproducible quality in accordance with accepted quality criteria.

Keywords: manufacturing; process; parameters; SCADA; concentrates; haemodialysis.

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CE P-3

The influence of extraction techniques on the antioxidant potential of Chaga mushroom extracts

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Chaga (*Inonotus obliquus*, family Hymenochaetaceae) is a brownish-black parasitic mushroom that has more than 200 compounds, including polyphenols, polysaccharides, triterpenes, melanins, sterols, lignins, minerals, and vitamins. This study aimed to compare the efficiency of two extraction techniques, maceration and ultrasound-assisted extraction (UAE), during estimation of the antioxidant potential of chaga mushroom extracts. Based on the previous knowledge, 50% (v/v) ethanol was used as a solvent of choice for the extraction of antioxidants from chaga mushrooms due to its non-toxicity and environmental acceptability. Unlike 24 h-extraction at room temperature (22±2 °C) in the maceration, the UAE was carried out at 50 °C for 20 min. The liquid-to-solid ratio of 10 mL/g was the same in both cases. The ultrasonic bath with a frequency of 40 kHz and power of 150 W was applied for the production of ultrasonic waves. The total antioxidant and total flavonoid content were 3.27±0.24 mg gallic acid equivalent per 100 g of dry weight

(mg GAE/100 g d.w.) and 0.34±0.11 mg rutin equivalent per 100 g of dry weight (mg RE/100 g d.w.), *i.e.*,3.58±0.26 mg GAE/100 g d.w. and 0.83±0.23 mg RE/100 g d.w. in the extracts obtained using maceration and UAE, respectively. The obtained results indicated that the UAE is a more efficient extraction technique compared to maceration since for shorter extraction time is achieved better yield of antioxidants and flavonoids. The difference in the total flavonoid content was significant by comparing two extraction techniques. Because of that, further studies will be focused on the optimization extraction conditions for antioxidants from used plant material.

Keywords: chaga mushroom, maceration, ultrasound-assisted extraction, antioxidants.

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CE P-4

Engineering Multi-Core Flower-like Magnetic Nanoparticles with High Intrinsic Loss Power

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In the last decades, self-heating magnetic nanoparticles (MNPs) were engineered and investigated for magnetic hyperthermia (MH) and other applications such as catalysis and chemical synthesis. To be applied as nanoheaters for *in vivo* MH in cancer therapy, MNPs should have high heating efficiency expressed by Intrinsic Loss Power (*ILP*). One of the requirements for *in vivo* applications of MNPs is their non-toxicity. Hence, the most investigated MNPs for MH are based on iron oxides (magnetite and maghemite), which are non-toxic or slightly toxic. This work aimed to apply thepolyol-mediated protocol to engineer mixed $Zn_{1-x}Mn_xFe_2O_4$ and analyze their heating abilities. To obtain a series of $Zn_{1-x}Mn_xFe_2O_4$ samples with a specific nominal composition, the initial components, salts of Zn, Mn and Fe, were mixed in the appropriate stoichiometric ratio. The deviation from the target stoichiometry and the formation of samples with polyvalent ions and possibly vacancies were determined after ICP analysis. By analyzing TEM micrographs, we found that the change in the chemical composition does not affect

the morphology. Multicore flower-like nanostructures with a size in the range of 47-63 nm were obtained. They consist of many cores (crystallites or nanoparticles) with a size of ~10 nm. The samples show good colloidal stability, which is significant for their medical applications. Magnetization measurements in different DC fields showed that the samples are superparamagnetic at 300K and that the saturation magnetization values are in the range of ~59-73 emu/g. The hyperthermic efficiency of the synthesized samples was tested in an external ac field of 252 kHz and a field strength of 15.9 kA/m. Significantly different values were obtained for the *ILP* parameter (in units nHm^2/Kg): 5.77 ($Zn_{0.098}Mn_{0.447}Fe_{2.455}O_4$) > 3.22 ($Mn_{0.624}Fe_{2.376}O_4$) > 2.04 ($Zn_{0.182}Mn_{0.344}Fe_{2.474}O_4$) > 1.36 ($Zn_{0.309}Mn_{0.240}Fe_{2.451}O_4$) > 1.01 ($Zn_{0.394}Mn_{0.138}Fe_{2.468}O_4$) > 0.34 ($Zn_{0.640}Fe_{2.360}O_4$). To explain the values of the *ILP* parameter, additional research is required, which includes the analysis of the influence of local defects and cation distribution on the magnetism of the investigated nanostructures. Also, significantly high *ILP* values indicate that some samples can be selected and further tested for *in vitro/in vivo* applications.

Keywords: magnetic nanoparticles, polyol synthesis, nanoflowers, magnetic hyperthermia.

CE P-5

Radiolabeled Surface-modified Single-core $(Mg, Fe)_3O_4$ Colloidal Nanoparticles as Vectors in RadionuclideTherapy of Cancer

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A series of $Mg_xFe_{3-x}O_4$ (x=0, 0.1, 0.2, 0.4, 0.6, 0.8, and 1) magnetic nanoparticles (MNP) were synthesized by a two-step procedure, a co-precipitation method followed by hydrothermal treatment in a microwave field. The MNP are single-core, with crystallite size gradually decreasing from 15.5(3) up to 2.5(3) nm with an increase of$x$. TEM images show pseudospherical log-normally distributed particles with an average particle diameter of 19.8 nm and a polydispersity index of 26.1% for magnetite. The particle diameter decreases with the increase of magnesium (x) in the formula unit. The colloidal stability of MNP was achieved by their surface modification with citric acid (CA), oleic acid (OA) and polyethylene glycol (PEG). The cytotoxic activity of uncoated and coated $Mg_{0.6}Fe_{2.4}O_4$ was tested against target malignant cells (HeLa, LC174, A549) and normal MRC5 cells. The investigated MNP show moderate cytotoxic activity against the tested malignant cells *in vitro*. In contrast, MNP didn't show any significant cytotoxic effect against normal cells. HeLa cells exhibited the highest susceptibility among the malignant

cells. $Mg_{0.6}Fe_{2.4}O_4$@OA show good cytotoxic activity against all examined malignant cells, significantly higher than other tested MNP. It can be seen that $Mg_{0.6}Fe_{2.4}O_4$@PEG show a lower cytotoxic activity compared to all analyzed MNP. A direct method was used for labeling with radionuclide ^{90}Y, which involves incubation of MNP with ^{90}Y at a certain temperature and time. The labeling yield of the ^{90}Y-coated MNP was determined by analyzing the radiochemical purity after labeling. ^{90}Y-$Mg_{0.2}Fe_{2.8}O_4$@PEG were labeled in high yield (100%), while the yield for ^{90}Y-$Mg_{0.2}Fe_{2.8}O_4$@CA was 83%. *In vitro* stability of ^{90}Y-coated MNP at room temperature in physiological solution and human serum was monitored within 72 h from the moment of labeling by determining the radiochemical purity of ITLC-SG by radio chromatographic method. The stability of ^{90}Y-$Mg_{0.2}Fe_{2.8}O_4$@PEG was about 97%, while ^{90}Y-$Mg_{0.2}Fe_{2.8}O_4$@CA stability was 73%. The results of this study indicate that radiolabeled surface-modified $(Mg, Fe)_3O_4$ can be used as vectors in radionuclide therapy of malignant diseases.

Keywords: iron oxide, surface modification, cytotoxicity, radiolabeling, cancer nanotechnology.

TE P-1

Keratin Extraction from Domestic Coarse and Fine Wool and the Influence of Keratin Concentration on the Formation of Keratin/PEO Blend Nanofibres Electrospun Mats

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Significant amounts of unused and discarded wool from domestic sheep in BiH represent waste and unused of this significant natural fibre. Keratin, which is an integral part of wool, is a renewable biopolymer with biocompatibility and biodegradability properties. Due to the content of a large number of functional groups, regenerated keratin can be used to make highly absorbent nanofibers for medical, ecological protection and other technical textiles. In this work, by using mercaptoethanol keratin in the time from 6 hours to 48 hours was extracted from wool in a form of solution, from which keratin films were further prepared.

Extraction from domestic coarse and fine wool for 48 hours provides sufficient utilization of keratin. Further, from a solution of keratin films in conc. formic acid and aqueous polyethylene oxide (PEO) solution in ratios of wt. % 25/75, 50/50 and 75/25 were prepared spinning solutions for making nanofibers using a single-needle electrospinning process. Due to the poor mechanical characteristics of pure keratin poly(ethylene oxide) is add to keratin aqueous solutions to enhance electrospinnability due to the increase in the viscosity of the solution.The nanofibers spun from the keratin / polyethylene oxide solution on nozzle devices were characterized by SEM microscopy and FT-IR spectroscopy methods to determine the nanofiber morphology. The obtained keratin/PEO nanofibers in the ratio of wt. % 75/25 promote the formation of continuous nanofibers without defects.

Keywords: nanofiber, wool, keratin

TE P-2

Examination of the Wavelength Dependence of K/S Values for Samples Dyed in a Two-Component System

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The constant K/S represents the relationship between the concentration of the color and its emission value, where K is the absorption constant for a certain wavelength and S is the vertical regulation constant also for a certain wavelength (only for the material, depending on the coloring of textiles, leather or paper). As early as 1931. Kubelka and Munk came to the mathematical dependence of these quantities (K and S) as well the quantity G, which is the absorption measure of color for a certain wavelength, as well as the proportionality constant B depending on the color, as well as the concentration of the color (C).In this test, polyester knit fabric (100% PES) was used as a substrate. Dyeing of polyester knit fabric was carried out by the exhaustion process at elevated temperature and under pressure (HT process). The dyeing fleet consists of a certain amount of TERASIL ROT W - 4BS and TERASIL GELB 4G disperse paints. For concentrations of 1.00% sample (1) and 4.00% for sample (2). When obtaining measurement results, the metric program "Super MATCH 6 supplement" was used, in which spectrophotometry is

used as an instrumental method. As a relatively new spectrophotometric technique, reflectometry is included, which is used to monitor the fabric dyeing process.[1] Measurements and processing of the results showed that sample (1) has a maximum K/S value of 17.31 and sample (2) has of 25.56 at a wavelength of 460 nm. The results of this research show that the staining matric provides the possibility of a quick and accurate calculation of the K/S constant for the tested samples.

Keywords: polyester knitwear, dispersed colors, reflection spectrophotometry

Acknowledgment: This work was supported by the Republic of Serbia - Ministry of Science and Technological Development, Program for financing scientific research work, number 451-03-47/2023- 01/200124.

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TE P-3

The Influence of the Characteristics of Knitwear in Parts of Classic Socks on Some Usage Properties

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Socks are an essential item of everyday clothing, and therefore, it is crucial that they are comfortable, long-lasting and affordable. In the study, five different cotton type socks were analyzed based on their raw material composition and structure. Samples of right-left knitted fabrics from the foot, heel and toes were used (on which the basic characteristics were checked: linear density yarn, density loop, loop length, surface mass, thickness, etc.), which were subjected to measurements of air permeability and abrasion resistance using methods in accordance with EN ISO and ISO standards. The results showed that the air permeability is higher in sock samples with a lower percentage of cotton fibers, as well as samples with lower densities and thicknesses compared to the others. In terms of abrasion resistance, samples with a lower percentage of cotton and a higher percentage of lycra exhibited greater changes in appearance (after 5000 cycles, the rating was 1-2). The samples of socks with polyamide fibers proved to be more resistant, as well as those with higher densities (rating 2-3). This research can be beneficial for companies and researchers involved in the design and production of socks, as it

investigates key factors in enhancing sock performance and provide additional information for potential future improvements.

Keywords: socks, right-left knitted fabric, air permeability, abrasion resistance.

Acknowledgement: Republic of Serbia - Ministry of Education, Science and Technological Development, Program for financing scientific research work, number 451-03-47/2023-01/200133.

TE P-4

Multifunctional cotton Impregnated with Multilayer Chitosan/Lignin Nanocoating and Ag Nanoparticles

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The demand for clothes with antimicrobial and UV protective properties is continually growing. In an attempt to develop a simple and efficient treatment for cotton fabrics, layer-by-layer deposition of chitosan and magnesium lignosulfonate followed by in situ synthesis of Ag nanoparticles (NPs) was performed. Magnesium lignosulfonate acts as a stabilizing agent and UV blocker while $NaBH_4$ is applied as a reducing agent. The influence of the number of bilayers (4 and 12) and the initial

concentration of $AgNO_3$ solution (10 mM and 20 mM) on UV protection factor (UPF) and antimicrobial activity against Gram-negative bacteria *Escherichia coli*, Gram-positive bacteria *Staphylococcus aureus* and yeast *Candida albicans* was studied. The presence of nanocoating on the surface of cotton fabric is confirmed by FTIR and XPS analyses. XPS and FESEM analyses reveal a successful synthesis of Ag NPs on the surface of cotton fibers with an average dimension of 35 nm. A four bilayer coating is sufficient to reach maximum 50+ UV protection. Maximum reduction of all investigated microorganisms is achieved with 12 bilayers and application of 20 mM $AgNO_3$ solution.

Keywords: cotton, chitosan/lignin nanocoatings, Ag nanoparticles, antimicrobial activity, UV protection

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TE P-5

Sodium Periodate Oxidation of Raw Jute Fabric – A Novel Approach for Tuning the Jute Structure and Properties

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This investigation represents a novel approach for tuning the jute structure and properties using sodium periodate ($NaIO_4$) oxidation. The obtained results revealed that the jute fabrics exhibited an increase in the aldehyde group content (for up to 114.7%) with an increase in the $NaIO_4$ concentration and/or oxidation duration. Due to the decline in the cellulose lateral order index (LOI) and fiber crystallinity index after oxidation, it can be concluded that jute crystalline areas are affected by sodium periodate oxidation. Both mentioned parameters are responsible for fabric mechanical properties, so, it was expected that by decreasing the LOI and jute fibers' crystallinity, their maximum force and stiffness will decrease too. This behavior is also attributed to the fiber damage, which is the most pronounced for the fabric treated with 0.4% $NaIO_4$ for 120 min. Besides slightly deteriorated

mechanical properties, fabrics oxidized with 0.2% $NaIO_4$ for 60 or 120 min and with 0.4% $NaIO_4$ for 60 min showed lower mass loss (6.78-12.22%) after 750 abrasion cycles compared to the raw jute (18.94%). Furthermore, oxidation led to obtaining fabrics with enhanced moisture sorption and water retention power that are inversely proportional to the fiber crystallinity. Due to the opportunity for tuning fiber structure and properties oxidized fabrics can be considered for various applications such as geo-prebiotic supports for cyanobacteria growth in biocarpet engineering, i.e., to promote a sustainable relationship between the microbiota and abiotic constituents on the degraded land surface.

Keywords: jute, sodium periodate, fiber structure, properties

Acknowledgement: This research was supported by the Science Fund of the Republic of Serbia, #7726976, Integrated Strategy for Rehabilitation of Disturbed Land Surfaces and Control of Air Pollution–RECAP and Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Contract No. 451-03-47/2023-01/200287, 451-03-47/2023-01/200135, 451-03-47/2023-01/200026).

EDU O-1

Computer Generated and Graded Online Physical Chemistry Exam

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During the COVID-19 pandemic circumstances, not only was the teaching process at universities suddenly converted to online teaching and learning, but examinations also had to be conducted online in most cases, although it was not always possible to ensure strict control.

In order to spare students, the supervision of two or more cameras focused on each student, or to expose them to the stress associated with timed remote examinations,[1] and yet ensure satisfactory exam proctoring[2] of written examinations in physical chemistry involving calculations, we prepared examinations in the Moodle environment with automatic grading. The numerical tasks in these exams contained the same text, but students were given randomly selected numbers in these tasks. Based on the given numbers, the correct numerical results were

calculated in the Moodle environment and compared with the students' answers, allowing some tolerance for the numerical result.

From the anonymous students' feedback, we can conclude that such an exam was conducted quite successfully without strict supervision and there were no critical problems related to the violation of the integrity of the exam. Most of the students' complaints were related to factors beyond the control of the examiners, while there is possible to improve such examinations in the area of controllable parameters.

Keywords: moodle, calculations, random choice

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EDU P-1

Identification of Difficulties and Misconceptions in the Study of Organic Chemistry in High School

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In much of educational research, organic chemistry is considered as one of the more difficult areas of chemistry. It is due to the amount of content to be taught, but mostly to its complexity, and consequently to the misconceptions in the basic concepts that might arise. Among the most difficult topics in organic chemistry are those concerning the concepts of stereochemistry, such as isomerism, and the concept of aromaticity of organic molecules. Stereochemistry is considered a difficult topic to study because it requires students to have the ability to mentally visualize the three-dimensional structures of organic molecules and accurately represent them with formulas.

In order to determine the specific difficulties that students face in understanding the spatial arrangement of atoms and the stereochemistry of organic

molecules, research was conducted using an anonymous test as a quantitative research method. The test was distributed to 194 students from three secondary schools in the Republic of Macedonia, where classes were conducted in different languages of instruction, namely Macedonian and Albanian.

The students' answers on the test were analyzed, and the results obtained revealed several difficulties and misconceptions in understanding stereochemistry concepts. It was found that most of the students cannot determine whether a cyclic molecule is planar or three-dimensional, based on a written structural formula, and consequently to determine its aromaticity according to Huckel's rule. The students do not identify the existence of isomerism when four different groups are connecter to two double-bonded carbon atoms. Therefore, it can be concluded that they do not clearly understand the restricted rotation around double bond, and the geometric isomerism, in general. In addition, some of the students think that only one type of isomerism can be present in a molecule. Most of the students are able to identify the most stable conformation based on Newman's formulas.

All these results point out that new methods of teaching stereochemistry must be introduce in the secondary school education, such as three-dimensional physical models, IT technology etc.

Keywords: education, organic chemistry, stereochemistry, isomerism, misconceptions

EDU P-2
Implementation of New Methodology of Testing of Body Cooling Systems into the Education Process

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The present research was conducted in order to evaluate possibility of implementation of new methodology of testing of body cooling systems into the education process at Military Academy in Belgrade. According to previous evaluation of personal body cooling systems based on different technologies and its effects on human's physiological suitability during exertional heat stress in hot

environment in the laboratory conditions, performed results are based on realized tests in especially unique designed testing ground. Ten healthy and prepared test subjects were subjected to exertional heat stress test consisted of specific working activities in hot environment. The students had significant roles in the collection and processing of data. Tests were performed with and without cooling system. As a physiological strain indicator the following parameters have been determined: mean skin temperature, auditive temperature, tympanic temperature, heart rate and sweat rate. Results confirmed that cooling vest worn under the protective clothes was able to attenuate the physiological strain levels during exercise, when compared to identical exposure without the cooling system. The lessons were recorded, uploaded to the advanced distance learning platform and are actively used in the teaching process.

Keywords: impermeable protective clothing, heat stress, cooling vest, strain indicators.

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EDU P-3

The importance of Quality, Safety and Environmental Aspects in Chemical Industry

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Pharmaceutical Chemical Cosmetic Industry ALKALOID AD Skopje plays an important role in the circular economy. One part of this industry encompasses production of a wide range of chemicals intended for laboratory, industry and consumer use, products used for agriculture production, cleaning agents and disinfectants.

Maintaining quality is essential to delivering quality, safe and efficient products, enhancing customer satisfaction and establishing a positive industry reputation, while optimizing operational efficiency and competitiveness in the market.[1]

Ensuring safety and health is paramount, mitigating risks, protecting workers and preventing accidents, while maintaining compliance and fostering a culture of responsibility.[2] The production and use of chemicals have impacts on the environment. By embracing sustainable practices such as green chemistry, waste reduction, management of environmental aspects, energy efficiency and responsible waste management, ALKALOID AD Skopje reduces its environmental footprint.[3]

ALKALOID AD Skopje is able to foster innovation, build trust, and contribute to a sustainable future by emphasizing quality, safety and environmental aspects.

Keywords: quality, safety, environmental, chemical, industry

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EDU P-4

Problem-Solving with Python: Modeling of Lanthanide Shift Reagent Complexes

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Herein we describe a program written in Python programming language that employs a simple complete-search algorithm for determining the geometry of a lanthanide-substrate (LS) complex. The program can be used as a work project in an introductory programming course for chemistry students to illustrate the concepts such as decision-making, repetition, functions, lists, file reading, and data visualization. Students are presented with the problem to determine the position of a lanthanide ion in an LS complex by using the results of the NMR titration experiment of menthol with $Eu(fod)_3$. The problem is subdivided into several stages: 1) assignment of the ^1H NMR shifts in the menthol molecule; 2) determination of $\Delta\delta$ values for each proton; 3) molecular modeling of menthol; 4)

writing a Python program that would calculate the Eu position which gives the best correlation with the experimental data. This project should not only improve the coding and problem-solving skills of the students but also offer them an opportunity to practice their NMR elucidation technique.

Keywords: Graduate Education, Organic Chemistry, Computer-Based Learning, Problem Solving, Computational Chemistry, NMR Spectroscopy

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EDU P-5

Analysis of the Application of Information Technologies in Teaching

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In the last decade, the rapid and fast development of information exchange, online communication technologies (ICT) and also multimedia content has definitely improved and modernized the quality of education worldwide. The needs for changes in all levels of education experienced an expansion, especially in the beginning of global pandemic in 2020, after the confirmation of the presence of the COVID-19 virus.[1,2] The goal of this paper includes new knowledges about the use of Google Classroom in classes at The Academy of Applied Technical Studies Belgrade on the subject of Chemistry, as well as examining the effect of distance learning on the passing of students in the aforementioned exam in the June term. In addition, the attitudes and opinions of teachers and students regarding the use of new technologies in teaching were examined. Results were obtained by analysis of data from the Faculty Information System and by the conducted questionary survey of students and teachers.

The obtained research results indicate that a greater number of students actively followed online classes and regularly did homework (78 - 85 %) compared to the traditional way of teaching (62 - 72 %). In addition, the passing rate of students in the June deadline increased from 31-36% (2018 and 2019) to 63-68% (2020 and 2021). Awareness has been developed among teachers and students about the advantages that ICT resources bring in teaching. According to the conducted research, teachers who are more interested in working with the use of ICT are mostly younger teachers and associates.

Keywords: information and communication technologies, online teaching, education

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