BOOK of ABSTRACTS

27th Congress of Chemists and Technologists of Macedonia

25-28 9 2024 OHRID, RN MACEDONIA

Сојуз на хемичарите и технолозите на Македонија

Society of Chemists and Technologists of Macedonia

27th Congress of SCTM

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25–28 September 2024

Metropol Lake Resort

Ohrid, N. Macedonia

Skopje, 2024

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The 27th Congress of SCTM is a EuChemS European Chemical Society **recognized event.**

Dear Esteemed Colleagues and Participants,

We are pleased to present the Book of Abstracts for the 27th Congress of the Society of Chemists and Technologists of Macedonia. Like our previous congresses over the past two decades, this event takes place in the cradle of Slavic literacy—a region with a rich history of intellectual accomplishments. We trust that the heritage, along with the beauty of Lake Ohrid and the city itself, will not only make your stay enjoyable but also serve as an added source of inspiration for your own work.

The SCTM congresses have grown into a prominent platform for regional researchers from all fields of chemistry and chemical engineering. We are honored to welcome plenary and invited speakers not only from Macedonia but also from countries like Czechia, Denmark, Italy, Serbia, Spain, and the United Kingdom. In addition, we are proud to feature a wide range of oral and poster presentations from researchers representing Austria, Azerbaijan, Bosnia and Herzegovina, Bulgaria, Croatia, Germany, Greece, Italy, Kosovo, Montenegro, Poland, Serbia, Slovenia, Spain, Romania, and Russia. With nearly 200 presentations from 550 authors and co-authors, it is especially gratifying to see many attendees returning as regular participants.

We hope this Book of Abstracts serves as both a source of inspiration and a record of the exceptional work presented at the 27th SCTM Congress. Let's use this opportunity to celebrate not only our achievements but also our resilience, determination, and steadfast commitment to advancing knowledge. Together, we can overcome challenges and, through our collective efforts, continue to drive innovations that make a positive impact on the world.

We extend our heartfelt gratitude to Prof. Jadranka Blaževska Gilev and Prof. Biljana Angjuševa for once again taking on the challenging task of organizing this year's congress. Their tireless efforts and dedication ensured the event's success. We also wish to thank all the members of the scientific and organizational committees who worked tirelessly behind the scenes, with special recognition to Assoc. Prof. Vojo Jovanov, Marija Prosheva and Despina Kostadinova for their management of the website, Book of Abstracts, and other essential tasks.

Our thanks also go to the reviewers and participants whose contributions have been vital to the success of this Congress. Your commitment to the scientific mission emphasizes the value of collaboration, especially during uncertain times. It is through the exchange of ideas, sharing of knowledge, and building of connections that we strengthen our community and advance our fields. Lastly, we express our sincere gratitude to the sponsors, acknowledged at the end of this book, for their generous support.

Prof. Zoran Zdravkovski, president

Society of Chemists and Technologists of Macedonia

CXTM

CONTENT

PLENARY LECTURES

INVITED LECTURES

ORAL AND POSTER PRESENTATIONS

ANALYTICAL AND ENVIRONMENTAL CHEMISTRY

ORAL PRESENTATIONS

POSTER PRESENTATIONS

BIOTECHNOLOGY AND FOOD TECHNOLOGY

ORAL PRESENTATIONS

POSTER PRESENTATIONS

CHEMICAL ENGINEERING

ORAL PRESENTATIONS

POSTER PRESENTATIONS

ORGANIC CHEMISTRY, BIOCHEMISTRY AND PHARMACEUTICAL CHEMISTRY

ORAL PRESENTATIONS

POSTER PRESENTATIONS

POLYMERS AND POLYMER MATERIALS

ORAL PRESENTATIONS

POSTER PRESENTATIONS

PHYSICAL, STRUCTURAL CHEMISTRY, SPECTROSCOPY AND ELECTROCHEMISTRY

ORAL PRESENTATIONS

PLENARY AND INVITED LECTURES

PL-1

Graphene-Based Nanomaterials for Water Purification

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We explored the physical and chemical properties of graphene oxide (GO) treated at low temperatures, without strong reductant agents or controlled environments. I-V measurements provided insights, showing that the resistance of GO was at its lowest (1.29×10^5 Ω) after 120 h of drying time. The latter can be attributed to the effective removal of oxygen functional groups. Our findings can be used to tailor the use of GO in various contexts by determining the optimal temperature and duration for a specific application.

From water purification perspective, we have demonstrated the effective and efficient removal of cationic pollutants, i.e., methylene blue (MB) and mercury-(II) (Hg-(II)) [1-3], from aqueous solutions using an eco-friendly and as-made reduced graphene oxide (rGO). The adsorbent material shows fast adsorption with saturation capacity of 121.95 mg g^{-1} and 109.49 mg g^{-1} at 298 K, suggesting a good affinity for MB molecules and Hg(II) ions. These results are superior to those recently reported for other graphene-based benchmark materials.

By means of several chemical physics analyses, we have also shown that rGO keeps a good efficiency over a wide range of initial cationic pollutant concentrations. Our results allowed us to conclude that the MB-rGO and Hg(II)-rGO adsorption interaction follows a combined physisorption-chemisorption process, due to the fact that the Gibbs free energy was found from -22.75 to -25.16 kJ mol-1 for MB and from -39.84 to -32.97 kJ mol-1 for Hg(II).

Keywords: graphene, pollutants

Acknowledgment: This work was supported by project funded by Romania's National Recovery a Resilience Plan (PNRR), component C9. Support for the private sector, research, development and innovation "I8. Development of a program to attract highly specialised human resources from abroad in research, development and innovation activities", entitled "Composite materials for the applications in the water management field", ID - 11/ 26.07.2023, contract number 760270/26.03.2024.

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PL-2

Emulsifier-Free Waterborne (Meth)Acrylic Formulations Enhanced with Zwitterionic Monomers

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Waterborne polymer, crucial for various industrial applications, are usually produced by emulsion polymerization relying on emulsifiers to provide colloidal stability. However, the migration of these emulsifiers during film formation not only affects the performance of the resulting polymer films but also poses environmental risks due to surfactant leakage. Therefore, novel strategies for synthesis of emulsifier-free polymeric dispersions are highly welcomed.

In light of this, we have developed an innovative approach based on use of zwitterionic monomers (ZM) in small quantity (1-5 wt%) to ensure colloidal stability of industrially relevant waterborne (meth)acrylic polymers, produced by seeded semi-continuous emulsion polymerization are shown. Fundamentals of the incorporation of highly hydrophilic ZM onto hydrophobic methyl methacrylate/*n*-butyl acrylate (MMA/BA) polymer particles and formation of in-situ stabilizing units are discussed. The main challenge is to avoid aqueous phase polymerization of ZM, hence, to achieve its high incorporation onto hydrophobic MMA/BA particles, as a key requirement for colloidal stabilization. The success of these processes relies on the careful selection of ZM type and quantity, initiator type, and ionic strength within the dispersion.

The outcome is the production of high-solids content polymer latex with exceptional colloidal stability, resulting in transparent coating films. The inherent properties of ZM confer unusual colloidal stability to the polymer dispersion even at high ionic strength, attributed to the anti-polyelectrolyte behavior of polymer chains containing ZM. Furthermore, the dispersions permanent stable through multiple cycles of freeze-thaw.

Owing to the rigid nature of the multiple ionic groups of ZM, significant improvements in the mechanical properties of the resulting coating films are attained, along with simultaneous anti-fouling protection. Moreover, the balanced number of opposite charges confer ionic neutrality and enhance hydrophobicity, leading to improved water resistance and reduced humidity permeation, thus paving the way for potent barrier coatings applications.

Keywords: emulsifier-free polymer dispersions; emulsion polymerization; (meth)acrylates; coatings

PL-3

Carboxylates Platform as Efficient Alternative to Sugar Platform when Targeting at Microbial Oils Production

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Oleochemicals, which market size is projected to significantly increase in the coming years, are mainly produced from animal fats and vegetable oil. To fulfill their increasing demand, microbial oils emerge as a promising candidate. However, obtaining low-cost microbial oils is crucial for achieving a successful expansion of green chemistry. Short-chain fatty acids (SCFAs) are carboxylates (C2 to C6) obtained in a shortened anaerobic digestion process of organic residues that have been recently shown to be good alternative carbon sources for a cost-effective microbial oil production. The maximum concentration of SCFAs that yeasts can stand without compromising process yields still remains unknown. Besides, the inhibitory effect of SCFAs has been reported to not only depend on the SCFAs concentration but also on the acid distribution profile in the media[1]. This talk will give an overview of the recent advances on the use of SCFAs for microbial oils production to get lipid content in yeast cells from 40% to 80% w/w[2]. The critical points for the process such as SCFAs concentration and profile, C:N ratio, phosphate limitation and strain background will be discussed[1-3]. This will open a new perspective for the utilization of SCFAs derived from low-cost substrates as alternative to the sugar platform to favor the economic viability of the lipid production process.

Keywords: microbial oils, short-chain fatty acids, oleaginous.

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PL-4

Cellulose: from Natural to Novel Cellulose-based Functional Materials

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Cellulose, the structural material of all plants, is the most abundant natural and renewable polymer. With its fascinating structure and many attractive properties such as renewability, biodegradability, biocompatibility, mechanical robustness (high specific strength, flexibility during processing, high specific stiffness, etc.), hydrophilicity, and broad chemical-modifying capacity, cellulose has attracted increased attention from both the industrial and scientific communities.

The current cellulose research is directed towards an advanced understanding and application of this most important bioresource. Emphasis is placed on cellulose functionalization and its conversion into novel high-performance cellulose materials with tailored properties such as fibers, films, membranes, composites, and micro- and nanofibrilated cellulose-based materials. Various physical and chemical treatments (ultrasound and plasma treatment, selective ($NaIO_4$ and 2,2,6,6-tetramethylpiperidine-1-oxyl-TEMPO radical) and non-selective (H_2O_2 and $KMnO_4$) oxidation, and their combinations) were used to adjust cellulose properties for different purposes.

Cellulose, bearing three hydroxyl groups per anhydroglucose unit, was easily functionalized, hydroxyl groups were activated or new moieties introduced. New functionalities were either used directly because of their special properties (e.g. hydrophilization or hydrophobization) or served as reactive “chemical hooks” for further chemical modification. Highly functionalized cellulosic products take advantage of the intrinsic properties of the polymer in combination with modern modifying reagents.

Keywords: cellulose functionalization, properties, application

Acknowledgment: This work was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Contract No. 451-03-65/2024-03/200135).

IL-1

Johnson Matthey Catalysis Research: How Novel Science and Characterisation Supports Technology

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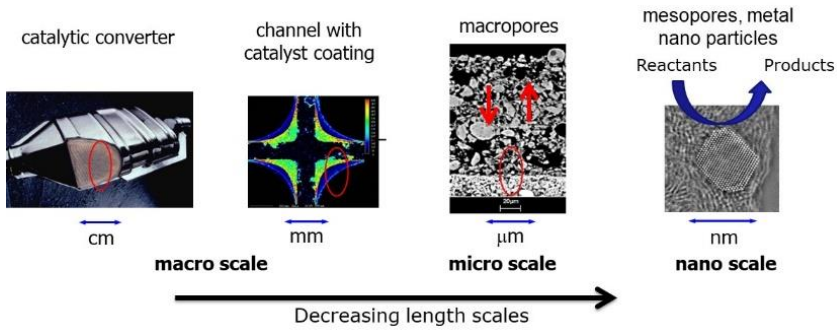
In this lecture I will give a range of examples of how Johnson Matthey applies advanced characterisation methods to bring greater understanding to our catalyst products and processes. Optimising our catalyst technology is a multi-scale problem, and therefore the examples will also cover a range of scales.



Much of the focus will be on catalysts for tackling emissions, especially for gasoline and diesel vehicles. This is still a highly relevant topic across the globe, with the internal combustion engine forecast to remain the foremost powertrain technology looking well into the future, while alternative drivetrains are being introduced alongside.

Some examples of where we have applied novel research will include:

- magnetic resonance imaging to visualise and understand exhaust gas hydrodynamics in particulate filter devices,
- spatially resolved capillary inlet mass spectrometry (Spaci-MS) for measuring concentration profiles and temperatures in gasoline three-way catalysts,
- neutron methods for i) measuring molecular diffusion in zeolite materials of relevance to the catalysis industry, and ii) for imaging adsorption/absorption of H_2 within a Pd/C packed catalyst bed in a stainless-steel reactor.

Keywords: catalysis, MRI, neutron scattering, neutron imaging, spacial resolution

IL-2

How to Attract EU Funds for Funding Your Innovative Research

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Horizon Europe is one of the biggest programme for funding research and innovation[1]. The programme is open in the period from 2021 to 2027 and more than 96 billions of EUR are provided for researchers from whole Europe and even outside of Europe. The structure of programme in three pillars and horizontal programme WIDERA will be presented. Examples of ongoing projects in the field of innovative technologies in textile electronics, food-based electronics, microfluidics and their application in biomedicine will be shown. What are the key aspects of a winning project proposal will be emphasized. Special focus will be on open calls for which institutions from Western Balkan countries can apply.

Keywords: Horizon Europe, Research and Innovation, MSCA, WIDERA

Acknowledgment: Acknowledgment to EC and Publication office of the European Union

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IL-3
Building Smarter

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The build environment sector is responsible for more than 1/3 of the global emissions of greenhouse gases. An important factor in this is that common civil engineering materials are used in huge amounts, and accordingly their production sums up to a high embodied energy and a high related carbon emission. Though concrete, for example, involves a release of only 0.13 kg CO_2/kg, it is on the bottom line responsible for about 7% of all non-natural CO_2-release since it is produced in annual amounts of gigatons – second to no other material in the world[1].

A suggested urgent pathway to decarbonize the built environment include improvement of building materials, and this transformation may involve the use of "smart materials" – materials which based on an external stimulus produce a designed, significant response[2]. Smart materials are quite opposite to building materials such as concrete, wood and fired bricks. Due to their production volume building materials have to be very low price and for the same reason they are often relatively ill-defined. Smart materials, however, are less cost constrained and may be delicately designed to possess very specific, extreme properties. The opposite features of smart materials and building materials make them a good match. With the use of a small amount of smart materials it is possible to modify building structures and building materials in a desired direction; low price, building materials become smart themselves. Many very different examples of this can be found in practice, and even more in the scientific literature[2]. This includes phase change materials for heat storage, superabsorbent polymers for moisture control, and memory metal for structures with a seismic load.

Undoubtedly, the future will being many new innovations of such kinds. The depletion of raw material sources, the need for recycling, and the tightening energy constraints will push for the appearance and use of more smart materials technologies within civil engineering.

Keywords: Construction materials, smart materials

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IL-4

Critical Importance of Environmental Data and Analysis for Addressing the Triple Planetary Crisis

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Chemical pollution from manmade or refined chemical substances, mixtures and undesired by-products as well as from their abiotic and metabolic transformation products is one of the major recognized societal challenges related directly or indirectly to the UN SDGs. The range of global chemical pollution and waste is making this environmental and health threat one of the areas referred to as the "Triple Crises".

This presentation will show how can researchers and data produced in the Central and Eastern Europe contribute effectively to make positive changes for state of protection of environment and humans. Expansion of the list of chemicals of concern also brings additional regulatory needs and requires more scientific information, including on exposure. Further activities will be presented such as the European Initiative for Human Biomonitoring (HBM4EU) aimed at harmonizing the accumulated experience, EU Chemical Strategy for Sustainability and a science-to-policy Partnership on assessment of risks of chemicals (PARC) with the aim to develop and endorse new methods for new generation risk assessment.

Further, contribution of the research infrastructure networks targeting environment and health i.e. EIRENE will be presented and discussed. Their linkages to existing global arrangements protecting human health and the environment will be also showcased.

Keywords: harmonization, EU Partnerships, human biomonitoring, research infrastructures, EIRENE

IL-5

The Secrets Behind the Eyes of Mona Lisa

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Forgery is a significant challenge in the art world, particularly concerning ancient artifacts, historical priceless works of art, and masterpieces. Today, despite the expertise of art professionals, the challenges connected with art restoration, attribution, and the detection of forgeries are growing in significance and may require the application of modern scientific methodologies. Thus, there is a rising imperative to use non-destructive analytical methods and tools capable of accurately distinguishing original works of art from forgeries.

Our work highlights the significance of NDT techniques in the preservation and conservation of movable cultural heritage objects, particularly historical and modern artworks and frescoes. The conclusions drawn are based on the investigation of original and non-original works of art analyzed in the mobile Laboratory for Testing Materials in Cultural Heritage, HeritageLab, over the past decade. Challenges such as variations in composition, surface degradation, and complex multilayered structures were effectively addressed through NDT techniques (FTIR, Raman spectroscopy, colorimetry and XRF).

In conclusion, the integration of non-destructive testing methods into the examination of paintings and cultural heritage artifacts is essential in the ongoing battle against forgery while simultaneously enriching efforts in cultural heritage preservation. Finally, an answer of the question of whether there are secret codes in the eyes of the Mona Lisa, along with a review of NDT usage in the examination of the most expensive masterpieces, is presented as a powerful tool for safeguarding the authenticity and longevity of humanity's artistic legacy.

Keywords: non-destructive testing, masterpieces, spectroscopy, cultural heritage, forgery

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IL-6

The Microplastic Visualization and Analytical Challenges

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Plastics have become indispensable in our daily life as they are inevitable in an exceptional amount of goods. Although plastics are considered non-biodegradable in the environment, they are affected by various biotic and abiotic processes that cause plastic fragmentation and create microplastics (MPs) and nanoplastics (NPs). MPs are commonly found in almost all aquatic and terrestrial ecosystems, where they become a part of the food chain. The detection and identification of the complex mixture of environmentally relevant MPs in biotic samples is currently one of the biggest challenges of microplastic research. There is an urgent need from the scientific community and (inter-)national health authorities for the development of reliable and sensitive approaches to identify and quantify environmentally relevant MPs within complex environmental, and specifically, biological matrices. The currently known methods do not allow precise localization of MPs within the biological samples or their chemical characterization. The aim of the presentation will be to introduce current MP detection technologies and their limitations and present the novel approaches - collaborative project PlastSensing. This project intends to implement state-of-the-art techniques that allow a complete characterization (spatially resolved visualization and identification of their composition) of environmentally relevant MPs, namely laser-based spectroscopy (elemental and chemical imaging) and X-ray computed tomography (structure visualization). Such approaches are currently being developed to monitor and identify MPs in preferably biotic matrices such as animal and human tissues. However, these approaches may also be applicable to environmental samples. This research was co-funded by the Slovenian Research and Innovation Agency (ARIS), the Czech Science Foundation (GAČR), and the Austrian Science Fund (FWF) under the PLASTsensing project (J1-4415, 23-13617L, I-6262-N, https://planterastics.fkkt.uni-lj.si).

Keywords: plastic particles, analysis, visualization

IL-7

Piezoelectric Polymeric Materials as Energy Harvesting Systems

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The development of tailored piezoelectric materials as energy harvesting systems has attracted considerable interest over the last two decades[1]. Their capability to capture and convert the mechanical energy into electricity has great potential in powering small electronic devices[2,3]. A variety of different piezoelectric materials such as piezo-ceramics, piezo-polymers and their composites have been extensively investigated for energy harvesting application[3,4]. Although certain ceramics have excellent piezo-properties, polymer piezoelectric materials are preferred for designing lightweight, easy-processable devices with superior mechanical flexibility over the brittle ceramic materials.

The main focus in this talk will be given to processing and post-processing routes to poly(vinylidene fluoride) (PVDF), poly(vinylidene fluoride-co-trifluoroethylene)(PVDF-TrFE) copolymers and their composites, aiming to achieve high content of piezo-active crystal phase and high overall degree of crystallinity responsible for their piezoelectric behavior.

Keywords: PVDF, piezo-active crystal phase

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IL-8

IR Reflectance Spectroscopy with Some Examples of Its Application

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Todays need of acquiring rapid information from different materials, pose necessity of techniques that are fast, non-invasive and precise. Infrared spectroscopy is one of them, and in particular, infrared reflectance spectroscopy. Nowadays, IR spectrometers are equipped with ATR and NIR-DRIFT attachments, quite suitable for fast IR spectra recording and identification of materials. On the other hand, reflection of electromagnetic radiation is a phenomenon that is sometimes needed (mirrors, metallic paints in auto industry, Mylar blanket), and sometimes suppressed (anti-reflectance coatings and stealth technology). Thus, in order to correctly use the reflection phenomenon either in the analysis of the materials or their construction, it is of vital importance to be acquainted with the physics of reflection.

Here, we would like to present some of our results obtained with methods that are used in the IR reflectance (ATR –attenuated total reflectance, DRIFT – diffuse reflectance infrared Fourier transform, SR – specular reflectance), in the context of their usage on different types of materials. We will concentrate our attention on the investigation of crystals with different symmetry in the obtainment of optical, dielectric and vibrational parameters using SR and ATR. We will show our results based on DRIFT spectra of modified powdered samples. We will also discuss the results obtained from thin films and nanomaterial investigations, using IR reflectance technique.

Keywords: IR reflectance spectroscopy, Specular reflectance, DRIFT, IR-ATR

IL-9

Harnessing Anoxygenic Phototropic Bacteria for Bioconversion of Food By-Products

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The food industry generates a significant amount of by-products, presenting both a challenge for waste management and an opportunity for resource utilization. Bioconversion processes offer sustainable solutions for waste management by transforming organic materials into valuable products. Phototrophic bacteria, with their unique metabolic capabilities, have emerged as promising agents for the bioconversion of these by-products. These bacteria utilize anoxygenic photosynthesis and anaerobic metabolic pathways to degrade and convert the by-products into biofuels, single-cell proteins, pigments, and other valuable compounds. Their ability to operate under varying environmental conditions further enhances their applicability.

Despite the promising benefits, challenges such as optimizing growth conditions, scalability, and substrate variability exist. Strategies to address these challenges through research and technological advancements are essential for maximizing bioconversion efficiency. Continued research and development in bioconversion technology using phototrophic bacteria are crucial for unlocking its full potential. With ongoing advancements and research, bioconversion using phototrophic bacteria holds great promise for contributing to a circular economy and environmental sustainability.

The aim of this presentation is to highlight the use of Purple Non-Sulfur Bacteria (PNSB) for the valorization of by-products. Following a literature review of the capabilities and properties of these bacteria, experimental data will be presented on co-culturing two species from the genera *Rhodobacter* and *Rhodospirillum* on molasses, a by-product of the sugar industry, for single-cell protein production. The presentation will also address the challenges that need to be overcome for the commercialization of these processes.

Keywords: phototrophic bacteria, food by-products, bioconversion

ANALYTICAL AND ENVIRONMENTAL CHEMISTRY

AEC O-1

Assessment of Volatile Organic Compounds in Indoor and Outdoor Air across N. Macedonia and Kosovo

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Exposure to volatile organic compounds has raised public concern due to their association with a range of acute and chronic adverse health effects.[1] This study investigates the mass percentage levels of volatile organic compounds (VOCs) in outdoor air across nine locations in N. Macedonia and Kosovo, spanning from April to December 2022. A total of 81 samples were collected during this period. Furthermore, measurements were conducted in 17 distinct indoor environments, encompassing educational, industrial, commercial, and residential settings, from March to December 2023, with a total of 60 samples collected from these sites. To achieve this, passive and diffusive samplers were employed to monitor VOCs. Subsequently, after appropriate desorption, the samples underwent analysis using gas chromatography-mass spectrometry (GC-MS). In total, approximately 70 VOCs were identified, encompassing BTEX, alkylbenzenes, glycol ethers, aldehydes, ketones, organosiloxane, monoterpenes, hydrocarbons, esters, and halogenated hydrocarbon. The sources of VOCs in outdoor air primarily originate from fossil fuels, particularly automotive fuels, with a minor fraction stemming from biogenic emissions, predominantly dominated by monoterpenes.[2] Indoor sources include household cleaners, tobacco smoke, air fresheners, toners, plastic materials, as well as external factors such as vehicular emissions.[3] The study highlights the need for quantitative analysis of VOCs in both indoor and outdoor air, as well as continuous monitoring throughout the year.

Keywords: VOC, indoor air, outdoor air, gas chromatography, passive sampling.

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AEC O-2

Mining Landfills in the Republic of Kosovo - A Case of the Artana Landfill

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Mining waste is unwanted, currently uneconomical, solid and liquid materials found in or near mines[1]. Kosovo has large reserves of mineral resources and as a result of their exploitation, many landfills have been created. These landfills pose a major risk of environmental pollution and also a potential for economic development[2]. The objective of this study was investigation of geochemistry and mineralogy of the flotation tailings from the Pb-Zn mine at the Artana landfill. A total of 38 tailings samples were analysed for their geochemical composition using: inductively coupled plasma - atomic emission spectroscopy (ICP-AES) and inductively coupled plasma–mass spectrometry (ICP-MS), as well as for their mineralogical composition using X-ray powder diffraction (XRPD) and scanning electron microscopy with energy-dispersive X-ray spectroscopy (SEM-EDX). The geochemical data show that the content of most elements is in the following range: iron 5.8-31.9 %, calcium 0.69-13.4%, aluminium 0.08-1.98%, potassium 0.11-1.34%, lead 0.26-1.75% and zinc 0.03-1.89%. The semi-quantitative X-ray diffraction (XRPD) analysis shows the information for the most common minerals with their average content: pyrite 37.38%, bassanite 25.28%, anhydrite 18.62% and quartz 16.93%.

Keywords: Pb-Zn tailings, ICP-AES, ICP-MS, XRPD, SEM-EDX, Artana landfill, Kosovo.

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AEC O-3

The Impact of Inoculated Biochar on Pesticide Adsorption and Biosorption in Soil

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This study investigates the use of biochar inoculated with *Bacillus megaterium* BD5 biofilm for pesticide sorption in soil. Experiments were conducted using stainless-steel columns (4 cm diameter, 20 cm length) filled with soil amended with 0.5% of inoculated biochar. A thiourea tracer at 4 mg/L was used, and pesticide solutions were passed through the columns. Eluates were collected and analyzed using GC/MS. A mathematical transport model solved the advection-dispersion equation to determine transport parameters like retardation (R_d) and biodegradation (λ). Retardation coefficients ranged from R_d=40-100, while biodegradation rates ranged from λ=0.2-3.3. There was no clear correlation between the octanol-water partition coefficient, retardation, and biodegradation, indicating that hydrophobicity alone did not determine sorption and transport characteristics.

In summary, inoculated biochar enhances both adsorption and biosorption of pesticides, effectively reducing pollutant leaching to the groundwater. This method shows promise for improving remediation efforts in contaminated environments.

Keywords: sorption, remediation, pesticides, soil, groundwater

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AEC O-4

Ecology of Soil Species of the Genus *Bacillus* and the Influence of Environmental Factors on their Biologically Active Compounds

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Soil chemistry has determining influence on soil microbial communities, and with that, affects the biogeochemical dynamics in natural ecosystems. *Bacillus* is one of the predominant bacterial genera that play a key role in soil biogeochemistry, making this genus one of the most commercially significant within the agro-biotechnology industry. The aim of this study was to explore the intricate relationship between the soil microorganisms of the genus *Bacillus* and environmental factors, highlighting the critical role of *Bacillus* in maintaining soil health and productivity. *Bacillus* strains were isolated from five different soil types across Republic of N. Macedonia before proceeding with characterization and evaluation of their antimicrobial and biosurfactant producing potentials. Soil physical and chemical properties were assessed with standardized methods. Our results show that the abundance of *Bacillus* spp. decreases with the reduction of humus percentage, indicating a direct correlation between these two parameters. The content of analysed heavy metals (Ni, Cu, Pb and Zn) has highest values in the mixed forests at Karadzica and Vodno localities. Strain biodiversity was found to be inversely correlated with the concentration of Ni and Pb at these localities, indicating that pollution may act as a bottleneck for soil microbial diversity. Understanding the ecology of *Bacillus* spp. can undoubtedly improve and assist current industrial practices with acquiring novel avenues for sustainable development. Furthermore, it elucidates the adaptive nature of microbial communities driven by their secondary metabolism in reaction to the soil chemistry. This study shows that the obtained results can be utilized for further research aimed at applying these microorganisms as agents for biological control and sources of green chemicals.

Keywords: biogeochemistry, soil bacterial community, heavy metals, biosurfactants, antimicrobials

AEC P-1

Adsorption of Diazepam onto Differently Modified Waste Cotton-based Yarn

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The constantly evolving fashion trends lead to an upsurge in textile production, particularly in the manufacturing of cotton-based materials, resulting in significant quantities of cotton-based waste. Therefore, this study explores the potential of repurposing waste cotton-based yarn to develop efficient adsorbents for the removal of diazepam from water.

Different chemical and thermal treatments were used for the modification of cotton and cotton/polyester yarn to improve their adsorption properties. Scanning electron microscopy and Fourier transform infrared spectroscopy were used to characterize unmodified and modified yarn, while adsorption characteristics were examined through the adsorption of diazepam. Applied chemical treatments induced the changes in yarn`s morphology and surface chemistry, while thermal treatment converted the used precursors into efficient carbon adsorbents. The influence of contact time, initial concentration, and the initial pH of the adsorption solution on diazepam adsorption was examined, and obtained data were analyzed by theoretical models. The study reveals that diazepam adsorption follows a pseudo-second-order kinetic model, and equilibrium data conforms to the Langmuir isotherm model. Applied chemical modification marginally enhanced the adsorption properties of cotton yarn, whereas thermal treatment yielded highly efficient cotton-based adsorbents.

Keywords: textile waste, cotton yarn, modification, adsorption, diazepam.

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AEC P-2

The Adsorption Efficiency of Selected Pharmaceuticals from Water Using Chemically Modified Potato Starch

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Pharmaceutical products are an important element of medical and veterinary practice, and their positive impact on human and animal health and food production is widely recognized. However, one area where there's a lack of general understanding is the ongoing impact of pharmaceuticals continuously being released into the environment due to production, consumption, excretion, and improper disposal of unused or expired products. Until people's awareness of this problem increases, it is necessary to work on removing pharmaceutical residues that end up in waterways. Low-cost natural polysaccharides became interesting for application as adsorbents in wastewater treatment due to their biodegradability and non-toxic nature. Starch is a biodegradable agricultural biopolymer with some limiting properties for its application such as poor chemical stability, low mechanical strength, and difficult recovery. However, chemical modification of starch can greatly improve these properties.

In the present study, potato starch was modified using environmentally acceptable chemical compounds, cysteine, histidine, and melamine, and obtained amino-modified starches were applied as adsorbents for the removal of selected pharmaceuticals (bromazepam, lorazepam, diclofenac, atorvastatin, clopidogrel) from aqueous solutions. The success of starch modification was confirmed by the surface and morphological characterization of the samples. It was found that applied chemical modification of starch contributed to an increase in the efficiency of pharmaceutical removal from aqueous solutions.

Keywords: biopolymer, potato starch, chemical modification, adsorption, pharmaceuticals.

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AEC P-3

Assessment of Heavy Metal Contamination in The Soils of Mitrovica City in The Republic of Kosovo

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Environmental pollution with heavy metals is one of the biggest challenges in modern society[1]. Heavy metals are one of the most serious environmental pollutants due to their toxic effects, persistent and abundant that can accumulate in aquatic ecosystems, soils and foods[2].

The concentrations of sixteen heavy metals (As, Ca, Cr, Cu, Fe, K, Mn, Ni, Pb, Rb, Sr, Ti, Y, V, Zn and Zr) were analyzed in the topsoil samples of four locations in Mitrovica city, by using X-ray fluorescence (XRF) technique. Statistical analysis was performed to better explain the data the maximum content of some heavy metals in the sediments exceeded the target values of the New Dutch List[3]. The soil contamination assessment was carried out using the pollution indicators such as contamination factor (*CF*) and geo accumulation index (*Igeo*). The soils were extremely contaminated with potential toxic elements: As, Cu, Mn, Ni, Pb and Zn, and the maximum value of *CF*, for these elements were: 41.6; 11.5; 5.7; 9.7; 197 and 91.3, respectively. The maximum values of *Igeo*, were for: lead (7.04), zinc (5.93), arsenic (4.79), and for copper (3.17).

Keywords: Heavy metals, soil, Mitrovica city, Niton XRF, Kosovo.

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AEC P-4

Assessing Volatile Methyl Siloxanes in Indoor Environments Using Passive Sampling

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Humans spend approximately 90% of their time indoors, consistently being exposed to volatile methyl siloxanes (VMSs) through ingestion, inhalation, or dermal contact, potentially posing health risks.[1,2]This study presents the mass percentages of VMSs identified in various indoor environments, utilizing passive and diffusive sampling techniques followed by gas chromatography-mass spectrometry analysis. VMSs can be categorized into cyclic (cVMSs) and linear (lVMSs) compounds based on their structure. The highest mass percentages of VMSs were detected in a barber shop, apartment, and house compared to other sampling locations. Three cyclic siloxanes (D4-D6) and four linear siloxanes (L2-L5) were detected in the sampled locations. Decamethylcylcopentasiloxane (D5) was identified as the predominant compound, comprising 60% to 90% of the total VMS mass. This compound is a major ingredient in some personal care products used daily, raising concerns about its ubiquitous presence in indoor environments.[3] Several cVMSs have garnered attention from regulatory bodies due to their potential persistence, bioaccumulation, and toxicity to both human health and the environment.[3,4] The ultimate objective is to conduct a comprehensive quantitative analysis of VMSs in indoor air environments over the course of a year.

Keywords: Siloxanes, cosmetic products, indoor air, toxicity, passive sampling.

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AEC P-5

Quantitative Determination of Microelements in Forest Berries from the Pešter Plateau in The Republic of Serbia by ICP-OES Method

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In this study the inductively coupled plasma optical emission spectrometry (ICP-OES) was used to determine the concentration of essential and potentially essential elements such as: Fe, Zn, Cu, Se, Cr and B, Co, Mn, Ni, Si, V. Forest fruit (strawberry (S1-S2), raspberry (R1-R2), and blackberry (B1-B2)) from different locations of the Pešter Plateau in the Republic of Serbia was selected for investigation. The range of microelements found in the analyzed forest berries was as follows: for **Cu**: S1 > R3 > S2 > R2 > B2 > B1 > R1; for **Fe**: R1 > S1 > S2 > R3 > R2 > B1 > B2; for **Cr**: S2 > S1 > R1 > R2 > R3 > B2 > B1; for **Zn**: R3 > R2 > S2 > R1 > B1 > S1 > B2; for **Se**: S1 > R1 > S2 > B1 > B2 > R2 > R3. The average results (concentration ± SD, μg g^{-1}) of essential elements obtained for forest berries are given in Table 1.

Table 1. Essential microelement contents (μg g^{-1}) in forest berries samples from the Pešter Plateau

Sampl.	Cu	Fe	Cr	Zn	Se
S1	3.17±0.13	6.83±0.33	0.312±0.002	2.53±0.02	0.454±0.039
S2	2.524±0.045	6.66±0.20	0.364±0.026	3.66±0.06	0.336±0.007
R1	0.903±0.020	7.842±0.055	0.2882±0.0024	3.58±0.07	0.391±0.004
R2	1.59±0.11	5.51±0.28	0.23±0.01	5.02±0.29	0.112±0.028
R3	2.511±0.069	6.66±0.60	0.190±0.002	6.75±0.14	0.045±0.029
B1	1.327±0.022	4.244±0.042	0.130±0.001	3.17±0.31	0.3030±0.0003
B2	1.360±0.096	3.43±0.77	0.139±0.007	1.74±0.08	0.302±0.010

S1, S2 = strawberry; R1, R2, R3 =raspberry; B1, B2 = blackberry.

Keywords: forest berries; microelements; ICP-OES; Pešter Plateau.

AEC P-6

Research of Macroelement and Microelement Composition in Domestic Fruit from the Pešter Plateau in the Republic of Serbia

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Concentrations of five macroelements (Ca, Mg, K, Na, P) and five essential microelements (Fe, Zn, Cu, Se, Cr) were determined in six types of domestic fruit, that were not chemically treated. Total mineral content, after samples mineralization, were analyzed by inductively coupled plasma optical emission spectrometry (ICP-OES).

Domestic fruit (raspberry, cherry, red plum, grape, aronia, red currant, black currant) from the Pešter Plateau in the Republic of Serbia, was selected for investigation. The results showed that aronia is the richest in the Se content, while sour cherries are the poorest. However, sour cherries were abundant in the content of other essential microelements.

Zn was the least abundant in grapes, while Cu, Fe, and Cr were the least abundant in red plum. As far as macroelements are concerned, it turned out that aronia was the richest in Na and Mg, while blackcurrant was abundant in the content of K, Ca, and P. According to the K content, it was observed that his amount in sour cherries are the least. The lowest content of all other examined macroelements was observed in the grape.

Keywords: domestic fruits; microelements; macroelements; ICP-OES; Pešter Plateau.

AEC P-7

Electroanalytical Approach for Quantification of Pesticide Maneb in River Water Sample Using Biochar-Modified Carbon Paste Electrode

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Manganese derivative fungicide, maneb (MAN) has a potentially toxic effect on living organisms such as aquatic species and humans.[1] Biochar (BC) has good electrical conductivity with a characteristic catalytic effect and could be used as an electrode modifier for sensing pollutants in river water samples.[2]

An optimal differential pulse adsorptive stripping voltammetric (DP-AdSV) parameters includes accumulation potential (E_{acc}) of -0.2 V and accumulation time (t_{acc}) of 90 s, Britton-Robinson buffer pH 7.0. The good linearity of the calibration curve was obtained in the concentration range from 0.049 to 1.84 μg mL^{-1} of MAN with a limit of detection of 0.015 μg mL^{-1} MAN and a relative standard deviation (RSD) of 3.2% at carbon paste electrode (CPE) bulk modified by 10% BC. Investigated interferences did not affect significantly the MAN signal intensity. The developed DP-AdSV method was successfully applied for the determination of MAN in spiked river water sample with the recovery of 99.49% and RSD of 1.02%.

Keywords: biochar, carbon paste electrode, voltammetry, maneb, river water sample

Acknowledgements: This research was supported by the Science Fund of the Republic of Serbia, #10810, Sustainable solutions in environmental chemistry: exploring biochar potential–EnviroChar.

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AEC P-8

Use of Hardwood Biochar for the Development of a Sensitive Electrochemical Sensor for the Determination of Pesticide Mancozeb in Wastewater Sample

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The levels of pesticides in water have increased due to their excessive use in the modern agricultural domain indicating the need for the development of simple and contemporary methods for their removal and determination.[1]

The electrochemical evaluation of fungicide mancozeb (MCZ) using a low-cost carbon paste electrode modified with biochar (BC-CPE) is a novel strategy to provide a sensitive response to water pollution. Biochar from a hardwood source was synthesized *via* pyrolysis process at 400 °C and 700 °C, and the resulting electrodes (unmodified CPE, BC400-CPE and BC700-CPE) were compared for MCZ sensing. BC700-CPE showed the best analytical performance and under optimized conditions of differential pulse adsorptive stripping voltammetric (DPAdSV) method (pH 7.0, E_{acc} = -0.2 V, t_{acc} = 30 s) the obtained linear range was from 0.025 to 2.78 μg mL^{-1} MCZ with detection limit of 7.5 ng mL^{-1}. The developed sensor was successfully applied as a sensitive electrochemical platform for the determination of MCZ in wastewater sample with a recovery of 101.7% and a relative standard deviation of 1.25%.

Keywords: biochar, carbon paste electrode, voltammetry, mancozeb, wastewater

Acknowledgement: This research was supported by the Science Fund of the Republic of Serbia, #10810, Sustainable solutions in environmental chemistry: exploring biochar potential–EnviroChar.

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AEC P-9

Analysis of Heavy Metal Pollution in the Drenica River by Feronikel and the Bioaccumulation of These Metals

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Environmental issues have consistently received significant attention and continue to be a major concern for scientists. Among these, water pollution remains a critical global challenge, exacerbated by various factors. Heavy metal pollution, in particular, poses a severe threat to the environment, triggering a chain of contamination that affects soil, water, and air, and ultimately impacts human lifestyles. Due to their toxicity, persistence in the environment, and propensity for accumulation in the human body through bioaccumulation, heavy metals can become extremely hazardous when combined with various environmental elements, such as water. Consequently, humans and other living organisms can be exposed directly or indirectly through the food chain.

In this review, we focus on research concerning water pollution in the Drenica River with heavy metals from the Feronikel enterprise, known for extracting metals like nickel (Ni), iron (Fe), zinc (Zn), lead (Pb), and others. The Drenica River, a crucial water source, faces significant challenges due to contamination with heavy metals. This issue has raised concerns within the community and has a direct impact on public health and well-being.

Our findings are alarming, showing an increasing concentration of metals in the river over the years. This is contrary to expectations that advancements in technology and environmental regulations would lead to improvements in water treatment before its discharge into the river.

Keywords: pollution, heavy metals, water, Drenica River, bioaccumulation, Feronikel

AEC P-10

Levels of Platinum, Palladium and Rhodium in Zagreb Air

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Platinum (Pt), palladium (Pd) and rhodium (Rh) are considered strategic metals because of their specialized applications in industry as well as significant role in the functioning of automotive catalytic converters designed to reduce gaseous pollutants. The hot exhaust gases that pass through catalytic converters cause damage to these systems which leads to the emission of Pt, Pd and/or Rh into the environment and an increase of their levels in the air. We investigated the spatial and temporal distributions of Pt, Pd and Rh in PM_{10} (particulate matter with aerodynamic diameter <10 micrometers) at three urban area stations (North, Center and South) over a sampling period of five years (2016 – 2020). A method was developed to determine Pt, Pd and Rh in airborne particles by inductively coupled plasma mass spectrometry (ICP-MS). This included the weekly sampling of particulate matter on quartz filters and microwave digestion in acid under high pressure and temperature. Quality control was done using two PM10-like certified reference materials: NIST 1648 (Urban particulate matter) and ERM CZ120 (fine dust) spiked with known quantities of Pt, Pd and Rh. Analytical recovery of Pt, Pd and Rh for spiked samples of ERM CZ120 was 96% - 105%, while the analytical recovery for the spiked samples of NIST 1648a was 95% - 104%. The average values of measured mass concentrations of the metals at the monitoring stations through the years were: 0.09-1.26 pg m^{-3} for Pt, 1.42-7.39 pg m^{-3} for Pd and 0.12-0.17 pg m^{-3} for Rh. Average concentrations of Pt, Pd and Rh in PM_{10} increased for all three elements in the direction north < center < south. Levels of Pt, Pd and Rh were statistically significantly different between the monitoring stations which was the result of the different traffic loads at the stations. Statistically significant seasonal variations with the highest values during the colder part of the year were found at all of the monitoring stations. This study was performed using the facilities and equipment funded within the European Regional Development Fund project KK.01.1.1.02.0007 "Research and Education Centre of Environmental Health and Radiation Protection – Reconstruction and Expansion of the Institute for Medical Research and Occupational Health"

Keywords: ICP-MS, microwave digestion, PM_{10}

AEC P-11

Removal of Toxic Textile Dyes from Aqueous Solution by Waste Hop-Based Biosorbent: Influence of Particle Size on Adsorption Efficiency

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Nowadays the treatment of dye-contaminated wastewater is a great concern, due to environmental pollution and dyes's harmful effects on public health[1]. Biosorption of toxic dyes on the waste hop biomass proved an effective method to minimize the harmful effects of dye-contaminated wastewater on the ecological environment and human health[2]. The main goal of this study was to evaluate the influence of particle size of waste hop-based biosorbent on the removal efficiency of malachite green (MG), methylene blue (MB), and crystal violet (CV) from an aqueous solution in a batch system. Four fractions of waste hop biomass (with a particle size of 1.03, 0.85, 0.519, <0.519 μm), were tested as biosorbents. Waste hop biosorbent showed great potential in removing the tested dyes with a removal efficiency that reached as high as 98.4 (MG), 98.8 (MB), and 98.5% (CV) for the smallest fraction used with a particle size smaller than 0.519 μm. The results also revealed that the efficiency of dye removal decreases with the increase in fractions particle size, thus for the largest particle size, it was 79.7, 81.3, and 80.1 % for MG, MB, and CV removal, respectively. The utilized fractions of biosorbent were proved to be an efficient natural material, which is also cheap and environmentally friendly, and its use is highly desirable considering that such biosorption reduces the costs of total wastewater treatment.

Keywords: dyes removal, biosorption, waste hop, particle size

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AEC P-12
Pollution Indicators of Heavy Metals in the Sediments of The Lepenec River in Republic of Kosovo

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Sediments are vital and integral parts of aquatic environments, and are the valuable indicators for monitoring pollutants in aquatic ecosystem[1]. In this study we investigated the sediments of Lepenec river in Republic of Kosovo, by using X-ray fluorescence (XRF) technique. The concentrations of eighteen metals (As, Ca, Cr, Cu, Fe, K, Mn, Nb, Ni, Pb, Rb, Sr, Th, Ti, V, Y, Zn and Zr) were analyzed in six different locations. Statistical analysis (Basic statistics, Pearson correlation and Cluster analysis) was performed to better explain the data the maximum content of some heavy metals in the sediments exceeded the target values of the New Dutch List[2-3]. Four groups of elements were identified by cluster analysis, based on their geogenic or anthropogenic origin. The sediments were mostly contaminated with potential toxic elements (As, Cr, Cu and Ni). The contamination factor (CF) for different metals and locations had values in ranges from 1.8 to 5.33, and the pollution load index (PLI) had values from 2.42 to 3.09. Nickel and chromium have contributed the most to sediment pollution, and their Igeo values in all locations are higher than 1. The most polluted locations were two locations which are no far from former nickel mine and cement factory.

Keywords: Heavy metals, sediment, Niton XRF, Lepenec river, Kosovo.

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AEC P-13

Presence of As, Hg, and Tl in Honey and Pollen in Kosovo

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This study aimed to estimate the concentration of three potentially toxic elements; As, Hg, and Tl, in honey and bee pollen samples. In total, we collected 99 honey and 67 bee pollen samples from the territory of the Republic of Kosovo. The digested samples were analysed using two spectroscopic techniques, ICP-AES and ICP-MS. The mean values for arsenic were 6.8 µg/kg, mercury 15 µg/kg and thallium 3.2 µg/kg in the honey samples. In the bee pollen samples, the mean values of the concentration in µg/kg were: 36; 23 and 3.7 for As; Hg and Tl, respectively. Higher concentrations were found in the pollen samples compared to those of honey, while when analysing the correlation between the same elements in the two components (honey and pollen), positive moderate correlation was found for Tl (0.49), very low positive correlation for Hg (0.15) and As (-0.03). Potential pollution sources are Trepca mine dump in the city of Mitrovica, the coal-fired power plant in the city of Obiliq, and a cement factory in the city of Elez Han[1,2].

Keywords: honey, bee pollen, potentially toxic elements, Kosovo

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AEC P-14

Analysis of Water Quality Using Physicochemical Parameters: A Study of the Lepenc River

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Water is a very important resourse with vital importance for human and other organisms[1]. In this study, we investigated the quality of water in the Lepenc river in the Republic of Kosovo, by using different physicochemical parameters. A total of 17 parameters were analyzed at six different locations: Temperature, pH, electrical conductivity (EC), total dissolved solids (TDS), total organic carbon (TOC), NO_3^-, NO_2^-, NH_4^+, PO_4^{3-}, SO_4^{2-}, As, Cd, Cr, Cu, Fe, Mn and Zn. Heavy metals were analyzed by inductively coupled plasma-atomic emission spectroscopy (ICP-AES). The mean values for some parameters that impacted in water pollution were: 392 µS/cm (EC); 15.8 mg/L (TDS), 3.22 mg/L (TOC), 1.46 mg/L (NO_2^-), 0.8 mg/L (PO_4^{3-}), 0.09 mg/L (Cr), 0.41 mg/L (Fe) and 2.49 mg/L (Zn). Statistical analysis (basic statistics, Pearson correlation and cluster analysis) was performed to better explain the data of different parameters[2]. The most polluted waters were found in samples S2 and S5 which are located close to the former nickel mine in Ivaja (municipality of Kaçanik) and the cement factory in Elez Han. Transport also has an impact on pollution in the investigated waters, because the Pristina-Skopje highway passes along the river, and the border between the Republic of Kosovo and N. Macedonia is located there.

Keywords: physicochemical parameters, water, ICP-AES, Lepenc river, Kosovo.

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AEC P-15

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 volatile organic compounds (VOCs).[1] The primary goal of this work was to achieve a 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 photocatalyst's surface to degrade the aforementioned impurities.[1] TiO_2, when irradiated with UV light, can decompose many organic compounds into 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 using leaching test, AAS and TOC analyses. Photocatalytic tests were conducted in a custom-made wind tunnel reactor with a simulated polluted atmosphere to confirm the activity. The successful immobilization of TiO_2 on the reference rubber tile was achieved, and the photocatalytic activity of the immobilized layer was confirmed by the successful degradation of ammonia.

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

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AEC P-16

Removal of Organic Pollutants from Water Using Wood-Derived Biochar

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Use of herbicides in agriculture is critical for ensuring high crop yields and supporting the global food supply. Despite their undeniable agricultural benefits, these chemicals pose significant environmental risks. Triazine herbicides such as atrazine and simazine were commonly used for weed control. The latest Joint Danube Survey[1] showed that these substances are still frequently detected throughout the Danube River Basin, even though the approval of atrazine at the EU level expired in 2004. The aim of this study was to assess the efficiency of wood-derived biochar produced at two temperatures in removing atrazine and simazine from water. Water samples with an initial concentration of 100 µg/L of each herbicide were treated with biochar at three doses (0.1, 0.2, and 0.4 g/L) for 48 h, then analyzed for residual concentrations using a gas chromatography/mass spectrometry system. Biochar produced at 400 ºC removed up to 25% of both substances, even at the highest dose. On the other hand, biochar produced at 700 ºC showed a significantly higher removal efficiency: 66.3% and 68.7% for atrazine and simazine, respectively, at the low dose, and >97% of both herbicides at higher biochar doses. Results indicate a high potential of wood-derived biochar produced at high temperatures for triazine herbicide removal from water.

Keywords: wood-derived biochar, triazine herbicides, water contamination

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AEC P-17

Immobilization of Toxic Pollutants (Pb, Cu, and Cd) from Wastewater by New Eco-friendly Materials Based on Red Mud, Fly Ash and Wood Ash

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This research aimed to examine the possibility of applying geopolymer synthesized based on red mud, fly ash, and wood ash for removing toxic pollutants, such as copper, lead and cadmium ions, from wastewater. The samples of different ratios of red mud (RM) and fly ash (FA), wood ash (WA) and fly ash (FA), were synthesized by alkaline activation process, geopolymer based on RM and FA (GPRMFA) and geopolymer based on WA and FA (GPWAFA). The physical-chemical characterization of geopolymers in terms of mineral composition and structure was performed using XRD, DRIFT and SEM analysis. BET analysis was used to define meso and microporosity, as well as the specific surfaces necessary for efficient adsorption. The batch equilibration method was used to determine the PZC value, which is a guide for predicting the adsorption process. The sorption experiments were performed at different operating parameters in order to determine the optimal values. The best adsorption efficiency for GPRMFA was achieved at pH = 4 (88.5%) i.e. at pH = 5 (99.4%) for Cu and Pb, respectively and for GPWAFA at pH = 6.5 (61.5%) for cadmium ions. Sorption kinetics depends on operating parameters and the order of the reaction and the most suitable kinetic model were determined within it. Performed analyses indicate that waste, such as red mud, fly ash and wood ash can be used as a raw material for obtaining a geopolymer that can be effectively used as a low-cost and eco-friendly material for immobilization of heavy metals (Pb, Cu, Cd) from wastewater.

Keywords: red mud, fly ash, wood ash, geopolymer, heavy metals

AEC P-18

Sorption Properties of Biocarbons Produced from Residues after Supercritical Extraction of Raw Plants

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The study presents a synthesis of adsorbents derived from residues resulting from the supercritical extraction of raw plants, including marigold, hops and chamomile. Biocarbons were obtained through the activation of precursors using carbon dioxide. The prepared biocarbons were studied using various techniques to determine their surface morphology, structure, elemental composition, porosity and acid-base properties. The kinetics and adsorption mechanism of methylene blue and Rhodamine B from an aqueous solution were investigated. The effect of reaction parameters such as temperature and pH changes, reaction time, dye concentration, adsorbent mass and sample shaking rate on the dye removal efficiency of the obtained adsorbents was evaluated.

The results demonstrated that the obtained adsorbents exhibited a mesoporous texture, and that the basic character of the synthesised adsorbents depended on the starting material. The pseudo-second-order kinetic model provided the best fit to the experimental results, indicating that the adsorption process followed a chemical process. Conversely, the Langmuir adsorption isotherm showed the best fit, indicating monolayer adsorption. The Langmuir adsorption isotherm demonstrated a high maximum adsorption capacity, with values of 195 mg/g for methylene blue and 173 mg/g for Rhodamine B. Negative Gibbs free energy values indicated that the removal of organic dyes could be thermodynamically favourable due to the spontaneous nature of the adsorption process.

Keywords: biocarbons, microwave heating, adsorption, methylene blue, Rhodamine B

AEC P-19

D-Optimal Experimental Design Utilization for Robustness Evaluation of a HPLC Method For Related Substances in Simvastatin Formulations

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The purpose of this work was to evaluate the robustness of a HPLC method for quantification of related substances in simvastatin formulations utilizing the D-optimal experimental design. This approach was used to assess the main, interaction and quadratic effects of the independent variables (concentration of acetonitrile in mobile phase, pH and molarity of buffer, flow rate, column temperature and column batch) on retention time, number of theoretical plates, asymmetry of the peak of simvastatin, and resolution of critical pairs of impurities A/I, E/F, B/J and J/C. Data fitting was performed by multiple linear regression with the software package Modde® 12.0.1. The statistical evaluation indicated that the coefficients of determination (R2) and predictability power (Q2) for all investigated dependent variables are acceptably high (>0.95) except for the dependent variable asymmetry of simvastatin peak (R2 = 0.89, Q2 = 0.67). The bias between the predicted and obtained experimental values was close for the investigated responses, confirming the robustness of the mathematical model, its validity and high predictive power. Based on the methodology of surface responses it was concluded that the HPLC method is robust within the investigated ranges for all independent variables. The findings showed that D-optimal experimental design can be applied for robustness evaluation of HPLC methods.

Keywords: D-optimal design, related substances, simvastatin, robustness, HPLC method

AEC P-20

Study of Elution Strength of Ethanol as "Green" Eluent in LC Analysis of Non-polar Acidic Compounds

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According to the Green analytical chemistry (GAC) principles, the toxic organic eluents (methanol, acetonitrile etc.) in liquid chromatography (LC) should be replaced with suitable "green" solvents[1]. The aim of this study was to evaluate the elution strength of ethanol as preferred green eluent and compared it with methanol. To achieve this objective, C18 column and phosphate buffer at pH 3.0 in different volume fractions with both organic eluents were used as a mobile phase. Various retention models were assessed to characterize the retention behavior of several non-polar, acidic active pharmaceutical compounds[2]. The retention behavior of the analytes, characterized with the log-log retention model, showed that similar retention factors for the analytes could be achieved with approximately 16% less volume fraction of ethanol compared to methanol. The findings confirmed that ethanol exhibits greater elution strength in comparison to methanol, a significant data for transition from conventional to green LC method.

Keywords: Green analytical chemistry, methanol, ethanol, elution strength, retention modeling

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AEC P-21

Noise Emissions from Equipment and Working Mechanisms During Quarry Operation

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Quarries during their work produce a certain level of noise, which can have a negative impact on the surrounding area as well as on the employees at the quarry location. Considering that there are several sources of noise, it is necessary to calculate the total emission level of noise. In this paper, an example of noise emissions from a quarry in the Berane area is given. The noise emission values from the complete machinery and equipment are given based on the catalog values of the noise level at a distance of 1 m. This noise level is calculated based on the equation:

$$Lr = 10 \cdot \log \sum_{j} 10^{0.1Lrj}; dB(A)$$

Where: Lr = Total emission noise level

Apart from the emission values of the noise level, the emission noise levels are also very important, the level of which can exceed the permitted values at certain distances from the place of origin. The use of machinery and equipment as a source of noise is included in the system of measures to protect the population from noise, which are contained in certain regulations. The system of measures includes techniques and organizational measures with the aim of ensuring that the noise in the environment in which a person lives does not exceed the permissible limit prescribed by the Law on Protection against Noise.

The aim of this work is to show the impact of noise on the working and living environment through the process of quarry work.

Keywords: quarry, noise emissions, working and living environment

AEC P-22

Waste Tires Management on the Montenegro Coast to Improve the Quality of the Environment

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Problems in the management of waste tires are increasingly evident in Montenegro, and therefore also in the cities on the Montenegrin coast. For this reason, a Base Study was made for the collection, transport, sorting and storage of waste tires, for solving the problem of waste tire management.

The risk of pollution due to inadequate treatment of waste tires on the territory of the municipalities of Bar, Ulcinj, Budva, Tivat and Kotor is very high at the moment, especially in the case of burning them. Gases and chemicals released by burning used tires are extremely toxic to human health and very harmful to the environment.

Environmental pollution occurs through pollution of all transmission routes - through air, water and soil. It is important to know that, according to expert estimates, burning a tire releases a significant amount of oil, and burning about 100 tires releases about 25 liters of oil, which can pollute the environment if it is not adequately cleaned. Apart from the direct pollution of soil and water by combustion products that are in a liquid state, we should also take into account the pollution of water and soil that occurs by washing away ash and unburned residues after rain or some other contact with water.

The aim of the paper is to show that through adequate management of waste tires, environmental pollution is prevented by their disposal in unauthorized and illegal places, as well as that recycling of waste tires enables the reuse of separated raw materials.

Keywords: waste tires, waste tire management, recycling, processing

AEC P-23

Two-Trace Two-Dimensional Correlation Spectroscopy as a Tool in Analytical Control Laboratories for Raw Materials

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In the present work, we employ two-trace two-dimensional (2T2D) correlation analysis, integrated with vibrational spectroscopy techniques (IR and Raman), to provide a robust analytical framework for the advanced control of raw materials in pharmaceuticals. This combined approach significantly enhances the detection and analysis of inconsistencies in raw materials, which are critical for managing unexpected results in quality control laboratories. The non-destructive and rapid nature of Raman and IR techniques allows for detailed, real-time analysis of molecular compositions and interactions. We demonstrate that by employing 2T2D correlation spectroscopy, a comprehensive two-dimensional spectral analysis can be achieved, that reveals even subtle differences between the samples which are not visible with traditional methods, thus facilitating a deeper understanding of materials' properties and variations. In particular, in our study we employ the complex plane phase vector representation of the spectra. It allows for a very convenient representation of the dynamic spectrum and the coherence measure as well as a simple comparison of the phase angles between two phase vectors derived from the original spectral pair.

In principle, this method supports rigorous compliance with regulatory standards and improves decision-making processes by providing precise and reliable data on raw material quality. Ultimately, the adoption of this sophisticated spectroscopic technique marks a significant advancement in the analytical capabilities of quality control in the pharmaceutical industry, ensuring higher production efficiency and reduced risk of quality deviations in final products.

Keywords: Two-trace two-dimensional spectroscopy, IR, Raman, raw materials, quality control.

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AEC P-24

Cleaning Validation of Laboratory Glassware

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The laboratory glassware used for quantitative analysis should meet the strict laboratory's requirements. Cleaning procedures and storages of volumetric equipment may be critical, particularly for trace analysis. The laboratories in quality control department perform cleaning validation of glassware by determining relevant chemical parameters (such as pH, conductivity, total organic carbon and specific HPLC analysis) in rinse samples.[1,2]

The aim of this study was to validate the cleaning procedure of the glassware machines type 26-03/PH by manufacturer Riebesam. The machines are designed for washing, rinsing, and drying metal, plastic or glass. The glassware machines have three types of shelves depending on the size of the glassware: shelf for large glassware, shelf for small glassware and shelf with box for pipettes. The procedure was performed with contamination of the glassware with worst-case product for cleaning, previously determined on the basis of solubility, PDE (Permitted daily exposure), difficulty of cleaning and frequency of production. The glassware was contaminated with highest concentration of sample solution used for regular analysis. About 10% of its nominal volume was filled with sample solution and shaked to contaminate the inner walls, emptied and allowed to dry. Then the glassware was washed in the washing machine. After the washing program was completed, rinse samples were taken from visually clean glassware and analyzed with specific HPLC method, pH, conductivity, and total organic carbon.

All obtained results from the performed tests were in the compliance with the acceptance criteria. This cleaning validation study confirmed that the washing program for laboratory glassware is effective and reproducible.

Keywords: cleaning validation, laboratory glassware, glassware machine, worst case product

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AEC P-25

Optimization of Cyclic Voltammetry versus Phenolic Profile and In Vitro Properties for Determining Antioxidant Activity of Rosa Dumalis Bechst. Fruit Samples

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Using cyclic voltammetry (CV), the antioxidant activity of water extracts of *Rosa dumalis* Bechst. fruit was investigated. To optimize the CV method, scan rates (25, 50, 75 mV/s) and pH values (2, 4.5, 7) were varied, with optimal conditions at 75 mV/s and pH 4.5. Voltammograms recorded from 0 to 1200 mV identified oxidation peaks for catechin-type flavonoids and quercetin between 0.465-1.045 V.

Spectrophotometric antioxidant assays (ABTS, DPPH, FRAP, CUPRAC) were conducted. ABTS results ranged from 280 to 460 mg TE/g, DPPH values were 75 to 140 mg TE/g, FRAP and CUPRAC results varied from 0.8 to 2.3 mmol FE/g and 230 to 620 mg TE/g, respectively. Total polyphenol content ranged from 86 to 217 mg GAE/g, flavonoid content from 37 to 82 mg CE/g, and vitamin C content from 2.72 to 3.85 mg/g. Significant correlations were found between spectrophotometric assays: ABTS and CUPRAC (R^2 = 0.949), ABTS and DPPH (R^2 = 0.948), DPPH and CUPRAC (R^2 = 0.909), and others. Cyclic voltammetry did not show significant correlation with in vitro antioxidant tests.

HPLC analysis identified phenolic compounds: procyanidin B2 (17.4-32.8 µg/g dw), quercetin (n.d.-26.1 µg/g dw), (-)-epicatechin (10.5-21.6 µg/g dw), (+)-catechin (4.10-10.01 µg/g dw), kaempferol (5.15-6.80 µg/g dw), rutin (3.26-3.99 µg/g dw), cyanidin-3-glucoside (1.59-2.01 µg/g dw), protocatechuic acid (n.d.-1.99 µg/g dw), and gallic acid (0.344-1.75 µg/g dw).

Keywords: *Rosa* L., antioxidants, cyclic voltammetry, PCA

AEC P-26

Development and Validation of an Analytical Method for Determination of the Particle Size Distribution of Atorvastatin Calcium Utilizing a Low-Toxicity Dispersant as an Alternative to *n*-Hexane

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Particle size distribution (PSD) analysis plays a crucial role in various industries, particularly in pharmaceuticals, where it directly impacts product quality and performance. Many methods of PSD analysis often involve the use of toxic dispersants like n-hexane, posing significant health risks and environmental concerns.

This study demonstrates the possibility to apply dry dispersion techniques utilizing compressed air, as a saferalternative.[2] In the current study atorvastatin calcium was used as a model active pharmaceutical ingredient (API), in order evaluate the ability of the newly developed dry dispersion method to provide comparable precision and repeatability in comparison to the originally used wet method based on n-hexane wet dispersion. The dry method ensures compliance with stringent safety and environmental regulations while simplifying sample handling and disposal procedures. Despite initial investment costs, the long-term benefits include decreased safety expenditures and enhanced operational efficiency, positioning dry dispersion methods as the preferred approach for PSD analysis in pharmaceutical research and development and routine testing.[3]

The method is validated by assessing the repeatability of the measurements, intermediate precision and robustness of the method.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.[1]

Keywords: PSD, Laser diffraction, dry dispersion, Atorvastatin Calcium, non-Toxic dispersants

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AEC P-27

Validation of an In-House Analytical Procedure for Assessing Residual Solvents in Codeine Phosphate Sesquihydrate Utilizing Gas Chromatography with Flame Ionization Detection

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This study validates an in-house analytical procedure for assessing residual solvents in codeine phosphate sesquihydrate API using gas chromatography with flame ionization detection (GC-FID). Following ICH and European Pharmacopoeia guidelines, the method's performance characteristics were evaluated.[1,2]

Specificity assessments confirmed the method's ability to discern target analytes in the presence of potential interferents.[3] Linearity studies demonstrated the method's ability to generate accurate and consistent responses over a defined concentration range, establishing its suitability for quantitative analysis.[1] Precision evaluations including repeatability and intermediate precision demonstrate the method's reproducibility and reliability.[1] Accuracy is validated through spike recovery experiments, ensuring the method's ability to recover known amounts of residual solvents with acceptable deviation.[2] Additionally, robustness studies evaluate the method's resilience to minor variations in analytical parameters, affirming its stability and dependability.[3]

The validation results collectively endorse the efficacy and reliability of the developed GC-FID method for quantifying residual solvents in codeine phosphate sesquihydrate API.

Keywords: Method validation, GC-FID, API, Codeine phosphate sesquihydrate, ICH

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AEC P-28

The Non-Aqueous Titrimetric Assay of API Using Perchloric Acid as Titrant

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The Active pharmaceutical ingredients (APIs) have pharmacological activity used with combination of other ingredients to diagnose, mitigate and cure the disease[1,2]. Hence, quantification of APIs is crucial for ensuring the safety and efficacy of pharmaceutical formulations [3]. Accurate measurement of APIs content is significant for ensuring that each tablet or capsule contains the correct amount of active ingredient. Potentiometric titration allows precise determination of APIs content in pharmaceutical products, ensuring that the product meets the required purity standards.

In this study caffeine is used as model API, for evaluating the potential of the non-aqueous potentiometric titration method for assay determination. The current study is focused on the feasibility of non-aqueous titration using perchloric acid as titrant for assay determination of caffeine. The obtained data is elaborated and evaluated in terms of results interpretation and the study of the potential advantages and limitations of perchloric acid titration in non-aqueous environment.

Overall, our findings suggest that non-aqueous potentiometric titration with perchloric acid can be considered as a promising and a viable method for the assay determination of different APIs.

Keywords: Active pharmaceutical ingredients, perchloric acid, potentiometric titration.

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AEC P-29

Practical Performance of a Volumetric Karl Fischer Titration for Water Content Determination in Pharmaceuticals

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Karl Fischer Titration is a widely used analytical method for quantifying water content in pharmaceutical products. It is of great significance in pharmaceutical development, production and quality control.

Water can adversely affect quality, stability and other physical and chemical properties of active pharmaceutical ingredients (API) and finished pharmaceutical products. Precise water determination is required by pharmacopoeias, ISO guidelines and ASTM (American society for testing and materials) to ensure the quality and stability of raw materials and finished products. Knowing the water content and understanding the hygroscopic nature of APIs, as well as for the final product in which the API is incorporated is essential quality prerequisite for obtaining chemically stable finished products.[1]

Pharmaceutical products are often characterized by complex formulations. By investigating the practical performance of volumetric Karl Fischer titration, this research will provide valuable insights for optimizing water content determination in Ibuprofen DC 90 as one of the most commonly used APIs in Alkaloid AD Skopje, ensuring product quality and consistency.The implementation of the Ph. Eur. suitability test proved that methanol and Hydranal – Composite 5 are suitable as solvent and titrant, respectively. The described KF method affords accurate and reproducible results and could be applied in pharmaceutical quality control laboratories.[2]

Keywords: Karl Fischer titration, active pharmaceutical ingredient, water content, ibuprofen

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AEC P-30

Quality by Design (QbD) Approach in Development, Optimization and Validation of Analytical Method for Determination of Content in Drug Product

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Simple, specific, robust and reproducible HPLC method for determination of content of biguanide active pharmaceutical ingredient (API) in drug pharmaceutical product is developed, using two different software for design of experiments (DoE). In drug products where a significantly large number of related and degradation impurities are expected, foremost approach to develop robust, specific and transferrable method is to apply DoE approach. The ranges of the relevant parameters and their interactions were investigated and evaluated.[1] After analysis of numerus experiments designed by Fusion QbD Chromatography-centric software, analytical method for determination of content of API is chosen. That method is optimized to fulfill the criteria for specificity, as well as chromatographic and separation data according to Ph. Eur. For its contribution cyano column as stationary phase and phosphate buffer pH 3.0 with organic modifier acetonitrile as mobile phase are selected. The other parameters such as column temperature and molarity of the buffer solution were set to implement proper resolution between the main peak of the API and adjoining peaks of the related and degradation impurities. After establishment of the method was made, its robustness was investigated with DoE software MODDE, using Plackett-Burman experimental design. Results from experiments in which different window intervals of the parameters were examined, showed fulfillment of the system suitability criteria.

As last step of this development, validation of the established analytical method for determination of content of biguanide API in drug pharmaceutical product was successfully performed according to ICH Q2 (R1) guideline.

Keywords: design of experiments, content, robustness, specificity

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AEC P-31

The Microelements Content in Mustard Seeds (*Semen Sinapsis*)

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In this experiment was used a sample mustard seeds, *Brassica nigra* (L.) Koch,[1] which was purchased in a health food store originated from Ukraine. The sample was prepared in a microwave digestion device, and the qualitative and quantitative determination of microelements was performed using the ICP-OES method.[2] All the 14 microelements were found, which were arranged in descending order of content in mg/kg: Fe (64.0), Zn(24.7), Si (23.7), Mn(18.4), Al(7.7), B(6.2), Cu(4.08), V(3.04), Ba(2.44), Ni(2.16), Se(0.51), Cd(0.179), Cr(0.084) and Pb(0.072). Elements: Co, As, Be, Hg and Ti were not detected in the tested sample.

Keywords:mustard seeds, ICP-OES, microelements

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AEC P-32

Method Verification for Particle Size Distribution for Ibuprofen Lysine Using Mechanical Sieving

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Particle size is arguably the most crucial physical property of powder samples and is routinely measured across various industries, often playing a pivotal role in the manufacturing of numerous products.

Precise control of particle size distribution is essential, particularly in the pharmaceutical industry, where it significantly influences both drug development and commercial production. Furthermore, in the analysis of powders, the particle size distribution is a key parameter for evaluating quality and performance.

The main objective of the verification of the analytical procedure is to demonstrate that the procedure is suitable for use in the quality control laboratory for routine testing. This is performed according to the Guidance on validation[1]. In this study, the verification of the procedure for mechanical sieving particle size distribution method for ibuprofen lysine active pharmaceutical ingredient (API) was performed on the parameter's repeatability and precision.

In order to study the testing method's repeatability and precision[1,2] six successive measurements of individually prepared samples were performed by the same operator, on the same instrument, in two different days.

The obtained results are within the specified limits and conform to the acceptance criteria. The test method is precise and can be used for its intended use.

Keywords: verification, particle size distribution, ibuprofen lysine, repeatability, precision, pharmaceutical industry

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AEC P-33

Development of Liquid Chromatographic Method for Codeine Related Compounds in Tablets: Optimization and Validation Using DoE and Computational Tools

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Codeine phosphate tablets are used to relieve mild to moderate pain, suppress coughing, and treat diarrhea under medical supervision due to the risk of side effects and dependency. During production, it is crucial to monitor both the active component and impurity levels. While many methods exist in the literature for separating and determining codeine's related compounds, none includes the separation of methylcodeine, morphine, codeine dimer, 3-O-(codein-2yl)-morphine, 10-hydroxycodeine, 14-hydroxycodeine, thebaine, norcodeine and codeinone in this type of matrix. The aim of this work was to develop and validate a liquid chromatographic (LC) method for the simultaneous separation and analysis of active compound and impurities in codeine phosphate tablets.

Satisfactory chromatographic separation was achieved using YMC TriartC18 column (75 × 3 mm, 1.9 µm) with gradient elution of acetate buffer and acetonitrile and flow rate 0.5 ml/min. Chromatograms were monitored at 284nm,a wavelength that minimizes interference from the mobile phase. These chromatographic conditions resulted in a linearity range of 0.3 µg/mL to 7.2 µg/mL, and realization of specificity, preciseness, sensitivity, and robustness requirements according to pharmacopeia and ICH guidelines.

During method validation, Dry Lab and Modde software tools were used for optimization and robustness testing. The design of experiments approach (DoE) with these tools provided insights into how the chromatographic conditions (temperature, gradient steepness, and mobile phase pH) affected parameter interactions and separation.

Keywords: UPLC, codeine phosphate, tablets, related compounds, DoE

AEC P-34

HPLC Method Development for Simultaneous Determination of Four Structurally Diverse Compounds in a Combined Dosage Form

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A high-performance liquid chromatography method for separation and simultaneous determination of ascorbic acid (AA), dextromethorphan hydrobromide (DEX), paracetamol (PAR) and pseudoephedrine hydrochloride (PSE) in a mixture was optimized. Due to the different properties of the target compounds, current methods require different chromatographic columns and conditions using a C18, SAX and SCX column for determination of the four compounds with three methods.

The goal of this work was to develop a suitable method for separation and quantification of these four compounds in a single run. Various RP-HPLC approaches were tested using a variety of reversed-phase columns with different nature and dimensions, mobile phases with buffers in the pH range from 2-6, methanol and acetonitrile, in order to establish optimal chromatographic conditions and satisfactory resolution. It was found that using Ascentis Phenyl 250 mm × 4.6 mm, 5 µm and mobile phase composed of 0.05M KH_2PO_4 with pH=4.5 and CH_3OH gives satisfactory results with a resolution of 2.18 for the critical pair PAR-PSE within a run time of less than 20 minutes. The developed method will be validated and its robustness confirmed in order to be introduced in regular quality control of combined pharmaceutical products containing these active compounds.

Keywords: RP-HPLC, method development, dextromethorphan hydrobromide, pseudoephedrine hydrochloride, paracetamol, ascorbic acid

AEC P-35

HS-GC-MS Analysis of Biogenic Volatile Organic Compounds in Macedonian Endemic *Stachys* Species

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Biogenic volatile organic compounds (BVOCs) produced by plants are crucial for plant defense, communication and ecosystem dynamics. They offer various biological activities useful to humans, presenting a sustainable and under-exploited source of bioactive compounds.

The aim of this work was to optimize and apply a headspace-gas-chromatography-mass-spectrometry (HS-GC-MS) method for BVOC profiling of the aerial parts of various endemic plants. Plant material from the endemic species *Stachys iva* Griseb. (100 mg), collected from Pletvar near Prilep, was used to optimize headspace temperature (120 °C, 140 °C, 160 °C, and 180 °C) and sampling time (10, 20, and 30 minutes). Additionally, injector temperatures of 210 °C and 250 °C were evaluated, and the impact of adding methanol to facilitate vaporization was examined. The results indicated that the optimal parameters were an incubation temperature of 180°C, an injection temperature of 250 °C, and a sampling time of 20 minutes.

The optimized method was applied to profile BVOCs in two endemic Macedonian plant species: *Stachys iva* Griseb. and *Stachys horvaticii* Micevski. Fifty different compounds were identified, with notable differences between the species. Both *S. iva* Griseb. and *S. horvaticii* Micevski contained caryophyllene (6.75% and 9.49%) and manoyl oxide (8.32% and 12.19%). The most abundant compounds were 3-furaldehyde (10.45%) in *S. iva* Griseb. and (4aS-trans)-1,2,3,4,4a,9,10,10a-octahydro-1,1,4a-trimethyl-7-(1-methylethyl)-phenanthrene (8.95%) in *S. horvaticii* Micevski.

Keywords: endemic plants, biogenic volatile organic compounds, HS-GC-MS

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AEC P-36

Determination of a Nitrosamine Drug Substance-Related Impurity in Antiarrhythmics by LC-HRMS

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Antiarrhythmics are commonly used drugs recommended in patients with atrial fibrillation and/or supraventricular tachycardias. The presence of a secondary amine in the structure of a drug makes it susceptible to *N*-nitrosamine (NA) formation, if nitrosating agents such as nitrites from certain excipients or packaging materials are present. N-Nitrosamines have been identified as potential human carcinogens and as such have triggered a regulatory response in the form of batch recalls and initiated a global risk assessment process[1].

A highly sensitive, rapid liquid chromatography – high resolution mass spectrometry (LC-HRMS) method was developed for the determination of a nitrosamine drug substance-related impurity (NDSRI) in an antiarrhythmic drug. Chromatographic separation was achieved on a Waters XSelect HSS T3 C18 column (150 mm × 3.0 mm, 2.5 µm) using gradient elution with a mobile phase consisting of 0.1 % formic acid and methanol. Thermo Scientific Orbitrap Exlporis 120 mass spectrometer was used with heated electrospray ionization (HESI) in positive mode. The method exhibits linearity over a range of 0.1-10 ng/mL. The limit of detection and quantification were 0.05 ng/mL and 0.1 ng/mL, respectively, which satisfy the regulatory requirements. No interferences were observed due to the high selectivity of mass spectrometric detection when applied for measurement of the selected target-ion of the NDSRI.

Keywords: antiarrhythmic, nitrosamines, HPLC, HRMS, NDSRI

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AEC P-37

A Simple and Sensitive HPLC Method For Determination of Tacrolimus in Pharmaceutical Dosage Forms

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Tacrolimus (TCL) is an immunosuppressive drug commonly used in organ transplant patient rejection.[1] A simple and sensitive RP–HPLC method with UV detection was developed for determination of tacrolimus in pharmaceuticals. The separation was performed on a Watters ODS 2 column (125 mm x 4.0 mm, 5µm) with a mobile phase consisted of acetonitrile and water acidified to pH of 4.0, 45:55 (*V/V*). The flow rate was set at 1 mL min^{-1} and UV detection was performed at 210 nm. The method was validated by determination of system suitability, specificity, linearity, precision, accuracy, limit of detection and limit of quantitation and robustness, following the ICH Q2(R1) guidelines.[2] The advantages of this method were: simple sample preparation, good precision (RSD < 2%) and high recovery (> 99%). Linearity was studied in the range of 0.0397 – 0.318 mg mL^{-1}. The limit of detection was 8.1 µg mL^{-1}, while limit of quantitation was 24.6 µg mL^{-1}. The limit of detection was compared with the one determined by DPV – Differential Pulse Voltammetry for the electrochemical nanosensor for the TCL. The main peak was obtained at 2.2 V for 0.0025M TCL. The method could be applied for routine quality control of pharmaceuticals and for evaluation of potentially counterfeit capsules containing TCL.

Keywords: Tacrolimus; High performance liquid chromatography; Immunosuppressive drugs

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AEC P-38

Optimizing Experimental Conditions for Accurate Mancozeb Detection in Soil Via HS-GC-MS

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Analysing different classes of pesticide residues in soil is an analytical challenge due to the complex physicochemical properties of these compounds, their variable stability and the complex soil matrix. Dithiocarbamates (DTCs) are one of the first classes of broad-spectrum fungicides widely used worldwide to control fungal diseases in a variety of crops. Despite their rapid degradation in the environment through processes such as photolysis and hydrolysis, DTCs remain one of the most commonly detected pesticides in the European Union (EU), which means that they need to be monitored.

DTCs fungicides, such as mancozeb and thiram, are polymeric metal-coordinated complexes that make direct analysis impossible. Their insolubility in both aqueous and organic solvents further complicates the analytical process and renders conventional multiresidue methods ineffective. For this reason, a method involving chemical cleavage of DTCs with stannous chloride and hydrochloric acid, followed by the partitioning of the released carbon disulphide (CS_2) in isooctane and its determination by gas chromatography, was developed for their analysis in food.

In this work, the method proposed for the determination of DTCs in food was adopted for sample preparation and determination of mancozeb in soil by measuring the released CS2. The quantitatively collected CS_2 from the soil samples was quantified by headspace gas chromatography coupled with mass spectrometry (HS-GC-MS) using the selected ion monitoring of the target analyte, carbon disulphide. The concentration of CS_2 was determined by external calibration using a standard solution of CS_2 in isooctane, with the residue expressed as CS_2 and calculated to be expressed as mancozeb. The analytical performance of the method was evaluated by testing its linearity, accuracy and precision. To demonstrate its applicability, it was used to analyse real soil samples after treatment with mancozeb.

Keywords: Dithiocarbamates (DTCs), mancozeb, soil, CS_2, HS-GC-MS

AEC P-39

Chemometric Approach to Modeling the Extraction Method Parameters for Toxic and Strategic Elements from Fly Ash Samples

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The modern development of industry brings with it an increasing energy demand. In Serbia, a significant portion of electricity is generated by burning coal in thermal power plants, which results in the production of large amounts of industrial waste: fly ash, bottom ash, and slag. These waste materials can contain both toxic and strategically important elements. By determining the quantity of toxic elements present, proper handling of this hazardous waste can be ensured. Additionally, extracting strategic elements from waste materials could offer an ecological alternative to mining.

In this study, a comparison of two digestion methods was conducted: HNO_3/HCl/HF and HNO_3/H_2SO_4 with V_2O_5. Additionally, modeling of microwave digestion parameters was performed, including temperature, time, catalyst, and type of mineral acids. The investigations were carried out on seven different fly ash samples.

The obtained results were processed using advanced techniques of multivariate chemometric analysis: artificial neural networks (ANN), cluster analysis (CA) and principal component analysis (PCA). The results indicated that lower temperatures and the method HNO_3/H_2SO_4 with V_2O_5 are more suitable for volatile toxic and some strategic elements, whereas higher temperatures and the method HNO_3/HCl/HF are more suitable for other elements, including most of the strategic elements.

Keywords: Fly ash, Strategic Elements, Artificial Neural Networks, Cluster Analysis, Principal Component Analysis

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).

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AEC P-40

Identification of Essential Oils Carried Out by Gas Ghromatography (GC)-FID Method

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This review describes analytical technique for the analysis of composition components in essential oils. Essential oils are complex mixture of volatile natural chemicals, mainly from plant materials[1]. Separation of components depends on the polarity and volatility of the analytes[2]. Gas chromatography is an analytical tool for quantitative analysis of this complex compounds[3], partitioning the solutes between the mobile and stationary phase. It is widely accepted tools for the separation of compounds because of its simplicity, sensitivity, and effectiveness. The qualitative analysis of essential oils by GC is based on the comparison of the peaks in the chromatogram for the essential oil with those of authentic standards separated with the same chromatographic conditions[4]. The detection of the composition component in essential oils with GC-flame ionization is a reproducible method for their determination. This method is specific for identification of essential oils compounds, based on the identification and chromatographic separation of three of its main components. This method procedure can be recommended for routine pharmaceutical analyses.

Keywords: Gas chromatography; Essential oils, Flame Ionization Detector

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AEC P-42

Occurrence, Identification and Distribution Characteristics of BTEX In Urban Shallow Lake Sediment

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BTEX group usually monitored in urban environment include benzene, toluene, ethylbenzene, and xylenes. Benzene is classified by International Agency for Research on Cancer (IARC) as human carcinogen (gr. 1) and poses a significant harmful risk to human health. Exposure to BTEX compounds can occur by ingestion, inhalation or absorption and rarely, across the skin. Once released to the environment, BTEX can volatilize, dissolve, attach to sediment/soil particles or degrade biologically. Increased pollution of surface water and sediments with such hazardous compounds therefore requires implementation of systematic monitoring and evaluation of the sediment quality[1]. Unplanned urbanization and large-scale industrialization made urban lakes sinks for untreated waste. The objectives of this study were to both identify and quantitatively analyze BTEXS in surface sediments of the urban shallow lake positioned in Central Serbia, using purge-and-trap (P&T) gas chromatography/mass spectrometry (GC/MS), and multivariate analysis to further identify pollution sources[2].

Keywords: VOCs; sediment quality; pollution sources; multivariate analysis.

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AEC P-43

A Comprehensive Analysis, Source Apportionment and Health Risk Assessment of Polycyclic Aromatic Hydrocarbons in Urban Shallow Lake Sediment

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Polycyclic aromatic hydrocarbons (PAHs) are ubiquitous environmental pollutants. Based on their toxicity and potential for human exposure, the US EPA and the EU have designated 16 priority PAHs. PAHs in the environment originate primarily from two sources, petrogenic and pyrogenic. Lake sediments are the most valuable natural archive documenting PAH contamination. PAHs can persist in lake sediment systems, posing a long-term threat to the environment. PAHs that were historically deposited can be remobilized upward in sediments and resuspended into the aquatic environment[1]. PAHs in sediment from urban shallow lake in Central Serbia were investigated in terms of their concentration, distribution, and potential effects on the environment and human health by calculating the toxic equivalent quantities (TEQs) and incremental lifetime cancer risk (ILCR). This study revealed the pollution characteristics of PAHs and their possible sources in lake sediments, clarified its correlation to regional anthropogenic activities, and provided corresponding risk management strategies for human and aquatic organisms.

Keywords: PAH; sediment quality; cancer risk; diagnostic ratio; multivariate statistics.

Acknowledgment: This research was financially supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Contract No:451-03-66/2024-03/200026 and 451-03-65/2024-03/200135).

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AEC P-44

Optimization of GC-MS Methods for Characterization of the Volatile Compounds in Macedonian White Wines

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Wine aroma is among most important attributes of wine quality. Identification and quantification of volatile compounds in wine is usually performed by gas chromatography coupled to mass spectrometry (GC-MS). A crucial step in the analysis is the appropriate sample preparation and for this purpose several techniques are usually applied, among which liquid-liquid extraction, solid-phase extraction, and solid-phase microextraction have been most commonly used.

Three approaches were used in this work to determine the aromatic profile of Macedonian white wines: liquid-liquid extraction with dichloromethane, liquid-liquid extraction with hexane and analysis of volatiles using headspace sampling followed by GC-MS. Headspace sampling was found as a much more convenient technique but with a limited number of detected compounds. Dichloromethane was found to be a more efficient extraction solvent with a higher number and yield of volatiles especially alcohols compared to hexane. A complex composition of the extracts after liquid-liquid extraction of the tested white wines has been identified with different groups of volatile compounds, such as alcohols, esters, aldehydes, lactones, phenols, and terpenes. Isopentanol, hexanol and phenethyl alcohol have been detected in all samples as well as isoamylacetate and ethyl esters of hexanoic, octanoic, decanoic and succinic acid. Linalool was also found in all samples whereas alpha-terpineol and citronelool were detected in selected samples. Differences between the wines have been evaluated in order to reveal specific variety related aroma compounds.

Keywords: aroma, volatile compounds, identification, LLE, headspace, GC-MS, white wine

AEC P-45

Optimization and Validation of Gas-Chromatographic Methods for Determination of Chlorination By-Products in Drinking Water

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Trihalomethanes (THMs) are chlorination by-products formed as a result of the reaction of residual chlorine, used as a drinking water disinfectant, with organic matter in raw water. The four main THMs ($CHCl_3$, $CHBrCl_2$, $CHBr_2Cl$ and $CHBr_3$) have been confirmed as human carcinogens and are meticulously controlled in drinking water. The development of the sensitive THMs quantification methods are useful in kinetic studies for the optimization of drinking water treatment and for monitoring and maintaining the lowest THM values. Gas chromatography with different detectors is the method of choice for separation and measurement of THMs and the sample preparation is mostly done by liquid-liquid extraction (LLE) in hexane.

In this work, two detection systems and two injection techniques for determination of THMs with gas chromatography have been optimized and the results compared. Liquid–liquid extraction followed by gas chromatography-mass spectrometry (GC-MS) and also by gas chromatography-electron capture detection (GC-ECD), as well as headspace-gas chromatography-mass spectrometry (HS-GC-MS) have been tested. The LLE and liquid injection proved to be more reliable and sensitive for quantification than headspace. Both MS (operated in the selective ion monitoring, SIM) and ECD were found applicable and with the required sensitivity in the range of 1 ppm. However, the electron-capture detector demonstrated better sensitivity in the range down to 0.5 ppm for chloroform and even better for the other THMs. Quantification method using LLE and GC-ECD was validated to demonstrate its ability to detect and reliably measure low concentrations of these toxic compounds.

Keywords: Chlorinated water, disinfection by-products, trihalomethanes, chloroform

AEC P-46

Optimization of a RP-HPLC Method For Trace Analysis of Pharmaceutical Compounds in Waters Using UV and ESI-QTOF-MS Detection

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Optimization of analytical methods for the analysis of pharmaceutical substances is crucial for ensuring their safety, efficacy, and quality, but also for addressing their growing impact as emerging water pollutants. The aim of this study was optimization of a reversed-phase high-performance liquid chromatography (RP-HPLC) method for simultaneous separation and analysis of 17 pharmaceutical substances from different classes, including cardiovascular, nonsteroidal anti-inflammatory drugs (NSAIDs), antibiotics and benzodiazepines that are widely prescribed and used. These compounds not only play crucial roles in medical treatments but are also increasingly detected as contaminants in water sources, posing environmental and public health risks.

Separation of the target compounds was achieved using C18 columns (250 mm × 4.6 mm, 5 µm, or 150 mm × 4.6 mm, 3.5 µm) with gradient elution with methanol and 0.1% formic acid in water. The detection method employed both, ultraviolet (UV) and quadrupole-time of flight mass spectrometry (QTOF) with electrospray ionization (ESI) in positive and negative mode. Complementary information was obtained for the optimal detection sensitivity for the target analytes. The optimized RP-HPLC method offers good chromatographic separation, short analysis times, and applicability to the trace analysis of the pharmaceutical substances. Both, the selectivity and the sensitivity together with the wide scope of the MS detection further enhance the versatility of the analytical approaches enabling the determination of contaminants of emerging concern in waters.

Keywords: pharmaceutical compounds, waters, HPLC-UV, HPLC-ESI-QTOF

AEC P-47

Vapor Recovery Unit – Process Principles

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Vapor Recovery Unit (VRU) is designed to recover evaporated gasoline vapors during trucks loading. The unit uses principles of Adsorption and Absorption, but most important step during operation of the unit is Regeneration (Desorption) of the saturated carbon bed that is filled into dedicated vessels named as Adsorbers.

VRU is equipped with two Adsorbers, Absorption column, separator for glycol/gasoline, feed vacuum seal fluid (ethylene glycol) pump, vacuum pump, gasoline supply and return pumps.

Evaporated gasoline vapors from the trucks are adsorbed into pre-activated carbon which is 90 % saturated. When the carbon riches 100% saturation than Hydrocarbon analyzer trips regeneration (desorption) of the saturated carbon. Regeneration of the carbon is based by reducing absolute pressure into adsorber up to 50 mbara. Reducing of required pressure is performing by vacuum pump that operates with seal fluid. As seal fluid is using pure ethylene glycol. At absolute pressure at 50 mbara desorption process at carbon bed starts and it last for 10 minutes. Crucial step is purging of the carbon bed with fresh air after elapsing of 10 minutes. Purging time is 5 minutes and purpose of this step is to remove desorbed gasoline that is on surface of the carbon. Removed gasolines together with the seal fluid go into gasoline/glycol separator that is designed with two compartments. At first compartment separation of the gasoline from glycol is performing and in the second compartment the absorption column is mounted. Purpose of absorption column is absorbing of gasoline vapors that appear into separator. Absorption is performing by flushing of gasoline vapors with fresh gasoline at the top of the column. Recovered gasoline with return gasoline pump is discharged into gasoline storage tanks.

Recovery performance of the unit is 2-3 m^3 gasoline per 100.000 m^3 loaded gasoline.

Keywords: Vapor Recovery Unit

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AEC P-48

Determination of Polycyclic Aromatic Hydrocarbon Types in Diesel fuel by HPLC Method with Refractive Index Detector and Operational Experiences

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The determination of polycyclic aromatic hydrocarbon types in diesel fuel with HPLC method using a refractive index detector is the most appropriate technique for the separation of these types of aromatic compounds as a part of the complex diesel mixture. According the EN 12916 method for determination PAH's, we used aminopropyl- bonded stationary phase as polar in the normal-partition mode with relatively nonpolar mobile phase, n-heptane. This column has a strong selectivity for aromatic hydrocarbons and modest affinity for non-aromatic hydrocarbons. As a result of this selectivity, the aromatic hydrocarbons are separated from the non- aromatic hydrocarbons according to their ring structure i.e. MAH, DAH and Three+ AH compounds. The column is connected to a RID that detects components as they elute from the column. The electronic signal from the detector is continually monitored by a data processor. The amplitudes of the signals from the aromatics in the sample are compared with those obtained from calibration standards in order to calculate the mass fraction of MAH, DAH and T+ AH in the sample. The sum of DAH and T+ AH mass fractions are reported as the mass fraction of POLY- AH and the sum of MAH, DAH and T+ AH mass fractions is reported as the mass fraction of total aromatic hydrocarbons. According to the regulations and standards for the quality of diesel fuel, this group of compounds that occur as a result of fuel combustion must be monitored due to the fact that they are significant environmental pollutants, and their presence in diesel fuel poses health risks due to their carcinogenic and mutagenic properties.

Keywords: RID, HPLC, MAH, DAH, T+ AH, Diesel fuel, Hydrocarbon.

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AEC P-49

Improvements of Precise Modeling Vs. Screening Models for Metals Depositions in Environment: Case Study Bregalnica River Basin

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In the last decade there has been a research expansion of methodologies that establish fast and effective methodological approaches for monitoring soil surface dust deposits. Long-term lithogenic degradation effectively disrupts a number of natural conditions in the environment. Certain surveys, especially in larger areas, require quick and easy screening of a given area. Analytical techniques are absolutely dominant when it comes to quantification of chemical elements.

This study focusses on extracting two differ chemometric approaches for identification of the affected zones of metals in environment with emphasis on air and soil metallic distribution. Long term investigated area has been selected along the river basin of Bregalnica River in N. Macedonia. The cross validation has been introduced for several metals: Pb, Cd, Cu, Fe and Zn.

The first represented approach extracts the chemometric model with precise quantification with application of ICP-MS and data visualization with application of artificial neural network – multilayer perceptron (ANN-MLP). Model obtained by ANN was tested for the lithologenic (soil samples) distribution and atmospheric (moss samples) distribution. The second approach represent a chemometric model using moss bioindication and FESEM analysis, as initial research for subsequent screening models. This chemometric model is suitable for screening for large areas in order to identify critically affected zones. Comparative overview reveals that quantitative chemical analysis with precise ANN-MLP visualization still remains an irreplaceable identification method for determining the multi-element distribution in the environment.

Keywords: soil, moss, metals, environmental distribution, ICP-MS, ANN-MLP, FESEM.

AEC P-50

Cellulose Recovery from Cigarette Butts

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A large consumption of cigarettes worldwide (5.7 trillion in 2020) contributes to the creation of huge amounts of cigarette butts as waste. Overall, 97% of cigarette filters are based on cellulose acetate a poorly biodegradable polymer[1]. The aim of this study is optimization of the cellulose isolation from cigarette butts.

The cleaned cigarette butts (CBs) free of unburnt tobacco and ash were water-swollen to paper unwind. After washing with hot water, squeezing, and soaking in 96% *v/v* ethanol the separated material was bleached with 1.25% *w/v* sodium hypochlorite solution (25°C, 6 h). The alkaline deacetylation (0.25 mol/dm^3 ethanolic solution of sodium hydroxide with pH=13, 1 h, 25°C) was carried out without or by applying an ultrasound. The cellulose acetate was converted to cellulose by hydrolysis with 55% *w/v* sulfuric acid (45°C, 1 h). The cellulose acetate and cellulose yields were gravimetrically determined, and the cellulose acetate substitution degree with ASTM D 871-96 method.

The determined yields of cellulose acetate and cellulose were 76.2% and 25.6%, respectively. Ultrasound applied in alkaline deacetylation increased the yields of cellulose acetate (78.0%) and cellulose (26.8%). Cellulose degradation was higher in the ultrasonic treatment, with the degree of substitution of 2.5 decreasing to 0.09 compared to the non-ultrasonic treatment where a higher value was determined (0.21). Cellulose recovery reduces the impact of cigarette butts on the environment.

Keywords: cigarette butts, cellulose acetate, cellulose, ultrasound, environmental impact.

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AEC P-51

Waste Stalks of Hot Red Pepper Fruits Potential Source of Nutritional and Bioactive Compounds

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Pepper (*Capsicum annuum* L.), an important vegetable used as food and spices is compose of valuable nutritional compounds and phytochemicals (capsaicinoids, phenolics, and carotenoids). The edible part is pericarp, while seeds, placenta, and stalk are waste generated during the pepper fruit processing.[1] This study aims to characterize the waste stalks of hot red pepper fruits in terms of nutritional and bioactive compounds.

The stalks of hot red pepper fruits (*Capsicum annuum* L. ssp. *microcarpum longum conoides*) manually separated by cutting with a knife were ground to a particle size of 0.1 mm. The nutritional chemical composition was determined by standard AOAC procedures. In stalk ethanolic extracts the content of total carotenoids (capsanthin extinction coefficient $^{1\%}E_{460nm}$ = 2300), and capsaicin (calibration curve of standard solutions of capsaicin in ethanol at 282 nm absorbance) was determined.

In the stalks, expressed in relation to the dry matter 17.81% protein, 3.79% fat, 9.94% ash, 25.34% cellulose, and 6.29% reducing sugars were determined. The quantity of total extract was 241.07 mg/kg, while the contents of total carotenoids and capsaicin were 230.75 and 29.47 mg/kg, respectively. The valorization of stalks in animal feed, nutritional supplements, or polymeric material will be highly valued instead of the negative environmental influence caused by their dumping as waste.

Keywords: hot red pepper fruit stalks, nutritional and bioactive profile, environmental influence.

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BIOTECHNOLOGY AND FOOD TECHNOLOGY

BFT O-1

Novel Non-Invasive Method for Determination of Immobilized Macromolecules

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Immobilized proteins are one of the most important affinity ligands. Despite that, there is no simple method that allows direct, non-invasive detection. Presented method is based on the pH transition, forming during change of solution ionic strength. The method utilizes the ionic character of the immobilized protein, while implementing biologically compatible buffers. Proteins glucose oxidase, horseradish peroxidase, bovine serum albumin, lysozyme and protein A were immobilized in different amounts on a porous polymeric matrix and their pH transition was measured using lactate buffer of various concentrations and pH values[1,2]. A linear correlation was found between the amount of immobilized protein and the amplitude of the pH transition, allowing the detection down to 2 nanomoles of immobilized protein. By changing the buffer concentration and pH, the sensitivity of the method can be tailored. Results were described by a mathematical model based solely on protein amino acid sequence, buffer pK_a value(s) and amount of immobilized protein. Since the proposed method is non-invasive, it can be routinely applied during optimization of immobilization protocol, for quality control, but also as an in-process monitoring tool.

Keywords: immobilized protein quantification, pH transition, mathematical model

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BFT O-2

Isolation Media for Purple Phototrophic Bacteria

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The isolation and cultivation of purple non-sulfur bacteria (PNSB) are pivotal for research advancements in microbial ecology, bioenergy, and biotechnology. This study summarizes the most used media for isolation and contributes by their optimization to enhance the growth and purity of PNSB populations.

The media are formulated to meet the specific metabolic needs of these phototrophic organisms, providing a balanced mix of organic and inorganic nutrients, including a carbon source, nitrogen, sulfur, and essential trace elements. To simulate the natural habitat of PNSB, anaerobic conditions and appropriate light intensity were maintained. Comparative analysis with established media such as Mineral Salt Medium (MSM), Pfennig's Medium[2], Rhodospirillaceae Medium (RS Medium)[1], and Van Niel's Medium[3] demonstrated the superior performance in selectively promoting PNSB growth while inhibiting non-target microorganisms. The efficacy of the isolation media was validated through successful isolation of several PNSB strains from environmental samples, confirmed by morphological and physiological characterization. These findings refine microbial isolation techniques and facilitate further exploration of PNSB's ecological roles and potential applications in sustainable technologies.

Keywords: Purple Phototrophic Bacteria, Isolation Media, Biotechnology

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BFT P-1

Technology of Chocolate Prunes Production

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The plum has no longer the economic importance it once had, but it is still our most widespread and important fruit. The drying process must be adapted to the physical and chemical properties of the fruits are determined based on their research. Chemical properties per 100g of plum: dry matter 14.5-20.2%, soluble dry matter 13.2-18.5%, ashes 0.37g, cellulose 0.42g, pH 3.90, total sugars 8,3-11,9%, pectic acid 0.33g, protopectin 0.21g.

Therefore, it can be stated that the same drying process does not have to be for every plum variety. Plums are dried most often with a stream of warm air (convection drying) and in exceptional cases, heating the medium (heat carrier) can also be another gas (nitrogen or carbon dioxide).

Dried plums are more suitable for further processing than fresh ones, because the drying process is used for preservation, thus extending the useful life of the fruit. Dried prunes are a dense source of essential nutrients. The phenolic compounds present in prunes act as antioxidants, helping to combat oxidative stress and may reduce the risk factors of certain chronic diseases.

A special type of chocolate is used for the topping, the so-called "tunk masa" [1]. It is obtained by a special technological procedure, i.e. by processing the cocoa mixture mass, sugar and cocoa butter. The product has a low viscosity, it is grainy, which allows to be used as a topping mass. "Tunk mass" must contain a minimum of 33% cocoa mass and the appropriate amount of cocoa butter, so the finished product must contain a minimum 35% cocoa butter. It must not contain more than 50% sugar.

Keywords: prunes, chocolate, food technology

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BFT P-2

Nutritional Values of Products Obtained by Incorporation of Nettle (*Urtica Dioica* L.) Seeds

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Nettle (lat. *Urtica*) is a perennial herb that belongs to the Urticaceae family[1]. Due to its nutritional and functional richness, nettle is the subject of increasing scientific interest and the development of new products. Food products must have a certain nutritional value to meet certain physiological needs of people. To improve the nutritional quality of wheat flour-based products, this work aimed the incorporate nettle seeds into such products. In this regard, the chemical composition (carbohydrates, proteins, oils, fibers, ash, moisture) and the mineral composition (essential minerals, essential trace and non-essential minerals) of products were determined and results were compared with the control product (product without nettle seeds).

The replacement of wheat flour with nettle seeds (30%) contributes to a statistically significant increase in the proteins (1.4 times), lipids (1.36 times), fibers (2.7 times), and ash (9.63 times) content, but not carbohydrates (compared to control product, the content was less for 1.1 times). Of the main essential and trace essential minerals, the most abundant were calcium (790.97 mg/100g) and iron (3.62 mg/100g). Compared to the control product, the content of calcium and iron was higher by 2.82 and 2.35 times, respectively. The results indicate that nettle seeds are an adequate incorporative component for the formation of wheat flour-based products with improved nutritional potential and such products are recommended especially because of the high content of fibers and minerals such as calcium and iron.

Keywords: nettle seeds, food products, nutritional properties, chemical composition, minerals

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BFT P-3

Antioxidant Activity of Edible Chitosan Films Obtained by Incorporation of Iva Grass (*Teucrium Montanum* L.) Extract

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The production of edible packaging based on polysaccharides has been developing greatly in recent years. With the use of edible—and therefore degradable—materials, it is possible to reduce the production of waste significantly. Chitosan belongs to the film-forming components that are most often proposed for use in the production of edible packaging[1]. *Teucrium montanum* L. (Iva grass) is a grass crop that has long been consumed both as an herbal medicine and as a nourishing food due to its antibacterial, antifungal, anti-inflammatory, and antioxidative activity[2]. In this work, the incorporation of different concentrations (3%, 3.75% and 5%) of iva grass extract into chitosan films (A, B, C) was carried out to obtain edible films with better physicochemical properties. The results were compared with the control chitosan film (without extract, film D).

The total phenolic content of iva grass amounts to 117.29 mg GAE g^{-1} of the sample, while films A, B, and C show the content of 18.42, 21.75, and 29.26 mg g^{-1}. The antioxidant potential expressed as EC_{50} value was 0.17 mg mL^{-1} for iva grass, while films A, B and C were 0.72, 0.18 and 0.08 mg mL^{-1}, respectively. Film D showed a maximum antioxidant potential of 34.33% (under 50% of neutralization of free radicals), indicating significantly low antioxidant potential. The incorporation of iva grass into the chitosan film contributes to a significant increase in the antioxidant potential of edible films, indicating a good potential for their application in the food industry.

Keywords: *Teucrium montanum* L., phenolic compounds, antioxidant potential, chitosan, edible films

Acknowledgements: This research was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia, Scientific Research Funding Program, ev. no. 451-03-65/2024-03/200133.

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BFT P-4

Phytochemical Potential of Wild Berries from the Area of the Pešter Plateau (Serbia)

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The past 20 years have seen a rise in interest in eating wild fruits because of their high bioactive nutrient content and significance as dietary antioxidants. In this study, the wild berry fruits (strawberry, blackberry, and rapsberry) from the Pšeter Plateau region were examined to determine the level of secondary metabolites. The total phenolics, flavonoids, tannins, and anthocyanins were evaluated. Samples of the same species were taken from localities that are at least 10 kilometers apart. The results of phytochemical analysis are shown in Table 1. The highest concentration of all examined secondary metabolites was recorded in blackberry fruits. Wild strawberry and raspberry fruits contain a similar amount of examined bioactive compounds.

Table 1. Total phenolic content (mg GA g^{-1} of extract), flavonoid concentration (mg Ru g^{-1} of extract), tannins (mg mL^{-1} of extract), total anthocyanins (μg mL^{-1} of extracts)

	Total phenolic content	Total flavonoid content	Tannin content	Total anthocyanin content
Fragaria vesca	46.51	4.43	0.31	2.97
Fragaria vesca	38.52	5.32	0.38	0.52
Rubus caesius	62.26	7.11	0.95	7.61
Rubus caesius	50.10	5.81	0.47	7.61
Rubus idaeus	38.41	3.50	0.20	2.36
Rubus idaeus	29.76	4.54	0.35	5.77
Rubus idaeus	38.74	3.76	0.52	0.79

Our results indicated promising perspectives for usage of wild berry fresh fruits from Pešter Plateau (which is known as an ecologically significant area) with considerable levels of bioactive compounds. Bearing in mind that wild berries grow without the addition of fertilizers, pesticides, and other additives, they could be an excellent nutritional alternative.

Keywords: wild berries, Pešter Plateau, secondary metabolites, bioactive compounds.

BFT P-5

Phytochemical Potential of Cultivated Berries from the Area of the Pešter Plateau (Serbia)

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The fruit-growing culture is widely represented throughout Serbia. Most often, raspberries are grown (for commercial purposes), but also blackberries and blueberries. In this study, the berry fruits (chokeberry, cherry, red currant, black currant, and raspberry) that are grown in the area of the Pšeter Plateau region were examined to determine the level of secondary metabolites. The total phenolics, flavonoids, tannins, and anthocyanins were evaluated. Fruit samples were taken at the time of full maturity. The highest concentration of all total phenols was recorded in chokeberry fruits (38.55 mg GA g^{-1} of extract). Chokeberry fruits also contain the highest concentration of anthocyanins (14.09 μg mL^{-1} of extracts). Blackcurrant fruits have the highest concentration of flavonoids (6.92 mg Ru g^{-1} of extract) and tannins (0.59 mg mL^{-1} of extract). Surprisingly low concentrations of phenols were recorded in the fruits of red and dark currants (0.71 and 3.75 mg GA g^{-1} of extract). The concentration of flavonoids is fairly uniform in all samples. The concentration of anthocyanin in the fruits of cherry, red currant, and raspberry has several times lower concentrations than chokeberry. The tannin concentration is uniform in the examined fruits and ranges from 0.062 mg mL^{-1} of extract (cherry) to 0.59 mg mL^{-1} of extract (blackcurrant).

Our results show that cultivated berries from the Pešter Plateau have high concentrations of bioactive substances, which makes them recommendable for dietary use. This result can be related to the fact that this fruit grows in unspoiled environmental conditions.

Keywords: cultivated berries, Pešter Plateu, secondary metabolites, bioactive compounds.

BFT P-6

Evaluation of the Antifungal Potential of *Streptomyces* sp.

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Secondary metabolites produced by the genus *Streptomyces* include a wide range of bioactive metabolites with antibacterial, antifungal, and antiviral activity, compounds with insecticidal and herbicidal properties, enzymes, antitumor agents, and immunomodulators[1]. The potential of *Streptomyces* antifungal compounds is high, given their genetic diversity and ability to synthesize various chemical structures. *Streptomyces* spp. and their antifungal compounds have great potential in agriculture and the food industry, against fungal pathogens and contamination. *Fusarium graminearum* and *Fusarium verticillioides* are important phytopathogenic fungi that cause great economic losses in cereals. Contamination of crops with *Fusarium* mycotoxins not only reduces the market value of products but also poses a challenge to food security and public health. *Streptomyces* biologically active substances represent potential biopesticides with minimum impact on ecosystems. In contrast, intensive soil management and applied food industry chemicals impact terrestrial and aquatic ecosystems and cause adverse effects on living organisms. This research aimed to determine the potential antifungal effectiveness of indigenous soil isolates of *Streptomyces* sp. on two strains of *F. graminearum* and *F. verticillioides in vitro*. The results did not provide a statistically significant inhibition of tested *Fusarium* isolates, so further research is needed to reisolate and identify more efficient *Streptomyces* strains.

Keywords: *Actinobacteria, Fusarium graminearum*, *Fusarium verticillioides*, biocontrol, cereals

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BFT P-7

Characterization of Silver Nanoparticles Biosynthesized by Aqueous Extracts *Rubus Spp*. Leaves

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Alternative biometallic nanoparticles are becoming increasingly interesting from the synthesis point of view since biomolecules reduce metal ions which is an environmentally friendly method[1]. Silver nanoparticles were stabilized by aqueous extracts of *Rubus spp*. Leaves at room temperature. Before that, the extract was obtained by maceration at room temperature. The nanoparticles thus obtained were subjected to characterization using X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray (EDX), dynamic light scattering (DLS) and zeta potential.

XRD analysis showed 2θ peaks at about 38.2°, 44.3°, 64.5, 77.4° corresponding to (111), (200), (220), (311) planes where the plane (111) has the most intense peak. The average size of crystallites obtained by biosynthesized AgNPs-E was 18.0±3 nm. SEM analysis showed that spherical nanoparticles dominate in the sample. The EDS spectrum confirms the presence of silver via the most intensive signal at about 3 keV. The atomic and mass content of silver in the sample were 89.6 and 97.9 %, respectively. Elemental mapping of nanoparticles shows the dominant presence of silver. The average value of the zeta potential was -25.9 mV, while the average nanoparticle's size was 50.93 nm. The average values of mobility and conductivity were -2.028 μmcm/Vs and 0.587 mS/cm, respectively. The bioactivity of nanoparticles synthesized in this way should be investigated for potential use in cosmetic preparations.

Keywords: silver nanoparticles, blackberry leaves, characterization

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BFT P-8

Implementation of the Circular Economy Principles in Production of Denitrifying Agent Microbial Biomass

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Denitrification ability of several bacterial species has found application in cultural heritage protection via biocleaning pathways for nitrate removal, considering nitrate salt efflorescence on the cultural heritage surface as the main cause of deterioration. *Pseudomonas stutzeri* ATCC 17588 is a well-known denitrifier with already investigated applications in cultural heritage biocleaning. Considering the direct dependence of biocleaning efficiency on the biomass concentration of the denitrifying agent, the question of techno-economically sustainable biotechnological production of viable denitrifier's microbial biomass is77tmostt importance. This study has investigated possible implementation of the circular economy principles in biomass production of *Pseudomonas stutzeri* ATCC 17588 by using several industrial effluents as cultivation media, including meat industry wastewater, whey from dairy industry, winery effluents, sugar industry effluents and wastewater from fruit processing. The highest number of viable cells was obtained using the wastewater from wine barrels washing (9.3 log(CFU/mL)), followed by meat industry effluents (9.2 log(CFU/mL)) and wastewater from fruit processing (9.1 log(CFU/mL)). The obtained results were highly comparable with commercial synthetic media nitrate broth and nutrient broth (9.3 log(CFU/mL)) and suggest potential of the aforementioned industrial effluents to be incorporated in the industrial symbiosis system aimed at production of denitrifying agents for cultural heritage biocleaning.

Keywords: *Pseudomonas stutzeri*, cultural heritage, industrial effluents, biocleaning

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BFT P-9

Determination of Total Phenolic Content, Antioxidant, and Antimicrobial Activities of Green Vegetables

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Modern trends in nutrition imply the daily intake of fresh fruits and vegetables, with the statement that they are important natural antioxidants that protect the body from oxidative stress. Green vegetables with a high total phenolic content (TPC), are especially highlighted. The TPC values of several types of green vegetables (brussels sprouts, cabbage, broccoli, parsley, borecole, and spinach) were determined by the Folin-Ciocalteu method. The antioxidative ability of chosen green vegetables were determined using DPPH and ABTS methods. The same samples were tested for antimicrobial activity against seven laboratory control strains of bacteria and one yeast. The obtained results indicate that there is a significant correlation between TPC and the antioxidant and antimicrobial potential of methanol-water extracts of selected green vegetables. *i.e.*, the high total phenolic content does influence the antioxidant activity of tested green vegetables from the *Brassicaceae, Amaranthaceae*, and *Apiacaae* families. Overall, these everyday consumed vegetables were shown as a good source of antioxidants for regulating free radicals in our body.

Keywords: green vegetables; total phenolic content; antioxidative activity; antimicrobial activity.

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BFT P-10

Effect of Extraction Process Parameters on the Recovery of Bioactive Phenolic Compounds from Blueberry Pomace

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Polyphenols are natural secondary metabolites produced by plants, well known for their strong antioxidant properties and potential health benefits, including the prevention of chronic illnesses such as cardiovascular diseases, osteoporosis, neurodegenerative diseases and some cancers.[1] Blueberries (*Vaccinium myrtillus* L.), can be processed into juice, wine, jam and marmalade. Berry processing generates large quantities of pomace, which consists of skin, seeds and some flesh.[2]

The aim of the present study was to assess the effects of solid-liquid extraction parameters (solvent composition, solid/liquid ratio and extraction temperature) on the total phenolic and total flavonoid contents isolated from blueberry juice pomace.

The content of extracted phenolic compounds directly depends on: extraction method, the solvent, the duration of the process, the extraction temperature etc. Results show that the maximum concentrations of total phenolic and flavonoids were extracted from blueberry pomace using 50% ethanol. An increased volume of solvent relative to the amount of plant material, results in a more efficient extraction process. The influence of the extraction temperature on the yield of extractive substances was examined in the range from 25°C to 45°C. The temperature increase resulted in growth of total phenolic and flavonoids yield in blueberry pomace extracts.

Keywords: blueberry pomace, phenolic compounds, extraction parameters

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BFT P-11

Future of Lectins: Plant Lectin Jacalin and Human Lectin Galectin 3 Interact with Biologically Important Molecules

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Lectins are carbohydrate-binding proteins, spread in plants, animals, humans, and bacteria. Jacalin is a plant lectin that specifically recognizes the tumor-associated Thomsen–Friedenreich antigen which is expressed on the glycosylated proteins in cancer cells. We studied the interaction of jacalin with curcumin. Our results have demonstrated that steady-state fluorescence and fluorescent labeling of jacalin are appropriate for studying jacalin-curcumin interactions. The affinity of jacalin for curcumin is in the micromolar range (registered by fluorescence and microscale thermophoresis). We also found that jacalin binds Au porphyrin, registered by fluorescence spectroscopy.

Human galectin-3 (hGal-3) is a mammalian lectin. Interestingly, multimerized extracellular hGal-3 is thought to crosslink cells by binding to glycoproteins/ glycosylated cancer antigens on the cell surface. Similar to jacalin, hGal-3 interacts with Au porphyrin, registered by spectroscopy method. Additionally, we found that Gal-3 binds to human C1q, a primary activator of the Complement system. We studied the recognition between Gal-3 and C1q, using ELISA and fluorescence spectroscopy, calculating KD value of 0.04 μM. Interaction of Gal-3 with C1q fragments: ghA and ghB was also studied.

In conclusion plant and human lectins recognize important biological molecules and are supposed to have important biological roles.

Keywords: lectins, galectin, spectroscopy, curcumin, jacalin.

BFT P-12

Utilization of SCFA-Rich Effluents from Brewery Spent Grains for Lipid Production by *Yarrowia lipolytica*: A Sustainable Approach

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Short-chain fatty acids (SCFAs), derived from anaerobic fermentation of organic residues, offer a promising avenue for cost-effective production oleochemicals, heralding a shift towards greener chemistry practices. This study investigates the potential of SCFA-rich effluents produced from Brewery Spent Grains (BSG) as a carbon source for lipid production using the oleaginous yeast *Yarrowia lipolytica*. The effluent, originating from the anaerobic reactor, underwent filtration (0.2 µm) before being employed in batch fermentation experiments. Samples were collected every 2 h to monitor SCFAs consumption and yeast growth via optical density measurements. Upon exhaustion of SCFAs, lipid extraction and quantification were performed. The effluent from reactor exhibited around 8 g/L of SCFAs that were rapidly consumed by the yeast within 29 h. Despite a carbon-to-nitrogen ratio (C/N) of 26.35, 18.74 ± 0.68% w/w of lipids were obtained, falling within the expected range for lipid production and an OD of 8.7. This conversion aligns with literature and suggests this material as an interesting feedstock to explore as an innovative carbon source for oils productions.

Keywords: SCFA-rich effluents, *Yarrowia lipolytica*, lipid production, sustainable biotechnology

BFT P-13

Study on the Kinetic Parameters of Drying Fruit Bars from Blue Plums with an Addition of Freshwater Algae

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Fruit bars based on prunes with the addition of 3 % freshwater algae *Chlorella* and *Spirulina Platensis* have been developed. The aim of this study is to investigate the kinetics of the drying parameters of the developed fruit bars depending on the type of added algae.

Depending on the temperature of the drying agent, the drying time for both variants of fruit bars with *Chlorella* and *Spirulina Platensis* varies from 7.0 to 18.0 hours. A second critical point was identified in all variants of the experiment. Two sub-periods were recorded: a sub-period of uniform decrease in moisture evaporation rate and a sub-period of non-uniform decrease in moisture evaporation rate. Regression models for the drying rate coefficients, degree of deformation, and sensory evaluation of fruit bars with *Chlorella* and *Spirulina Platensis* were obtained. These models describe the investigated process with sufficient accuracy. The most significant influence in both variants is exerted by the linear effects of the thickness of the fruit bars, the drying temperature, the quadratic effect of the bar thickness, and the interaction between the drying temperature and the bar thickness.

Keywords: drying kinetics, fruit bars, algae

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CHEMICAL ENGINEERING

CE O-1

Solid Iron Dissolution in Acid Media to Support Fenton Process for Methyl Orange Oxidation

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One of the most known advanced oxidation processes for organic pollutants removal form aquatic environment is the Fenton process. It is based on the reagents; H_2O_2 and Fe^{2+}, which produce hydroxyl radicals $^{\bullet}OH$, very strong oxidizing species which degrade organics[1,2]. Usually Fe^{2+} is added into the solution to be treated at very small quantities as catalyst, in form of some soluble iron salt such as $FeSO_4$. However, the exploitation of other sources of Fe^{2+} than iron salts, can make the method more economical, more effective, and easier to operate. In this research common construction iron nails were used as a source of Fe^{2+} for the Fenton process. They are cheap, and they are frequently found as scrap material. First, the dissolution of iron from nails was studied in order to measure the availability of Fe^{2+} when solid Fe^0 is put in an acidic solution. Then the degradation kinetics of methyl orange (MTO) was studied at various iron bar surface areas and pH-s. It was found that iron nails are very effective in MTO and the degradation kinetics changed from a zero to order degradation reaction for small iron bar surface areas, to first order reaction when larger iron bar surface areas were applied. There was also determined that no efficiency is lost during many consecutive degradation experiments with the same iron bar.

Keywords: Fenton, radicals, degradation, pollutant

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CE P-1

The Influence of The Activation Function Within Deep Learning on Predicting Natural Rubber Rheological Properties

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This research aimed to develop and explore an advanced Deep Learning (DL) for the prediction of vulcanization in commercially available rubber gum used in tire manufacturing. The DL was created utilizing TensorFlow with Keras in a Python framework, employing two hidden layers consisting of 10 neurons each. Sequential and adam were employed as the model and optimizer, respectively. The investigation involved varying the activation functions to assess their impact on vulcanization prediction. The activation functions employed were ReLU, Sigmoid, Softplus, and Hyperbolic Tangent. Notably, the DL model with the Softplus activation function exhibited the highest accuracy. Training the network was carried out at temperatures of 130, 150, and 170 °C, with experimental data at 140 and 160 °C utilized to determine numerical errors. The proposed DL successfully predicted torque dependence on time at temperatures within the range of 140 to 160 °C. The accuracy of the predictions was confirmed using different numerical methods at all tested temperatures, with MAPE and MSE values below 4.6 % and R2 values exceeding 0.92.

Keywords: Activation function, Deep Learning, Rheological properties, Natural rubber

CE P-2

Experimental Investigation of the Solids Circulation Rate and the Minimum Spouting Velocity in the Modified Spouted Bed

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When designing a particle-fluid contactor with a spouted bed, the basic parameters are the solids circulation rate and the minimum spouting velocity, i.e. the velocity at which the spout forms along the entire bed[1,2]. When a draft tube is placed along the spouted bed column, the minimum spouting velocity is the velocity at which the particle bed reaches the top of the draft tube and forms a spout at the exit of the tube. This paper presents the results of an experimental test on the solids circulation rate and the minimum spouting velocity in a column with a draft tube. The system consisted of a cylindrical column with a diameter of 100 mm, on the conical bottom of which a smaller column with a diameter of 60 mm and a draft tube with a diameter of 20 mm and 25 mm, and adjustable distance from the bottom. Spherical glass particles were used in the experiments, and air introduced at the bottom of the column and into the annular space was used as a fountaining agent. The influence of the diameter and the distance of the draft tube from the bottom on the solids circulation rate and the minimum spouting velocity was determined and a comparison of the experimentally obtained values of the minimum spouting velocity with the Matur-Gischler correlation was given.

Keywords: spouted bed; minimum spouted velocity; solids circulation rate

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CE P-3

Extraction Gallic Acid, Punicalin, Punicalagin I Ellagic Acid from Pomegranate Peel in Packed Bed Systems and by Recirculation of the Liquid Phase

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There are many healthy and medicinal polyphenols in the peel of the pomegranate, so that the peel is not treated as waste. In this manuscript has been studied extraction the following polyphenols from pomegranate peel: gallic acid, punicalin, punicalagin and ellagic acid with the aim to examine possible industrial production of these medicinals polyphenols from pomegranate peels. The extraction is done in packed bed composed of grains pomegranate peels with recirculation liquid solvent throught bed. Internal diametar (ID) column in which the extraction carried out is 40 mm, mean diametar grains pomegranate peel is 2 mm. The experimental apparatus is equipped with a heater and temperature regulation. In this way the temperature changes in the system. The experiment is done at three different temperatures and with three different solvents. The solvents used are: water, water solution ethanol of 50 vol% and 96 vol% ethanol. The dependencies of the concentration mentioned polyphenols as a function of times for three different temperatures and three different solvents are shown. The influence of the temperature and the choice of solvent on the yield of the extraction mentioned polyphenols is shown. Optimal working conditions were determined with a tendency to develop equations that describe the extraction mentioned polyphenols in this system. The diffusivity coefficient of these four polyphenols in the used solvents was calculated.

Keywords: extraction; pomegranate peel; polyphenols; mass transfer; diffusion coefficient

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CE P-5

Solvent-Free Synthesis of Cu(II) Complex with 3,5-Pyrazoledicarboxilic Acid as Ligand

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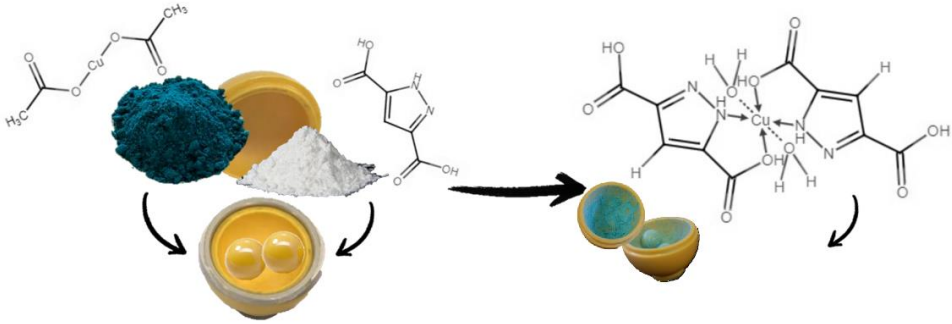
Complex pyrazole compounds are primarily synthesized by traditional methods from solution. In order to increase the efficiency of the syntheses by improving the yield, reducing the reaction time and reducing the use of toxic solvents, mechanochemical methods are being investigated as an environmentally friendly alternative.

This research investigates the mechanochemical synthesis of Cu(II) complexes with 3,5-pyrazoledicarboxylic acid as a ligand. Cu(II) salts and the ligand were mixed in a ball mill without the addition of solvent. Different synthesis conditions were tested. Analysis showed that coordination occurred within 3 minutes of mixing. The product was analyzed before and after conducting work-up and it was shown that a pure product was obtained, which increases the efficiency of the synthesis. Characterization of the compound was carried out by elemental analysis, IR spectroscopy and UV-Vis spectroscopy.



Keywords: mechanochemistry, complex, pyrazole, solvent-free synthesis

CE P-6

Extraction Techniques Impact on Oregano Post-Distillation Waste Biomass Valorization

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Aromatic plants contain various phytochemicals endowed with potent biological activity, making them promising candidates for the treatment of a variety of chronic diseases.[1] The extraction of essential oil (EOs) constitutes one of the main reasons for the large-scale aromatic herbs. Due to their low cost and simplicity, hydrodistillation continue to be the primary technologies that satisfy industrial needs for EOs.[2] However, various post-distillation by-products, including spent plant materials (solid residues, waste biomass) and aqueous condensates (hydrolates, hydrosols) are generated in large amounts. By providing raw materials for agriculture, cosmetics, and pharmaceuticals, this agroindustry can contribute to broader sustainability goals.[1]

The aim of the present study was to investigate polyphenolic content of post-distillation waste extracts of oregano (*Origanum vulgare*), growing wild in Montenegro. Three different extraction techniques were used to obtain extracts of origano post-distillation waste: Soxhlet extraction, ultrasonic extraction and maceration. Obtained results suggest that post-distillation waste of oregano leaves could be used as a source rich in bioactive compounds as polyphenols.

Keywords: oregano, postdistillation waste, bioactive compounds, extraction techniques

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EDUCATION

EDU O-1

The Role Self-Esteem Plays in Academic Achievement

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Teaching is the process of facilitating learning, knowledge acquisition, and skill development in individuals. It involves the deliberate and systematic transfer of ideas, values, and skills from a teacher or instructor to learners. Teaching can take place in various forms, yet the literature mentions mainly two of them: teacher-centered and learner-centered teaching. Teacher-centered instruction is an approach where the teacher takes on a central role in the classroom whereas student-centred teaching places the learner at the center of the learning process. To achieve student-centred learning, it is important to understand how instructional practices and learning theories complete each other. Among others, humanistic learning theory stands out as this approach mainly focuses on learner-centred instruction by transferring power from teachers to students. Considering the importance of attaining success in the teaching and learning processes, this study focused on factors which make students in SABAH groups (These groups were created to cultivate students' intellectual and creative abilities while ensuring the acquisition of specialties) more successful compared to conventional groups. The purpose of this qualitative small-scale research was to gain an understanding of educational achievements, educational performance and learning from the faculty's perspectives. The research was guided by A. Maslow's and C. Roger's humanistic theories. The research questions focused on two areas: instructors' perceptions and the perceived difference in instruction in Sabah groups.

Keywords: self-esteem, student-centered learning, academic achievement, learning theories, humanistic learning theory.

EDU P-1

Implementation of Lean Management Approaches into Optimization of Processes Used in Quality Control Laboratories in Alkaloid AD Skopje

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The implementation of Lean Management techniques into manufacturing facilities all over the world is a prime topic for cost and waste reduction. From the far eastern to the modern western companies, from start-ups to corporations, lean management is the most desired change to the industry especially in times of constant economical disbalance and difficulties in "just in time" (JIT) procurements and delivery.[1]

The heart of lean management and lean manufacturing is quantity control and value-added products[2]. The laboratory for quality control of chemicals at Alkaloid AD Skopje besides the quality control obtained and certified by following ISO standards coupled into the integrated management system has to deliver JIT results by reducing the seven lean wastes and by adding up value to the product. With steps of coupling of different lean techniques such as 5S, Kanban, visual management and SMED[2] (single minute exchange of dye) the output of the key activities in the laboratory was increased. With lowering the wastes such as movement, over-processing, waiting and inventory inside the laboratory standard operating procedures (SOP) while maintaining the high-end quality, successful implementation of lean management techniques was established.

Keywords: Lean-management, Kanban, 5S, SMED.

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EDU P-2

Evaluating Green Chemistry Education through Student Interventions

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The implementation of green chemistry in education is a significant step toward sustainable and innovative practices, teaching students the importance of environmental protection and responsible use of natural resources[1]. This approach aligns with IUPAC project[2] recommendations to promote green chemistry globally. In this research, 211 students were divided into a control group (CG, N=107) and an experimental group (EG, N=104). The study involved creating teaching interventions and monitoring their effects on students, as well as examining students' opinions before and after the intervention. Data were collected using quantitative techniques: knowledge tests and questionnaires, and qualitative methods: individual and group interviews. Data analysis of mid-term grades used an independent-samples *t*-test and showed no significant differences in initial achievement between CG and EG students.This study further analyzes questionnaire results with descriptive statistics and Cronbach's alpha to evaluate intervention effectiveness. Additionally, the interviewed students' responses provide valuable insights into their attitudes, experiences, and motivation during the activities.

Keywords: Green chemistry, questionnaire, sustainability, teachers.

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EDU P-3

The Presence of Organic Stereochemistry Issues at the International Level Competition

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The stereochemistry syllabus often causes confusion among students, since for a comprehensive understanding of stereochemical problems and to acquire knowledge in this field, the students should combine and harmonize the three learning areas. The problems students encounter in studying and mastering stereochemistry topics have prompted educational researchers to pay more attention to research in this field.

Stereochemistry receives limited attention in high school education in the Republic of Macedonia, but its importance is increasingly recognized internationally. In order to investigate the presence of stereochemistry problems, theoretical and practical problems from the past 55th International Chemistry Olympiads (IChO) were analyzed. In addition, each of these problems was analyzed from the perspective of Bloom's taxonomy and an analysis of the results achieved at the 55th International Chemistry Olympiad was carried out.

Based on the analysis and the obtained results, it can be concluded that in recent years, the number of stereochemical questions has increased and most of them are theoretical problems. These problems are from the higher levels of Bloom's taxonomy. However, the response to the IChO questions shows that even the most talented students in the world have difficulty solving stereochemical problems. The practical problems usually regard to some real problems e.g. sterochemical synthesis, which is even more complicated for the students.

Taking into consideration, these facts, in recent years, the stereochemistry problems are more present in international education compared to the previous.

Keywords: Bloom's taxonomy, International Olympiads, organic chemistry, stereochemistry.

INORGANIC CHEMISTRY AND TECHNOLOGY, INORGANIC MATERIALS AND METALLURGY

ICTM O-1

Mining and Metallurgical Waste as Potential Secondary Sources of Metals in the West Balkan

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The main objective of this manuscript is to collect, classify, and compile all available data about secondary mineral sources of valuable metals in the West Balkan countries. The material is generated from the extracting and processing sector, which might be transformed into an important raw material for another industry. The management inventory guide will strengthen communication and dissemination efforts, contribute to Europe's self-sufficiency, and support transitioning to green and digital technology. Identification of the knowledge gaps associated with secondary sources of sulphide valuable metals (Au, Ag, Bi, Cu, Mo, Pb, In, etc.) and REEs in West Balkan will contribute to connections between all partners being involved at the beginning, during the lifetime of products and at the end of the life cycle, represented with deposit owners, technology developers and potential processors, producers, and potential users.

In the investigated area it was found 1835 individual landfills, most of them belonging to waste rocks. The total quantity of all material in SRM is about 3.2 billion tonnes over an area of about 100 km^2. More than half of this material is characterised as conventional mining waste, 40% belongs to the processing tailings, and less than 10% to metallurgical waste. Most of these tailing sites are unclaimed, presenting a source of contamination for the surrounding communities. The largest 95 individual landfills were selected as potential prospective landfills, containing approximately 1600 million tonnes of material.

Keywords: secondary mineral deposits, Rees, sulphides, economic perspective, West Balkan

ICTM P-1

Optical Microscopy Control and Sieve Analysis of Milled Diatomaceous Earth Sample After the Elutriation Process

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A series of experiments and calculations related to the granulometric separation of a non-metallic complex raw material - diatomaceous earth from Slavishko Pole - have been carried out in order to determine the technological preparation of the sample.

An operation of opening the raw material (crushing and milling) was performed, after which the separated fraction -400 μm was subjected to wet sieve and the elutriation process. A series of sieves with perforation size of: 0.25 mm, 0.2 mm, 0.16 mm, 0.125 mm, 0.1 mm, 0.071 mm, 0.05 mm and 0.032 mm were used. The coarsest fraction (+0.25 mm) and the finest fraction (-0.032 mm) with around 17 wt. % of each were more prevalent. However, the other grain fractions did not exceed 10 wt. %, with the exception of the fraction (-0.071 +0.05 mm) whose mass percent was approximately 15. The different grain size fractions obtained from the wet sieve analysis and the elutriation process were simultaneously examined by an optical microscope. The settling velocities of the grains with the corresponding diameter range were also calculated according to the precipitation equation. At a water velocity of 3.13 cm/s, only mineral grains with a diameter greater than 210 μm were deposited, at a velocity of 2.41 cm/s grains with a diameter greater than 190 μm, and at the speed of the countercurrent movement of water through elutriation column of 1.68 cm/s, mineral grains with a diameter greater than 160 μm were deposited. The obtained deposition speed values indicate a dominant influence of the shape factor of the particles, namely their morphology.

The technological preparation of the diatomaceous earth can be conducted to a specific regime with precisely defined parameters, in order to obtain appropriate dimensional fractions of grains.

Keywords: granulometric separation, wet sieve analysis, elutriation, settling velocity, shape factor

ICTM P-2

Preparation Of Separate Fraction from Selected Non-metallic Raw Materials According to Granulometric Composition, Suitable for the Elutriation Process

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The quality of the production process is improved with adequate preparation of the raw inorganic materials, which is of positive impact on the final product. This research is based on the preparation of separate fractions of raw inorganic materials, namely granite, mica, quartzite, calcite and bentonite clay appropriate for the elutriation process.

A general overview of the basic characteristics of non-metallic raw materials has been made. The optimal parameters in the crushing and milling processes of the raw materials have been determined, precisely a jaw type crusher to a grain size of -1 cm was used, followed by a combined milling mode, i.e. predominantly cataracting regime. A wet sieve analysis using series of sieves with perforation size of: 0.1 mm, 0.071 mm, 0.05 mm and 0.032 mm was performed, as an ultimate preparation procedure for obtaining the appropriate combinations of materials with different mineralogical composition and different particle size range for a visible separation during the countercurrent gravity concentration process in a water medium.

The coarse fractions were dominantly present in the granite and mica, as opposed to the quartzite, calcite and bentonite clay, where the fine fractions were far more prevalent. Nevertheless, the efficiency of the elutriation process as a method of countercurrent gravity concentration in a water medium depends most directly on the grain size and the mineralogical composition of the materials.

Keywords: raw inorganic materials, wet sieve analysis, countercurrent gravity concentration

ICTM P-3

Reactive Orange 16 Photodegradation Mechanism in the Presence of TiO_2/Polypyrrole Nanocomposite

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With the aim of determining the mechanism of photodegradation of toxic azo dye Reactive Orange 16 (RO16), the TiO_2/PPy nanocomposite (PPy = Polypyrrole), containing 1 wt.% of PPy, was produced from the hydrothermally prepared TiO_2 and PPy, obtained by chemical oxidative polymerization. Based on XRPD results, the TiO_2 was obtained in nanoanatase form with crystallites of 26 nm while FTIR analysis confirmed the presence of PPy. The UV-Vis absorption spectrum of TiO_2/PPy nanocomposite showed a shift of band to higher wavelengths indicating that the presence of PPy enhanced the absorption capacity for visible light. This is important, considering that TiO_2 is mainly active in the UV region[1]. The calculated band gap energy value was 3.08(3) eV. The TiO_2/PPy demonstrated excellent photocatalytic activity by completely degrading RO16 within 120 minutes under simulated solar light, with degradation described by the pseudo-first-order reaction kinetics and a rate constant of 0.056(5) min^{-1}. A detailed analysis of the mechanism showed the following distribution of reactive oxidative species: 73 % of h^+, 20 % of $O_2^{\bullet-}$, and 7 % of $^{\bullet}OH$. It also revealed that the photodegradation followed a modified direct Z-scheme heterojunction in which PPy played an active and irreplaceable role by opening a new reaction pathway.

Keywords: TiO_2, Polypyrrole, Photocatalysis, Reactive Orange 16

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ICTM P-4

Microstructural Alterations of Ti-Based Implant Alloy Induced by High-Pressure Torsion

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The β-type Ti-based alloys that contain bio-inert alloying elements have been attracting significant attention in recent years as potential hard-tissue implant materials due to their biomechanical compatibility. The Ti-Nb alloys are singled out as the most promising implant alloys of this group. Even though these alloys show exceptional biocompatible characteristics, their properties can be further enhanced by altering their microstructure. Severe plastic deformation (SPD) processing is a microstructural refining method that can successfully convert the coarse-grained materials into ultrafine- or even nano-grained metallic materials, thereby altering their response to harsh working bio-conditions.

With this in mind, the scope of the present research was to investigate the influence of the high-pressure torsion (HPT), as one of the SPD processing methods, on the Ti-45Nb (wt.%) alloy's microstructural characteristics and consequently on its interaction with living cells. Microstructural alterations achieved during HPT were examined using small-angle (SAXS) and wide-angle (WAXS) X-ray scattering, combined with texture measurements conducted using X-ray diffraction (XRD), while the alloy's interaction with living cells was investigated *in vitro* using MRC-5 human fibroblasts. The results revealed intensive texture property changes and the achievement of ~4.3 times smaller grains in the alloy's microstructure due to the HPT processing which consequently led to a significant improvement of cell viability when in contact with the investigated Ti-45Nb alloy. Even though the alloy showed excellent cytocompatibility in both HPT-unprocessed and HPT-processed conditions, the investigations revealed the significant potential of the HPT method for improving the compatibility of metallic implants with biological systems.

Keywords: Ti-Nb alloy, HPT processing, SAXS/WAXS analysis, microstructural refinement

ICTM P-5

Physico-Chemical and Structural Analysis of Sm_2O_3-Doped Geopolymers for Advanced Material Applications

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In the current era of extensive materials exploration, geopolymers have emerged as a notable category of inorganic polymers, attracting significant interest in the fields of materials science. Geopolymers, known for their high strength, corrosion resistance, and thermal stability, are synthesized through the alkali activation of metakaolin, incorporating Sm_2O_3 to investigate the impact on their physico-chemical properties. This study examines the synthesis and physico-chemical characterization of geopolymer materials doped with Sm_2O_3. Two samples with 1% and 5% Sm_2O_3 by weight, S_1 and S_2, respectively, were analyzed. Characterization techniques such as energy dispersive X-ray fluorescence spectrometry (EDXRF), diffuse reflectance infrared Fourier transform spectroscopy (DRIFT), scanning electron microscopy (SEM) for the physico-chemical characterization of the geopolymers. The structural analysis indicates a homogeneous integration of Sm_2O_3, which did not significantly affect the material's density or porosity. This study demonstrates the potential of Sm_2O_3-doped geopolymers in various applications, positioning them as suitable materials with enhanced properties.

Keywords: geopolymer, Sm_2O_3, EDXRF, DRIFT, SEM

ICTM P-6

Method Development for In-House Determination of Heavy Metals in Talk Powder

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The determination of heavy metals in talk powder is very important for usage of talk powder in pharmaceutical and cosmetic products. As one of the main fillers of the products for topical usage the presence of iron, magnesium, aluminum, calcium cadmium, chromium, nickel, and lead[1] is strictly monitored by European pharmacopeia and US food & drug administration.

Three sample preparation methods were developed for determination on ICP-OES in comparison to the European pharmacopeia methods based on AAS[2] determination. The first method was developed by dissolving the sample into concentrated nitric acid and digested into microwave oven. The second method was developed by dissolving the sample into concentrated nitric acid and by ignition the sample into ignition oven. The third sample was prepared by simple dissolving into concentrated nitric acid without any thermal treatment. Afterwards the samples were filtrated through blue ribbon filter paper, and properly dissolved to reach the calibration curve.

The obtained results were compared to spiked samples to determine the best preparation method for determination of heavy metals in talk powder. The most optimum method in preparing the samples and obtaining the results is in accordance with the expected results and limits by European Pharmacopeia[2]. Further validation of the method with most optimal results will be implemented.

Keywords: Method development, ICP-OES, Talk powder, heavy metals.

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ICTM P-7

Aluminum-Based Composites Reinforced with Waste Basalt Fiber

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Modern technology has placed increasing demands on materials. The properties of conventional metallic materials can be improved by the method of reinforcing fibers into metals and alloys[1]. As previously stated, it has resulted in broad spectrum composite materials manufacturing. The mechanical properties of fiber-reinforced metal matrix composites (MMCs) make them suitable for applications in many fields. Basalt fiber (BF) has gained significant attention as reinforcement in construction engineering composites because it is non-toxic, eco-friendly, easy to process, and costs less than other fibers[2].

For this study, aluminum 2024 alloy chips with the chemical composition per the ASTM standard were used as the base matrix alloy. These chips were ball-milled for 6 h to obtain powder particles with a round shape. Waste basalt short fibers from stone wool were used as reinforcement. The percentage of reinforcement varied from 5 to 30 wt. % in steps of 5%. The composites were then prepared using the Spark Plasma Sintering (SPS) technique, which involves applying high pressure and temperature to consolidate powder particles at 500ºC. This process was followed by a subsequent heat treatment at 550ºC.

The paper overviews obtaining waste basalt fiber-reinforced aluminum-based composite materials (AMMCs). It delves into the manufacturing method, microstructural (LM, SEM/EDS), structural (XRD), and mechanical properties (HV) of these materials, providing a thorough understanding of their characteristics and potential applications.

Keywords: aluminum-based composite materials (AMMCs), basal fibers, reinforcement

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ICTM P-8

Synthesis and Study of 2-Dimensional Hybrid Lead Based Materials

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Organic–inorganic hybrid materials are among the most promising materials for many technological applications. The combination of the organic and inorganic components in molecular level results in materials with tailor made structures and novel properties different from those of the single components. Due to these properties, they have been used in photovoltaic materials, light-emitting materials, photodetectors and other optoelectronic applications.

2-dimensional organic inorganic compounds with the formulas $APbX_4$ and $A_6Pb_5I_{21}{\cdot}I{\cdot}3H_2O$ (A= 2-aminomethyl-pyridine and X=Br, Cl) were synthesized and studied. Their structure was solved by X-Ray analysis showing a perovskite-like, 2-dimensional, structure. Their optical, vibronic and thermal properties were studied. Based on the experimental structure, we performed theoretical DFT calculations to obtain the electronic and vibronic properties. The theoretical results are in accordance with the experimental results.

Keywords: Low dimensional materials, Perovskites X-Ray analysis, optical spectroscopy, FT-IR, Raman.

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ICTM P-9

Development and Validation of ICP-OES Method for Determination of Elemental Impurities in Topical Antiseptic

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These days, the presence of elemental impurities in pharmaceuticals is a major cause for worry. During development and manufacturing of pharmaceuticals, various sources can cause contamination with elemental impurities. These impurities can be toxic and it is important that the concentration in pharmaceuticals is controlled and kept at a low level[1]. The goal of this study was to quantitatively determine elements from class 1, Cadmium (Cd), Lead (Pb), Arsenic (As), Mercury (Hg) and class 2A, Cobalt (Co),Vanadium (V), Nickel (Ni) that the analyzed topical antiseptic contained[2]. The method included inductively coupled plasma with optical emission spectrometry (ICP-OES) and microwave digestion[3]. The validation experiments involve: specificity with provided evident difference between the spectra (intensity) of the diluents and standard solution. Results for LoQ under 30% of the element specification level, LoD results that not exceed LoQ. Linearity and range with correlation coefficient is ≥ 0.99. Precision (method and system precision) with a criterion for RSD achieved, and accuracy experiments between 75.8% and 133.3% recovery for individual results, within all acceptance limits[4]. The statistical analysis showed that the developed ICP-OES method for measuring elements is selective and accurate and can be used for determination of elemental impurities from class 1 and 2Ain the topical antiseptic.

Keywords: ICPOES, Elemental impurities, Topical antiseptic

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ICTM P-10

Synthesis and Characterization of Hybrid Organic-Inorganic Perovskites with Gadolinium(III) in the B Position

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Since the discovery of hybrid organic-inorganic perovskites (HOIPs) as sensitizers for photovoltaic cells, research interest in these compounds has significantly increased. Extensive studies have been conducted to understand their optoelectronic properties. This study focuses on the synthesis and characterization of HOIPs featuring gadolinium(III) as the B-site cation and iodide (I^-) in the X position, with variable A-site cations such as morpholinium, pyridinium, and pyrrolidinium, were synthesized and investigated. Additionally, mixed B-site cation perovskites incorporating both silver and gadolinium(III) cations, with iodide in the X position were considered.

The synthesis of the HOIPs was conducted in acetonitrile as a solvent, to which the iodide salts of silver and the organic cations were added. Gadolinium(III) iodide was generated *in situ* from gadolinium(III) hydroxide and hydroiodic acid, due to the difficulty of working with the deliquescent halide salt. The reaction mixtures were either heated until crystallization began, or the crystallization was induced using the anti-solvent vapor-assisted crystallization method with dichloromethane as the anti-solvent.

The obtained compounds were analyzed by X-ray powder diffraction XRPD and vibrational spectroscopy (IR and Raman) in a wide temperature range (LNT to 200 ºC). Thin films of the HOIPs were obtained by spin coating technique and investigated by UV-VIS spectroscopy. These data were used to construct Tauc plots, from which the direct and indirect band gaps were determined.

Keywords: gadolinium iodide organic-inorganic perovskites, XRPD, vibrational spectroscopy, thin films

ICTM P-11
Superalloy Development by Combustion of Aluminothermic Mixtures - Characterization

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This work concerns an attempt to develop a superalloy similar to Udimet 720, based on Ni-Co-Cr + additions (Mo, W, Ti, Al, and C), thanks to the combustion of aluminothermic mixtures composed of oxides and aluminum. The reduction reactions of the NiO-Co_3O_4-Cr_2O_3 mixture by aluminum are initiated using an electric arc. The thermal explosion produced by the reduction process generates a temperature that greatly exceeds the melting temperatures of the targeted metals. X-ray diffraction analyses of the reduction product after solidification revealed the presence of the solid solution peaks based on Ni, as well as peaks of lower intensity, attributed to $Cr_{23}C_6$ carbide. Metallographic analyses using optical microscopy and electron scanning microscopy coupled with a semi-quantitative EDS assessment, revealed an oriented dendritic structure, resulting from rapid solidification of the liquid alloy. Free forging at 1150°C and recrystallization annealing at 850 °C, under argon flow, made it possible to eliminate the solidification texture and ensure a uniform distribution of the main alloying elements. A consolidation regime was carried out based on hyper quenching at 1080°C for 4 hours, followed by aging at 850 °C, with holding times varying from 2 to 6 hours. However, under these conditions, no effect of intermetallics or carbides precipitation was observed. All alloying elements remained in solution. The Vickers hardness of the obtained alloy does not exceed 2000 MPa, even after annealing for 6 hours. This technique could potentially reduce the manufacturing cycle of these materials.

Keywords: superalloy, combustion, aluminothermic process, microstructure, vickers hardness.

ICTM P-12

Mechanochemical Synthesis of Cu(II) dithiocarbamato complex: Advantages Over Traditional Solution-Based Methods

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According to IUPAC, mechanochemistry is identified as one of the top 10 emerging technologies in chemistry with a positive impact on sustainable development. In previous studies, the coordination of ammonium-iminodiacetate dithiocarbamate with Cu(II) ions was investigated using traditional solvent-based methods that required the addition of HCl during complex formation.[1] To avoid the use of solvents and harsh chemicals, mechanochemical syntheses were conducted by directly mixing ligand with various Cu(II) salts in a planetary ball mill.

IR spectra were recorded after 15 min, 30 min, and 1 h, showing completion of the reaction within only 15 min under all conditions (different jar materials, numbers of balls, and mixing durations). The complexes were characterized by elemental analysis, IR and UV-Vis spectroscopy, which confirmed that Cu(II) ions are coordinated through sulfur as donor atoms (regardless of the conditions of mechanochemical synthesis).

Keywords: mechanochemistry, complex, dithiocarbamate, green synthesis

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ICTM P-13

Efficient Solvent-Free Synthesis of Ni(II)- Dithiocarbamato Complexes using Mechanochemistry

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Previous research has confirmed the possible coordination of the ligand ammonium-iminodiacetatedithiocarbamate, $(NH_4)_3$idadtc, with transition metals, including Ni.[1] Mechnanochemical synthesis of $(NH_4)_3$idadtc and Ni(II) ions was examined with the aim of optimizing the synthesis, avoiding the use of HCl and obtaining a purer product. The application of mechanochemistry, which is also known as “green chemistry", leads to saving time and energy, as well as reducing the use of organic solvents and results in low waste.

This experimental work was carried out in a planetary ball mill. Numerous syntheses were performed with different conditions. Jars and balls made of zirconium oxide and stainless steel were used. Reactions with different number and size of balls as well as grinding speed and time were tested. IR spectra were recorded between 5 minutes and 1 hour, showing that the same product is obtained regardless of the synthesis conditions. The complexes were characterized by elemental analysis, IR and UV-Vis spectroscopy. Analysis confirmed that Ni(II) ions are coordinated through the sulfur atoms. All applied conditions resulted in high purity products which did not require additional post-synthetic treatment. This research showed a great potential of mechanochemistry as a novel clean synthetic approach for sustainable synthesis.

Keywords: mechanochemistry, dithiocarbamates, green chemistry

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ICTM P-14

Thermally Treated Low Carbon Geopolymer Foams Doped with Nd_2O_3 and Sm_2O_3

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Geopolymers represent an innovative group of porous ceramic materials characterized by low energy consumption during production for construction purposes; they are cheap and environmentally friendly with low emissions of CO_2. The tested material, which was thermally treated at three different temperatures (300°C, 600°C and 900°C) showed an additional decrease in the amount of carbon in its composition. Geopolymer foam structure doped with neodymium and samarium were examined in detail by X-ray photoelectron spectroscopy (XPS) and showed and confirmed the existence of incorporation of Nd and Sm into the polymer matrix. The reduction of total carbon was also confirmed. SEM analysis revealed the initiation of micro-cracks, both on the surface and in the bulk of the material. Increase in porosity is observed, which can be described as the formation of a sponge-likestructure in the initial phase. HR-TEM of samples treated at 900°C proved the existence of polycrystalline grains of SiO_2 and Al_2O_3. Micrographs emphasize the unique structure characterized by spherical formations dispersed throughout a sponge-like microstructure containing nano-sized pores. From the difference in contrast, one can clearly distinguish two different phases. Brighter colored grains represent Al_2O_3, while the dark colored areas mostly present SiO_2 as quartz.

Keywords: geopolymer foam, Nd_2O_3, Sm_2O_3, XPS, HR-TEM

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ICTM P-15

Development of Porous Ceramics from Clay and Coal Fly Ash Using Various Pore Creators: A Study on Microstructure and Mechanical Properties

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The utilization of coal fly ash in the production of porous ceramics has garnered significant attention due to its environmental and economic benefits. This study explores the utilization of coal fly ash (FA) and clay (CL) as primary raw materials in the fabrication of porous ceramics, employing various pore creators to tailor the porosity and mechanical properties of the final product. Different pore creators, including coal (C) and sawdust (D) from different origins, were systematically investigated for their effectiveness in enhancing the porosity, pore size distribution, and structural integrity of the ceramics. The prepared samples were characterized using techniques such as scanning electron microscopy (SEM), density measurements and mechanical testing to evaluate their microstructure, porosity and bending strength.

The results indicate that a highly porous structure with an integral porosity of 45% can be obtained from fly ash and 20 wt.% of coal (FA20C), sintered at 1100°C for 1 hour, while the porosity of the structure obtained with 2 wt.% was 28%, sintered under the same conditions. It can be concluded that the type and concentration of pore creators significantly influence the mechanical properties of the ceramics. A reduction in mechanical properties was observed, with bending strength decreasing from 20.6 to 6.28 MPa for FA2C and FA20C, and from 47.7 to 6.55 MPa for porous structures CL2C and CL20C, respectively. The optimized porous ceramics demonstrated potential applications in filtration, thermal insulation, and lightweight structural components.

Keywords: coal fly ash, ceramics, pore creators, mechanical properties

ICTM P-16

Enhancing Environmental Management of Mining Legacies: Database, Mapping, and Monitoring Insights from COST Action REMINDNET

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Since the beginning of human history, metals and minerals have been extracted from the Earth's crust. However, the environmental residues left by the mining sector, such as tailings, waste dumps, and contaminated water, the management of mine closure and post-closure is becoming more and more significant. Many regions in Europe and around the world are struggling with these problems, frequently lacking the resources and expertise needed to properly manage old mine sites effectively.

The aim of this paper aligns with the primary objective of the REMINDNET action and Working Group 3 (WG 3) which is to map best practices for mine site rehabilitation and provide cost-effective monitoring methods and risk management tools.

The QGIS database, following best practices for mining rehabilitation, will be continually updated throughout the duration of the COST Action and is visualized in a Web GIS app using the open-source software GeoServer and MapStore. Furthermore, a Python script that makes use of the Landsat satellite constellation has been developed for efficient monitoring of mining locations. All of these methods improve Europe's capacity to track, restore, and manage the environmental effects of mining legacies.

Keywords: Mine Rehabilitation, Environmental Monitoring, Risk Management, QGIS Database

Acknowledgments: This work was supported by COST Action CA22138: Recovery of Mining District Network (REMINDNET). We thank the network of scientists and practitioners for their collaboration and contributions. Additional information about the COST Action can be found at https://www.remindnet.eu/.

ICTM P-17

Use Of Waste Glass and Dolomite as Cement Substitutes in Mortars with a Lower Environmental Impact

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Portland cement (PC) is the most commonly used binder, but it is responsible for 8-10% of the global CO_2 emissions. Partial substitution of PC with byproducts presents one of the most promising technologies for lowering CO_2 emissions. Waste glass and dolomite present excellent alternatives for cement substitutions in mortars, with resulting environment benefit.

In this light, the influence of 10wt.% glass and 10 wt.% dolomite as well as the mixture of 5 wt.% waste glass and 5 wt.% dolomite on fresh mortar properties (density, air permeability, consistency and setting time) and harden mechanical properties were followed. The water to cement ratio was 0.5 for all mortar mix design. The both waste materials present the domestic secondary raw materials taken from ACRON glass recycling company and waste tailing dolomite. The mean diameter (D_{50}) and specific gravity of glass particles were 53μm and 2.12 g/cm^3, respectively. Dolomite was pretreated by grinding and milling up to granulation less than 125 μm. The addition of waste glass and dolomite increased the mortar consistency up to 160 mm and caused drastic delay of setting time in mortars. Relating to the mechanical properties, all the mortars were in accordance with the expected values of mechanical properties of conventional mortars.

The actual study presents the example for secondary raw materials utilization as cement replacement in line to the principles of circular economy, resource efficiency and decrease of CO_2 footprint in our country.

Keywords: waste glass, dolomite, mortar, circular economy, CO_2 emission

ICTM P-18

Photocatalytic Activity of Zeolite-Based Nanocomposites for Reduction of Organic Pollutants in Solution

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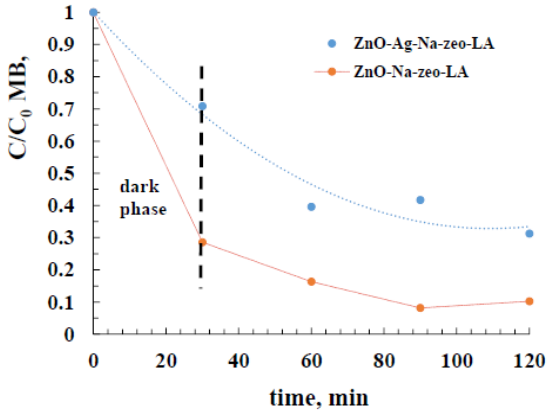
Photocatalysis is an effective method for decomposition of organic pollutants, which is a process initiated by irradiation of semiconductors with energy equal to or higher than its band gap. In this study, we investigated the photocatalytic activity of ZnO deposited onto natural zeolite as well as Ag decorated ZnO loaded onto zeolite support. These nanocomposites were produced by formation of ZnO nanoparticles through laser ablation in liquid method, which is environmentally friendly approach for nanoparticles fabrication. As-prepared nanomaterials were characterized by various techniques (UV-vis, SEM, TEM, XPS) and their photocatalytic activity in degradation of methylene blue by ultraviolet light irradiation was tested. The results revealed that the decrease of methylene blue concentration in solution is a combination of both adsorption of organic molecule onto the zeolite and its photocatalytic degradation by ZnO. Addition of silver nanoparticles onto zeolite hinders the adsorption process and enhances the photocatalytic activity of silver-containing nanocomposite.



Keywords: photocatalyst, ZnO, zeolite, dye degradation.

ICTM P-19

Photocatalytic Coating Based on Natural Illite Clay Impregnated with TiO_2

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Urban pollution has an adverse impact on the environment and the buildings. Recently, heterogeneous photocatalytic active coatings have been widely employed for air and water remediation due to their effectiveness in the oxidation of urban pollutants, self-cleaning properties, lack of toxicity, and low cost. In this light, it is of great interest to develop novel coating materials with enhanced photocatalytic performance for indoor and outdoor application.

For this purpose, natural illite clay impregnated with TiO_2 (3 and 10 wt.%) by mechanical activation was used. The obtained coating was applied on three types of substrates: non-porous (glass), porous (clay roofing tile), and highly porous (clay–fly ash composite). Photocatalytic efficiency was assessed by UV photodegradation of the pollutant Rodamin B (RdB), performed before and after durability tests. The durability tests were performed in laboratory conditions by measuring active properties after water rinsing and tape adhesion procedures while the self-cleaning was assessed by measuring the contact angle, before and after water rinsing and tape adhesion.

The obtained results of self-cleaning assessment (31° contact angle/24hUV), photocatalytic activity (32% RdB activity/24hUV), and durability tests (26.43% activity after both tests) show that the properties of the new illite clay/TiO_2 coating have good consistency when applied on clay roofing tile, which confirms its good compatibility and stability with that substrate.

Keywords: Illite clay/TiO_2, photocatalytic activity, self-cleaning, durability, coatings

ICTM P-20

Characterization of Fragments from Archeological Site Stobi by Non-Destructive Testing Methods

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The archeological site of Stobi is located near the confluence of the Crna River with the Vardar River and is abundant with ceramics dating from the early 3rd century BC to the 6th century AD.

In this research were used fragments from three samples, which, based on previous typological and chronological identifications, belong to an original Terra Sigillata vessel imported to Stobi, a fragment of a local imitation of the Terra Sigillata vessel, and a fragment of the local pottery production of Stobi, respectively. Samples of imports and imitations of Terra Sigillata are dated to the 1st-2nd century AD, and the last sample is dated to the 2nd-3rd century AD. In this study non-destructive testing (colorimetry, contact angle measurements, XRF and DRIFT FTIR analyses) was performed in order to characterize the pottery samples.

The Terra Sigillata sample imported to Stobi shows the most intensive red color and low hydrophilicity on both surfaces (73.9º/69.0º) in relation to other two samples that have red yellowish color and higher hydrophilicity. In all samples, silicon (Si), aluminum (Al) and iron (Fe) were detected as dominant elements, followed by potassium (K) and Calcium (Ca). The presence of illite/mica, quartz, feldspars and calcite were detected in all samples.

Keywords: archeological pottery, non-destructive testing, colorimetry, hydrophilicity, FTIR, XRF

ICTM P-21

Green Synthesis of CeO_2-ZnO Using *Veronica Officinalis* L. Extract: Photocatalytic Ability

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Green synthesis has many advantages in comparison with the physical and chemical methods: it is environmentally-friendly, pollution-free, non-toxic, economical and more sustainable [1]. The green approach was used to prepare the CeO_2-ZnO nanoparticles using *Veronica officinalis* L. plant extract and combining hydrothermal and thermal treatment. The obtained material was characterized by powder X-ray diffraction analysis and Fourier-transform Infrared spectroscopy. The synthesized CeO_2-ZnO was additionally ozonated. The photocatalytic ability of ozone treated and non-treated CeO_2-ZnO materials were tested and compared in the reaction of photocatalytic degradation of Reactive Black 5 dye as model contaminant in aqueous solutions under UV irradiation.

Keywords: green synthesis, *Veronica officinalis* L., CeO_2-ZnO, ozonation, photocatalytic activity

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ICTM P-22

Effect of Mixed-Phase Zno Nanoparticles on The Animal Pathogens *Erysipelothrix Rhusiopathiae* and *Aeromonas Caviae*

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The aim of this study is to evaluate the impact of green-synthesized wurtzite-hydrozincite mixed-phase ZnO nanoparticles on selected apathogenic and pathogenic Gram(+) and Gram(-) bacteria. The ZnO particles were obtained using a *Mentha arvensis* extract, followed by hydrothermal treatment at 180◦C. The resulting powder samples were characterized by X-ray diffraction (XRD) analysis and by Transmission Electron Microscopy (TEM). The particles sizes of biosynthesized powders decreased upon the increase in the plant extract concentration. Powders containing 10%, 20% and 30% plant extract are denoted as G-Z1, G-Z2 and G-Z3, respectively. The samples had highest antibacterial activity against the G(-) test microorganisms. The action of G-Z1 on *A. caviae* is bactericidal, while that of G-Z3 is bacteriostatic. The sample with the smallest particle sizes (G-Z3) exhibits the most effective inhibition. The combination of factors: the presence of two phases, reactive oxygen species formation; small particles sizes have positive effect on enhancement of their antibacterial properties.

Keywords: green synthesis, wurtzite-hydrozincite nanoparticles, antibacterial activity, *Aeromonas caviae, Erysipelothrix rhusiopathiae*

Acknowledgement This study was accomplished with the financial support of Project KP-06-H69/8"Novel polymer-hybrid materials containing (bio)synthesized metal oxide particles with improved photocatalytic and antimicrobial potential" of the National Science Fund, Ministry of Education and Science, Bulgaria

ORGANIC CHEMISTRY, BIOCHEMISTRY AND PHARMACEUTICAL CHEMISTRY

OBPC O-1

Monitoring Lipid Phase Transitions with Fluorescent Dyes

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The interaction with cellular membranes or membrane models is one of the most studied topics in biomedical research, especially in drug delivery studies. Recently, the importance of lipid formulations has been further emphasized with the introduction of mRNA vaccines based on lipoplexes, where self-organizing lipids function as drug delivery systems and protective agents. Fluorescent dyes incorporated in multilamellar liposomes can be used to monitor phase transitions and report on their environment. Steady-state or time-resolved fluorescence spectroscopy and microscopy are among the most widely used techniques for visualization and evaluation of membrane integrity, structure, organization, and dynamics[1]. Fluorescent probes diverse in polarity, lipophilicity, and their position within the lipid multibilayers were used to record temperature-dependent fluorescence spectra of the liposomal suspensions constituted from 1,2-dipalmitoyl-sn-glycero-3phosphocholine (DPPC), and 1,2-dipalmitoyl-sn-glycero-3-phosphoethanolamine (DPPE) in different buffer formulations.

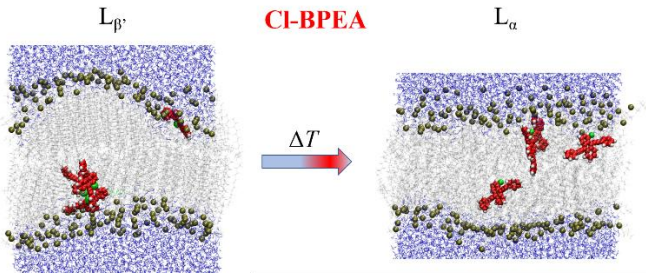

Figure. Snapshot of Cl-BPEA + DPPC in the gel (left) and the fluid (right) phase of DPPC bilayer

Keywords: fluorescent, cyanine dyes, spectroscopic techniques

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OBPC P-1

Recognition of Double-Stranded and Multi-Stranded DNA and RNA Structures by Cyanine Dyes

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Cyanine dyes react differently (intercalation, minor groove binding) with nucleic acids based on changes in cyanine structure (polymethine chain length, substituents) and the nucleic acid's sequence composition. The most recent findings for cyanine structural motifs that preferentially bind to duplex and multistranded DNA and RNA structures are presented here.[1,2] The spectroscopic techniques (fluorescence, UV/vis, and circular dichroism) were used to study the binding modes of cyanine dyes to nucleic acid structures. The relationship between the antiproliferative effect of cyanine dyes in cell culture and their high binding potential was investigated. Halogen-substituted cyanine dyes induced the triplex formation of consecutive rA/dA-containing nucleic acid helices. The presence of the rA chain in studied polynucleotides significantly enhances the tendency to form H-aggregates. Cyanine with methyl substituent of the selenium-substituted cyanine dyes shows 100-fold selectivity for G-quadruplex over duplex DNA. It exhibits submicromolar cytotoxic activity and accumulates in nucleoli.

Keywords: nucleic acid recognition, cyanine dyes, spectroscopic techniques

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OBPC P-2

Synthesis and Immunomodulating Properties of Mono- and Di-Mannosylated Desmuramyl Peptides

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Muramyl dipeptide (MDP, N-acetylmuramyl-L-alanyl-D-isoglutamine) is the smallest immunologically active peptidoglycan fragment[1]. Desmuramyl peptides are MDP analogs without N-acetylmuramic part. MDP acts as a pathogen-associated molecular pattern and activates the NOD2 (Nucleotide Binding Oligomerization Domain Containing 2) receptor. Following the activation, NOD2 binds to the protein kinase RIP2 (receptor-interacting protein 2) to coordinate NF-κB (nuclear factor κ B)-mediated cytokine responses. L-Ala-D-isoGln pharmacophore contributes mostly to the NOD2 binding[2]. Mannose receptors present on immunocompetent cells also represent a class of pattern-recognition receptors, as well as NOD2. Therefore, we have designed and synthesized mannosylated desmuramyl peptides with one and two mannose units, in order to explore the contribution of mannosylation to immunostimulation. Immunostimulating properties of synthesized compounds are evaluated in the mouse model. Mannosylated DMPs exhibit improved immunological activity and the di-mannoslyated derivative showed to be the most active one. Man2AdDMP has induced the highest production of total anti-OVA IgG antibodies, and it directs the immunoreaction toward the Th2 type response.

Keywords: Synthesis, Immunomodulating properties, Mono- and di-mannosylated desmuramyl peptides

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OBPC P-3

Examining the Inhibitory Activity of Furanocoumarin Derivatives from *Kampo Extract Medicines* on Beta-Secretase 1 Enzyme Involved in Alzheimer's Disease Pathogenesis

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The present study aimed to evaluate the inhibitory effect of natural furanocoumarin coumarin derivatives, namely isoimperatorin (***Iso*IMP**), oxypeucedanin (**OXY**), oxypeucedanin hydrate (**OXY*h***), imperatorin (**IMP**), heraclenin (**HER*n***), and heraclenol (**HER*l***) isolated from *Kampo Extract Medicines*, on human enzyme Beta-Secretase 1 (**BACE1**) through molecular docking simulation. **BACE1** plays a pivotal role in the pathogenesis of Alzheimer's disease by catalyzing the production of amyloid-beta peptides, which form the hallmark plaques in the brains of Alzheimer's patients. Based on the Gibbs binding energies (ΔG_{bind}, kcal mol^{-1}), the inhibitory potential against the **BACE1** enzyme decreases in the following order: **OXY** (-7.65) > **HER*n*** (-7.55) > ***iso*OXY** (-7.27) > ***iso*IMP** (-7.20) > **IMP** (-7.05) > **HER*l*** (-6.78). While all investigated compounds exhibit nearly identical, albeit slightly lower, inhibitory effects towards the **BACE1** enzyme compared to Isophthalamide (**IsoP**, -9.71), they still demonstrate significant inhibitory activity. In summary, the examined compounds display strong inhibitory activity against the **BACE1** enzyme and show structural similarities to commercial inhibitors. Furthermore, considering the crucial role of **BACE1** in Alzheimer's disease pathogenesis, their potential as **BACE1** inhibitors opens avenues for further research and suggests possible therapeutic applications in Alzheimer's treatment.

Keywords: furanocoumarins, molecular docking, Kampo Medicines.

OBPC P-4

Design and Synthesis of Some Novel Compounds Derived from Hybdrid Coumarin-Thiazole Structures

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Coumarins are molecules that belongs to a special family of compounds which, due to the conjugated double bond become interesting molecules for many fields of study. Their structure and physical properties make them a privileged scaffold in medicinal chemistry. Also, they exhibit a wide range of biological activity including free radical scavenging. Recent research has focused attention on the anticancer activity of coumarin and coumarin- derived compounds due to their high level of cytotoxicity. Thiazole rings, on the other hand, had also showed remarkable anticancer activity on various cancer cells. Based on this, the idea was to combine those two heterocyclic units in one hybrid unique molecular structure with high anticancer potential. The synthetic strategy was simple, applying the reaction of diazotation of 2-aminothizoles and using the corresponding diazonium salts as good electrophiles to attack the 4-hydoxycoumarin at position 3. Furthermore, it was revealed by previous investigation that the alkyl substituent at the thiazole ring is playing key role. Namely, by increasing of the nonpolar tail at that part of the molecule, the biological activity is also increased. Based on this, some 4-substituated-2-aminothiazoles were synthesized by optimization of the Hantzsch reaction, prior to diazotation and coupling with the coumarin core. All of the newly synthetized compounds were purified by crystallization and the melting point was determined. Finally, the obtained compounds were characterized by spectroscopic means.

Keywords: synthesis, coumarin, thiazole, Hantzsch reaction, anticancer activity

OBPC P-5

Chemical Profiling and Antioxidant Capacity of Lichen Extracts from Genus *Physcia*

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Lichens, which are symbiotic organisms, are increasingly being recognized for their wide range of chemical compounds, biological functions, and possible therapeutic uses[1]. This study examines the chemical composition, total phenolic and flavonoid content, as well as the antioxidant activity of acetone and hexane extracts derived from the lichen *Physcia dubia*. The chemical characterization of the extracts was conducted using high-performance liquid chromatography coupled with a UV detector (HPLC-UV), while the quantification of total phenolic (TPC) and flavonoid contents (TFC) was performed using a spectrophotometric method. HPLC assessment of the extracts from *P. dubia* lichen indicated the presence of methyl beta carboxylate, haematommic acid, methyl haematommate, parietin, and atranorin as the main components. The most abundant components of the acetone and hexane extracts was the di-depside atranorin (65.25 % and 96.85 %) and methyl beta carboxylate (20.15 % and 2.03 %). The TPC and TFC analyses indicated that the acetone extract displayed higher values, with a TPC of 69.69 mg GA/g and a TFC of 38.36 mg RE/g, and 6.61 mg QE/g. Antioxidant activity was assessed through in vitro assays including DPPH and ABTS radical scavenging activities. The acetone extract exhibited a slightly superior level of antioxidant activity ($IC_{50\ DPPH}$= 237.35 µg/mL; $IC_{50\ ABTS}$= 219.51 µg/mL). This study adds to the broader understanding of both this lichen species and the genus *Physcia*.

Keywords: Physcia, HPLC, Antioxidant Activity, Total phenols

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OBPC P-6

QSAR study for the antiproliferative activity of 2-aryl benzothiazole derivatives

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Quantitative Structure-Activity Relationship (QSAR) analysis for the antiproliferative effects of benzothiazole derivatives evaluated on the human MCF7 breast cancer cell line and hepatocellular carcinoma cell line, HepG2. QSAR provides insight into structural characteristics related to enhanced anticancer activity. The best model obtained for cytotoxic activity on the MCF7 cell line is: $\log IC_{50} = 8.212 - 0.059$ *RDF025u* – 32.01 *G2m* ($N_{tr} = 27$; $N_{ex} = 5$; $R^2 = 0.76$; $F = 37.86$; $R^2_{ext} = 0.87$); while for the activity on the HepG2 cell line: $\log IC_{50} = 5.821 + 1.741$ *Mor26m*– 27.607 *G2m* ($N_{tr} = 27$; $N_{ex} = 5$; $R^2 = 0.77$; $F = 41.11$; $R^2_{ext} = 0.91$). WHIM descriptor *G2m,* presented in both models, transmits information about the three-dimensional symmetrical dispersion of atomic mass along the y-axis. Thus, the projection of the atomic mass along the y-axis is absent for the most active compound **26** (Figure 1). QSAR models also revealed that the increased number of atoms distributed in the inner part of a molecule enhanced antiproliferative activities.

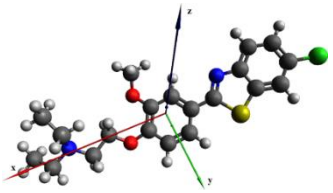

Figure 1. The three-dimensional representation of the optimized structure with principal axes of the most active compound **26**.

Keywords: anticancer activity, benzothiazoles, QSAR, WHIM descriptor

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OBPC P-7

Molecular Docking Study for the Antiproliferative Activity of 2-Aryl Benzothiazole Derivatives

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To elucidate the inhibition mode of the 27 derivatives of benzothiazole against human breast cancer cell, they were docked into the binding site of the estrogen receptor alpha (ERα) (pdb: 5U2B). Compound **33**, which showed strong inhibitory activity against the human MCF7 breast cancer cell line (IC_{50} = 4.71 μM), is the sixth best-ranked compound after the standard ligand PA-E2, according to its binding energy (-86.74 and -104.72 kcal mol^{-1}, respectively). Compound **33** binds at the C-terminal ligand binding domain (LBD) of ERα, partially encased within the narrower half of the LBD in a predominantly hydrophobic cavity (**Figure 1**). For this binding, an important structural feature of benzothiazoles is nitrogen from the thiazol ring.

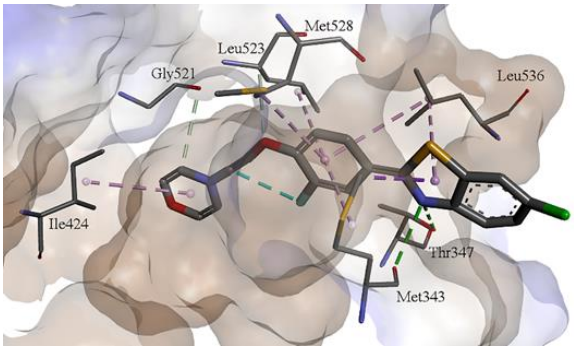

Figure 1. Hydrophobic surface representation of LBD with the docked compound **33**.

Keywords: breast cancer, antiproliferative activity, benzothiazoles, molecular docking

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OBPC P-8

Impact of Deep Eutectic Solvent Pretreatment on the Extraction of Polyphenolic Compounds and Antioxidant Activity from Wild Apple (*Malus Sylvestris*) Waste

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Deep eutectic solvents (DES) and natural deep eutectic solvents (NADES) enhance polyphenolic compound extraction from biomass by disrupting cell walls and increasing solubility, providing a sustainable alternative to conventional methods and significantly improving yields and antioxidant activity[1]. In this study, we investigated the impact of pretreatment with four different eutectic solvents on the ultrasound-assisted extraction of total phenolic (TPC) and flavonoid (TFC) contents and the antioxidant (DPPH and ABTS assays) activity of wild apple waste generated during the production of filter tea. The extracts obtained with DES pretreatment have a significantly higher content of TPC (from 808.21 to 969.64 mg GAE/ml LE) and TFC (from 295.93 to 586.39 mg QE/ml LE) compared to the extracts without pretreatment (TPC=252.51 GAE/ml LE and TFC=62.66). Additionally, the DES pretreatment extracts exhibit stronger capability in neutralizing DPPH (IC_{50} µg/ml=26.93-130.144) and ABTS (IC_{50} µg/ml=32.48-148.65) compared to the extracts without pretreatment (IC_{50} µg/ml_{DPPH}= 154.68 and IC_{50} µg/ml_{ABTS}=188.13).The obtained results indicate that pretreatment with deep eutectic solvents significantly enhances the extraction efficiency of polyphenolic compounds as well as the antioxidant activity of wild apple waste, demonstrating superior performance compared to conventional methods.

Keywords: deep eutectic solvents, polyphenolic compounds, antioxidant activity, *malus sylvestris*, pretreatment extraction

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OBPC P-9

Insight into the Interactions of Cornelian Cherry Anthocyanins with Dipeptidyl Peptidase III

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Dipeptidyl peptidase III (DPP III) is a zinc-hydrolase involved in various physiological and pathological processes. Its overexpression in several cancers and sepsis positions the enzyme as a promising target for drug development. In our previous work, we have found that cornelian cherry (*Cornus mas* L.) extracts inhibit human DPP III (hDPP III), and that its anthocyanin components have an affinity to form a complex with the open form of the enzyme[1]. In this study, molecular docking was used to explore interactions between cornelian cherry anthocyanins and the semi-closed form of hDPP III, the dominant form in aqueous solution. The obtained results revealed that all anthocyanins have a better affinity to form complexes with the semi-closed form of hDPP III compared to the open form of the enzyme. Among the tested anthocyanins, pelargonidin 3-robinobioside (Pg3rob) exhibited the highest binding affinity of -9.5 kcal/mol. Interactions of the aglycone core of this compound include hydrogen bond with Gln566, and π-anion, amide π-stacking, π-π-stacking, and π-alkyl interactions with Glu316, Ser317, Tyr318, and Ala567, respectively. Additionally, robinobiosyl moiety of Pg3rob forms hydrogen bonds with Ala388, Gly389, and Glu451, and π-sigma interaction with His568.Overall, this research provide suseful insight into the interactions of anthocyanins with semi-closed form of hDPP III, which may explain the observed *in vitro* inhibitory activity of these plant-derived compounds.

Keywords:anthocyanins, cornelian cherry, dipeptidyl peptidase III, molecular docking

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OBPC P-10

Molecular Docking Study on the Potential Mechanism of Coumarin-1,2,4-Triazoles Antifungal Activity

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Pathogenic fungi cause severe crop damage and production losses in agriculture, requiring treatment with fungicides. Due to the withdrawal of many fungicides because of adverse environmental effects, there is a continuous search for new antifungal agents. Recently we have shown that hybrid coumarin and 1,2,4-triazole compounds inhibit the mycelial growth of some plant pathogenic fungi, and utilizing molecular docking proposed lanosterol 14α-demethylase as the most probable target.[1] However, the purpose of hybrid compound research is, among others, to find compounds with multiple targets contributing to the desired activity. Thus, the potential mechanism of antifungal activity was further investigated by docking the compounds to other enzymes involved in mycelial growth, specific allychitinases (A and B), and *N*-myristoyltransferase. Most of the tested compounds fit well into the active sites of both chitinases. However, despite good binding affinities, the compounds did not interact with important residues in the active site of *N*-myristoyltransferase. Al together, results indicate that coumarin-1,2,4-triazoles potentially inhibit two antifungal activity targets, sterol 14α-demethylase and chitinases, which is promising for their further research in this field.

Keywords: coumarin-1,2,4-triazoles, antifungal activity, molecular docking, chitinase, *N*-myristoyltransferase

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OBPC P-11

New Powerful Building Block Molecules in 1,8-Naphthalimide Chemistry

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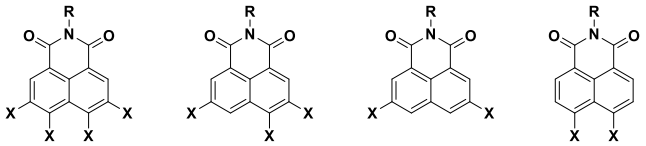
In recent years, much attention has been paid to the design and preparation of new substituted 1,8-naphthalimide architectures and the studies on the properties of materials[1,2]. Wide possibilities of changing the optical and fluorescence, thermal, electrochemical, electroluminescent, and photoelectrical properties of 1,8-naphthalimide compounds can be materialized by introducing different electron-donating or electron-accepting moieties at the 1,8-naphthalimide core. At the same time, derivatives of substituted 1,8-naphthalimide have found application in other optoelectronic devices, such as organic light emitting diodes, organic solar cells, as well as in memory devices. 1,8-Naphthalimides can have wide energy gaps and low reduction potentials, making them good candidates for use as *n*-type materials in OLEDs.



In our laboratory we have developed several new building block molecules[1, 2] that have found wide application for the synthesis of various naphthalene based fluorophores and chromophores.

Keywords: 1,8-naphthalimides, building block molecules, anticancer drugs, OLEDs

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OBPC P-12

Design Of Peri-Disubstituted Tellurolo-1,8-Naphtalimides

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Polyacenes possessing peri-dichalcogen bridges are well documented in the literature and are known for their extremely high electron donating abilities[1].

Substituted 1,8-naphtalimides, on the other hand, have found plenty of applications throughout the years thanks to their exceptionally diverse and rich photoelectronic properties.

Thus, combining the great electron donating abilities of tellurium heterocycles as well as the naphthalimide core, novel series of peri-disubstituted ditellurols were synthesised. Contrary to the aforementioned polycyclic aromatics, they show higher degree of solubility and are thus much easier to characterise. The imide group not only enhances the optoelectronic properties of the molecule by acting as an electron sink but also increases the overall solubility by means of controlling the alkyl length of the attached amine. Introducing a strong acceptor lowers the LUMO of the molecule that changes observably the CT excited states. Ditelluride are easily reduced in presence of current and reoxidized again since throughout the whole process both tellurium atoms remain in close proximity to each other held tightly by the naphthalene core.

Based on all these facts we suppose that such structures might show better battery capacity and could find applications as potential cathode materials in electronic materials.

Keywords: 1,8-naphtalimides, ditellurols, electronic materials

Acknowledgments: „This study is financed by the European Union-NextGenerationEU, through the National Recovery and Resilience Plan of the Republic of Bulgaria, project No BG-RRP-2.004-0008“

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OBPC P-13

Heterocyclic Fused 1,8-Naphthalimides As Anticancer Agents

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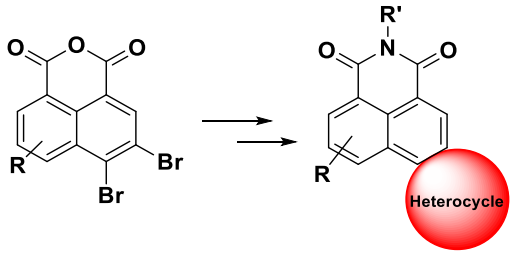
Recent anticancer research has focused on small molecules that interact with DNA. Among these, 1,8-naphthalimides and their derivatives have demonstrated significant anticancer activity against various human and murine cells. Studies show that their efficacy is greatly affected by the fusion of aromatic or heteroaromatic rings and by modifications to the position and size of their side chains.

In our laboratory, we have developed an excellent building block for the synthesis of heterocyclic extended 1,8-naphthalimides. The target structures are highly suitable as DNA intercalators.



Keywords: 1,8-naphthalimides, anticancer activities, heterocyclic compounds

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OBPC P-14

Synthesis and Optical Properties of PEG Alkoxylated 1,8-Naphthalimides

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1,8-Naphthalimides have found wide application as emissive materials in OLEDs, chemosensors for cations and anions, fluorescent cellular imaging agents and DNA intercalators. The NMI core have proven itself as versatile photoactive structure upon which many fluorescent compounds can be built. The addition of electron donating substituents to the electron acceptor already present in the aromatic ring forms a push-pull system with good photostability and high fluorescence quantum yields.

Here we present the synthesis of double *peri*-PEG substituted naphthalimides containing both hydrophilic and hydrophobic substituents. The substances are highly fluorescent, both in solution (including water) and in the solid state, making them highly suitable for bio application. The synthesis, optical properties and potential applications of several derivatives will be discuses in this poster.

Keywords: 1,8-naphthalimides, peryleneimides, dichalcogenides

Acknowledgements: Authors are grateful to the Bulgarian National Science Fund project KP-06-H79/8.

OBPC P-15

Peri-Substituted Dichalcogenides of Ryleneimides

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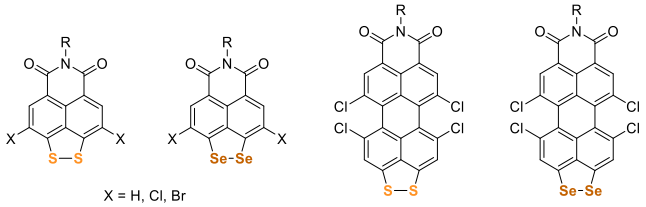
Tuning of solid-state properties using molecular modification is a key to develop organic functional dyes such as light emitting diodes, solar cells, and memory devices. Herein, we describe the first naphthalene monoimide dithiolato or diselenolate derivatives as well as the preparation of novel NMI-dithiolate and diselenate containing two additional halogen atoms in the *ortho* positions to the two chalcogens. We also recently reported a facile strategy for synthesis of perylene monoimide dithiolato or diselenolate derivatives.



The synthesis, optical properties and potential applications of several derivatives will be discuses in this poster.

Keywords: 1,8-naphthalimides, peryleneimides, dichalcogenides

Acknowledgements: Authors are grateful to the Bulgarian National Science Fund project NSF KP 06-N69/1.

OBPC P-16

Implementation of Supervised and Unsupervised Machine Learning Techniques in the Development of Pharmaceutical Dosage Forms

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Principal component analysis (PCA) and Partial-least squares-Discriminant analysis (PLS-DA)[1] using Simca® 17 software were applied for evaluation of the X-Ray powder diffraction (XRPD) diffractograms obtained from a compatibility study designed for the active pharmaceutical ingredient (API) ibuprofen with selected excipients, commonly used in the formulation of pharmaceutical dosage products.

Based on the obtained results changes in the XRPD diffractograms were better explained by the optimal PLS-DA model (R^2X = 0.833, R^2Y = 0.991 and Q^2 = 0.960), compared to the corresponding PCA model (R^2X = 0.894 and Q^2 = 0.687), implying that the supervised machine learning-based techniques are a more adequate choice. The prediction power of the optimal PLS-DA model for XRPD experimental data was further confirmed by estimation of the Root mean squared error of prediction (RMSEP = 0.35%).

The obtained results have shown that the implementation of XRPD in this type of studies, coupled with machine learning-based algorithms, is a promising approach to obtain valuable information about the structural changes in the tested samples and therefore can be used during the routine analysis in the formulation development.

Keywords: X-Ray powder diffraction, machine learning, PCA, PLS-DA

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OBPC P-17

A Series of Esters of Regioisomeric Furanmethanols: Mass Spectral Libraries and Gas Chromatographic Data

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Volatile furan derivatives are highly esteemed by food chemists and technologists due to their notable organoleptic properties. Furfural and its derivatives hold significant economic value in the flavor industry, as they are extensively used as aroma and taste enhancers, contributing notably to the sensory qualities of heated foods. These compounds play a crucial role in determining consumer acceptance of various foods and products. Consequently, the characterization of aromatic profiles, precise compound identification, and sensory evaluations are essential aspects of food research, quality control, and product development. Accurate identification of furfural and related compounds is particularly important given that, under certain conditions, they can negatively impact human health.

A review of the literature on the retention index (RI) data for esters of regioisomeric furanmethanols (furan-2-ylmethanol and furan-3-ylmethanol) revealed a lack of comprehensive references and data on their mass spectra and gas chromatography retention. This survey highlighted frequent instances of partial identification or even misidentification in existing studies. To address this gap, we synthesized a series of esters of regioisomeric furanmethanols with selected short- and medium-chain fatty acids and various aromatic acids. This work resulted in a detailed collection of gas chromatographic RI data obtained via GC-MS using commonly employed capillary columns of different polarities. The compilations of retention indices and electron ionization mass spectra generated can facilitate automated profiling, advancing the field of food chemistry.

Keywords: regioisomeric furanmethanols, furfuryl esters, EI Mass Spectral Libraries, GC RI Libraries, MS and GC data collections

OBPC P-18

Evaluating *Cinchona*-9-amines as Butyrylcholinesteras Inhibitors

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Cinchona alkaloids are natural products with interesting structure which includes aromatic quinoline ring and bicyclic aliphatic quinuclidine ring connected with a chiral carbon atom having hydroxyl group.[1] These alkaloids and their derivatives are useful in organic chemistry as chiral stationary phases for chromatographic separations or organocatalysts in stereoselective syntheses[2] but due to their various bioactive properties they are also very important in medicinal chemistry. Some derivatives of *Cinchona* alkaloids have been previously identified also as inhibitors of cholinesterases.[3]

To investigate a new class of potentially bioactive *Cinchona* alkaloids, a series of cinchonidine-9-amine and their corresponding pseudo-enantiomeric cinchonine-9-amine have been prepared. They were used as starting material for the Menshutkin reaction in which the quinuclidine nitrogen atom is quaternized with differently substituted benzyl bromides. Structural properties of prepared compounds were studied by FT-IR, 1D and 2D ^{1}H and ^{13}C NMR spectroscopy and mass spectrometry. All prepared compounds were evaluated as butyrylcholinesterase (EC 3.1.1.8) inhibitors.

Keywords: *Cinchona*-9-amines, Menshutkin reaction, butyrylcholinesterase inhibitors

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OBPC P-19

The Reducing Power of Black Pepper (*Piper Nigrum* L.) Essential Oil and Hydrolate

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NOT PRESENTED

OBPC P-20

Chemical Composition and Antioxidant Activity of *Geranium Robertianum* L. Leaves Hydrolate

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NOT PRESENTED

OBPC P-21

Chemical Composition and Antioxidant Activity of Hydrodistillation Wastewater from *Herniariae Herba* (*Herniaria Glabra* L.)

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The present paper aimed to determine the chemical composition and antioxidant activity of hydrodistillation wastewater (HDWW) from *Herniariae herba*. The plant material was purchased from the Institute for Medicinal Plants Research, "Dr. Josif Pancic", Belgrade, Serbia. The essential oil was isolated by Clevenger hydrodistillation for 2 hours using a hydromodulus of 1:10 m/V. The chemical composition of the HDWW was determined by the UHPLC-DAD-ESI-MS method. The contents of total phenols (TPC) and total flavonoids (TFC) were determined by the Folin-Ciocalteu method and the $AlCl_3$ method, respectively, while the antioxidant activity was determined by the DPPH assay. According to the results obtained, HDWW was rich in phenolic acids (such as 4-*O*-caffeoyl-quinic acid) and flavonoids (such as oxytroflavoside A). The TPC and TFC were 77.6 mg GAE/g of dry extract and 16.3 mg QE/g of dry extract, respectively. According to the EC_{50} values obtained, HDWW showed better antioxidant activity (0.22 mg/cm^3) in comparison to synthetic antioxidant butylated hydroxytoluene (0.43 mg/cm^3) after 20 minutes of incubation with the DPPH radical. It could be concluded that hydrodistillation wastewater from *Herniariae herba* should be considered as a potential source of natural alternative to synthetic antioxidants.

Keywords: liquid waste, rupturewort, hydrodistillation by-product

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OBPC P-22

Why Does Gallium Exert an Antibacterial Effect: Insights from a DFT Study

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The main objective of the current research is the abiogenic metal cation gallium(III) and its mechanism of antibacterial therapeutic action. As an iron mimicry species it is well known that gallium strongly binds to the iron-transporter in blood, transferrin, which appears as its main carrier in the bloodstream. Gallium's antibacterial action, however, is more focused on the interaction between the abiogenic ion and the iron-scavenging siderophores that possess different affinity depending on the type of bacterium secreting it, but also on the intimate structure of the siderophores and the gallium-based initial complex. Consequently, it was found that different *P.aeruginosa* strains, genetically modified to lack the ability of synthesizing either pyochelin, pyoverdin, or both, show specific susceptibility toward Ga-based therapy. Another bacterium prone to such therapy is *A.baumannii* secreting acinetobactin in two forms depending on the pH of the surrounding medium. Although experimental evidence has been extensively provided, the intimate mechanism of the process of Ga^{3+}/ Fe^{3+} competition for binding bacterial siderophores has not been revealed. Herewith, we apply reliable DFT methodology in an attempt to shed light on the metal rivalry for binding these intriguing ligands of biological significance and to disclose the factors that predispose gallium's application as a novel therapeutic agent.

Keywords: gallium, iron, siderophores, DFT analysis

Acknowledgments: This research is funded by the Bulgarian National Science Fund, grant number KP−06-M69/1 (project "*In silico* study of the antibacterial action of Ga-based complexes applied against ESKAPE microorganisms"). N.K. gratefully acknowledges the additional funding provided by the Program "For Women in Science" 2023, granted by L'Oreal and UNESCO.

OBPC P-23

Ru(II)-catalyzed Synthesis of Heteroarylated 2-Pyridones via Consecutive C–O/C–N/C–C Bond Formation Reactions

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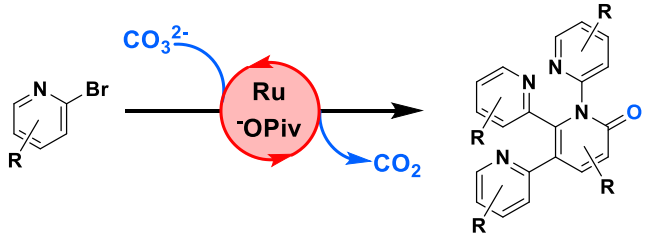
Reactions that lead to the formation of hetero(aryl)-hetero(aryl) systems in a simple manner are interesting from a synthetic point of view, since such systems occur in many biologically active compounds and natural products[1].

A novel strategy for the synthesis of 2-pyridones decorated with 2-pyridyl groups is presented starting from substituted 2-bromopyridines using a simple Ru(II)–pivalate–carbonate catalyst system. Unsubstituted 2-bromopyridine was successfully converted to the penta-heteroarylated 2-pyridone product using this method. Preliminary mechanistic studies revealed a possible synthetic pathway leading to the multiply heteroarylated 2-pyridone products involving consecutive oxygen incorporation, Buchwald-Hartwig type reaction and C–H bond activation.



Keywords: 2-pyridone, C–H activation, Ru-catalysis

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OBPC P-24

Tetramic and Tetronic Acids in Enantioselective Organocatalyzed Transformations

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Tetramic and tetronic acids represent an important and structurally diverse group of naturally occurring compounds that have been isolated from various terrestrial and marine species. They have attracted considerable attention due to their diverse and promising bioactivities.[1] Simple unsubstituted tetramic acids are prepared in two steps by *C*-acylation of Meldrumic acid with the activated, *N*-protected α-amino acid followed by subsequent thermal decomposition of the Meldrumate intermediate.[2] Together with tetronic acid, they represent useful building blocks for the construction of libraries of more complex tetramic/tetronic acid derivatives. Continuing the application of pyrrolone derivatives in organocatalyzed asymmetric transformations, the use of *N*-substituted tetramic acids and tetronic acid in organocatalyzed conjugative addition to nitroalkene acceptors followed by *O*-alkylation/acylation (59–94% *ee*) is presented. The resulting polyfunctionalized tetramic acids were incorporated into model dipeptide and depsipeptide sequences, while detailed quantum chemical studies provided mechanistic insights into the organocatalyzed transformation.[3]

Keywords: Asymmetric organocatalysis; Bifunctional noncovalent organocatalysts; Tetramic acids; Tetronic acids; Amidation

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OBPC P-25

Quaternary 3-Quinuclidinone Compounds: Potent Antibacterial Agents Against *Staphylococcus aureus* and *Listeria monocytogenes*

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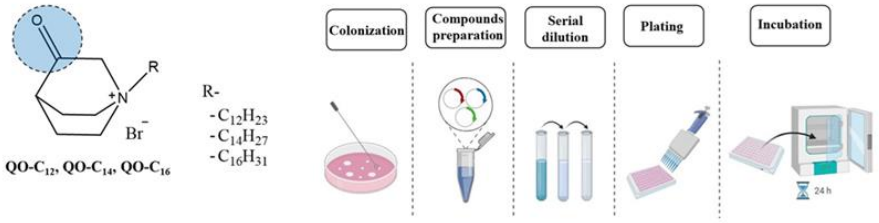
Quaternary ammonium compounds (QACs) are a class of organic compounds known for their potent antibacterial properties. However, their high toxicity, attributed to a membranolytic mode of action, raises significant concerns. Speculating that the polarity and hydrogen bonding potential of the substituent can affect antibacterial activity, we synthesized QACs which are unable to form hydrogen bonds with surrounding water molecules.The newly synthesized 3-quinuclidinone QACs with alkyl chain were tested for their antibacterial activity. The obtained minimum inhibitory concentrations (MICs) were better compared to previously synthesized QACs[1], indicating the role of substituent's hydrogen bonding potential. Among the candidates, QO-C_{16} exhibited excellent antibacterial activity against all tested strains of *Staphylococcus aureus* (ATCC 25923 and 33591, including Clinical/MRSA) at a concentration of 7.81 µM, which is equal to or better than conventional QACs (10-25 µM). This candidate also showed strong activity against the foodborne pathogen *Listeria monocytogenes* (ATCC 7644) with MIC of 3.9 µM, outperforming the activity of commercial QACs.Our study demonstrates that QO-C_{16}, exhibit superior antibacterial activity, underscoring their potential as effective and safer alternatives for combating bacterial infections and reducing resistance.



Keywords: QAC, antibacterial activity, minimum inhibitory concentrations

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OBPC P-26

DFT Prediction of Laser Dyes - Cucurbit[7]Uril Binding Affinities

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One of the important applications of supramolecular host-guest complexes is the control of the photo-physical properties of light-emitting dyes. Host-guest supramolecular complexes are dynamic systems composed of macrocyclic host molecules that encapsulate smaller guest molecules. Fluorescent supramolecular complexes based on classical synthetic macrocyclic host molecules (cyclodextrins, calixarenes, etc.) or more versatile host systems (cucurbiturils and bambusurils) have been described in the literature. Among macrocycles, cucurbiturils are carriers with the highest affinity (typically 6 orders of magnitude higher), so they have great potential for applications in biology, medicine, and materials science. Supramolecular host-guest complexes typically result from the selective encapsulation of fluorescent dye molecules in solution. When deposited on solid matrices, however, the efficiency of the dyes decreases, limiting their use in fluorescent applications. Inspired by the discovery of Paatelainen et al. that complexation between CB[7] and acrylated Rhodamine B (RhBa) dye leads to an enhancement of fluorescence as well as an improvement of photostability in swollen hydrogel films, we decided to computationally model supramolecular host-guest complexes of CB[7] with different laser dyes as guests and to evaluate the binding affinities (the strength of the interaction between host and guest molecules). Furthermore, the possibility of the host molecule to incorporate a side chain of the water-soluble PAZO polymer into its cavity was considered.

Keywords: DFT prediction, laser dyes.

Acknowledgements: This research was funded by Bulgarian National Science Fund, grant number KP−06-N39/10 (project "BIRDCagE"). S.A. gratefully acknowledges the funding by the European Union-NextGenerationEU, through the National Recovery and Resilience Plan of the Republic of Bulgaria, project № BG-RRP-2.004-0002, "BiOrgaMCT". The authors gratefully acknowledge the provided access to the e-infrastructure of the NCHDC–part of the Bulgarian National Roadmap for RIs, with the financial support by Grant No D01−325/01.12.2023.

OBPC P-27

Naphthalimide-Based Amphiphiles: Synthesis and DFT Studies of the Aggregation and Interactions with Water Molecules

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The synthesis of novel fluorescent amphiphilic naphthalimide-based probes with 1,8-naphthalimide as the fluorescence signal reporting group, octyl as hydrophobic head, and PEG as hydrophilic tail is described. 1,8-Naphthalamides themselves represent an important class of biologically active compounds with favorable photophysical properties, that makes them extremely useful bifunctional therapeutic agents and fluorescence imaging agents. Both unsubstituted and substituted naphthalimide units tend to aggregate due to intermolecular π–π interactions among the naphthalimide cores. In our study, we focus on the core 1,8-naphthalimide fragment and on the PEG hydrophilic tail(s), and substitutions at the nitrogen atom will enable further functionalization in the future. The designed molecules represent a new class of self-assembling structures with some promising characteristics. The successful synthesis of such structures is fundamental to synthetic chemistry, and the computational study of the aggregation and binding of water molecules are shedding light on the ability of these new systems to function as membrane water channels. This study not only expands the list of 1,8-naphthalamide derivatives but may also serve as a new platform for the development of PEG-functionalized naphthalamide-based membrane additives.

Keywords: 1,8-Naphthalamides, PEG-functionalized naphthalamide

Acknowledgements: This research was funded by Bulgarian National Science Fund, grant numbers KP−06-N39/10 (project "BIRDCagE") and KP-06-H79/8 of 15.12.2023 (project "BioTIARA").

OBPC P-28

Elucidating the Metal Specificity in PHLPP2

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Aberrant (abnormal) phosphorylation of proteins is one of the hallmarks of cancer cells and in many cases is a prerequisite for maintaining tumor development and progression. Protein phosphatases catalyze selective dephosphorylation and are key regulators of cell signaling. Yet, their contribution to aberrant signaling in cancer cells is generally less explored and hence their therapeutic potential remains largely unknown/untapped. Furthermore, the stoichiometry and identity of the bound metal ion(s), mechanism of action, and enzymatic specificity of these proteins is not known. Here, we take into consideration PHLPP2 as a potent representative of the family and try to elucidate its metal cation specificity by employing the reliable tools of the DFT methodology in conjunction with experimental techniques. We show some intriguing features of the protein under study mostly related to the active site composition, metal cation specificity, catalytic function, and its role in tumor suppression. Overall, the obtained results provide clues to the biological function of PHLPP2 of immense significance and disclose the factors that predispose its application in antitumor therapy.

Keywords: metal specificity, PHLPP2, DFT analysis

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OBPC P-29

Application of Voltammetric Methods in Electrochemical Analyzes of Cannabinoids

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The advantage of voltammetric analysis is rapid, sensitive and inexpensive methods contributed to their versatile applications: detection of cannabinoids in biological samples, quality control of cannabis product and analysis of their antioxidant properties.

A carbon-based electrode modified by initial electrodeposition of Δ^9-tetrahydrocannabinol (THC) has been established to enhance the affinity of the examined THC molecules to the sensing electrode surface. Amplified square-wave voltammetry (SWV) signal contributed to its application in detection of THC in artificial or real saliva samples.[1] SWVmethod for detection of cannabinoids in food products has been developed based on voltammetry of immobilized microparticles of cannabinol (CBN) and cannabidiol (CBD) at paraffin-impregnated graphite electrode. Cannabinoids have exhibited net peak potentials at 0.538 V and 0.556 V, for CBN and CBD respectively, attributed to electro-oxidation of a phenolic group to a phenoxy radical.[2] Cyclic voltammetry and differential pulse voltammetry have been utilized in examination of the antioxidant properties of isolated cannabinoids or Cannabis extract.

Although there are some challenges in practical application of these methods, analysis in forensic purposes and development of electrochemical sensors for detection of THC in biological samples have been deeply investigated and improved, nowadays.

Keywords: cannabinoids, forensic analysis, sensors, voltammetric techniques.

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OBPC P-30

Effects of Various Nitrite Scavengers on Mitigation of *N*-Nitrosamine Formation in Pharmaceutical Drug Product

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N-Nitrosamines, a class of chemical compounds recognized as potential human carcinogens, can form under specific conditions, particularly through the reaction of secondary or tertiary amines with a nitrosating agent, typically under acidic conditions. They have been detected in various products, including pharmaceuticals. In 2018, they were initially discovered in sartan-based drugs, and since then, pharmaceutical industries have faced challenges in controlling and mitigating the presence of these impurities.

The aim of our study was to understand the impact of using nitrite scavengers in drug product formulation to inhibit or control the formation of *N*-nitrosodimethylamine (NDMA) impurity in the drug product.

For chromatographic separation, detection and quantification of NDMA, liquid chromatography with high-resolution mass spectrometry (LC-HRMS) was utilized to achieve quantification of trace levels of the impurity. Liquid-liquid extraction using ethyl acetate as a solvent was employed for sample preparation in order to eliminate the interference of the sample matrix.

A stability study was conducted on three drug product formulations containing different nitrite scavengers, including ascorbic acid, propyl gallate and acetyl cysteine, to determine which nitrite scavenger performs best in mitigating the formation of NDMA. According to the stability study results, ascorbic acid was shown to be the most effective nitrite scavenger.

Keywords: *N*-nitrosamines, drug product, NDMA, nitrite scavengers

OBPC P-31

QSAR Modeling of Substituted Hydrazones- Biological Activity and Selected Descriptors

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Due to their many biological uses (antimicrobial, anti-inflammatory, antimalarial, anticancer, anticonvulsant, antidepressant ….) substituted hydrazones are of great interest[1]. In addition, hydrazones have been employed as herbicides, nematocides, rodenticides, insecticides, and regulators of plant growth. Potential uses for the metal complexes of hydrazones include molecular sensors, luminescent probes, and catalysts[2].

QSAR analysis of a substituted hydrazones tested for growth inhibitory activity against *Bacillus subtilis* was performed using several: *spectroscopic* and *physicochemical* descriptors. Multiple linear regression method was used to linearly correlate the selected descriptors and biological activity expressed as $\log 1/C_{MIC}$.

In all QSAR model, R^2 and R^2adj. values are > 0.98.

Keywords: QSAR, hydrazones, $\log 1/c_{MIC}$,

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OBPC P-32

QSTR Study of Alkaloids

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Diterpenoid alkaloids (DAs) are substances produced by various natural plants with significant thematic difficulties, bioactivity, and somewhat disreputable toxicity. Many DAs demonstrate different pharmacological properties[1,2]. DAs can be divided into a subgroups represented by molecules with the lycoctonine, heteratisine and napelline diterpene skeletons. DAs, for the last few decades, have been the target of considerable interest by medicinal chemists.

We present the results of a structure –toxicity relationships (QSTR) study carried out for 19 alkaloids with the lycoctonine skeleton. Alkaloids are subdivided into two groups in accordance with the functionality nature at C4. All original LD_{50} toxicity data (mg/kg) has been converted to $logLD_{50}$ response variables[3]. According the toxicity data, compounds of the second group are more toxic than the first group alkaloids. Several variable selection methods: Stepwise, Forward, Backward and Best model selection methods were performed by XLSTAT program package. In all QSAR model, R^2 values are > 0.85. The VIF (variance inflation factor) values were calculated for all model descriptors. To accept the QSTR model, the VIF value of should be between 1 and 5. Only QSTR model with 2 descriptors is statistically significant.

Keywords: QSTR, Diterpenoid alkaloids (DAs), $logLD_{50}$, VIF value

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OBPC P-33

Evaluation of the Molecular Properties and Bioactivity Score of the Set of Herbicides

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Lipinski's rule describes the molecular properties important to the pharmacokinetics of drugs in the human body, including their absorption, distribution, metabolism, and excretion (ADME)[1]. According to Lipinski, a compound is more likely to be membrane permeable and easily absorbed by the body if it meets criteria such as: (i) MW < 500; (ii) Log P < 5; (iii) HBA < 10 and (iv) HBD < 5. Lipinski's rule was quickly adopted in the design of herbicides and insecticides. Colin Tice defined the criteria for the identification of herbicides - modified Lipinski's rule (MLr): MW 150 ÷ 500; Log P ≤ 3,5; HBD ≤ 3; HBA 2 ÷ 12. According calculated values for 75 investigated herbicides, 12 herbicides of 75 heave one MLr violation; and only one herbicide is with two MLr violation.

Molinspiration is a web-based tool used for the calculation of bioactivity score (BS) of compounds including herbicides[3]. If BS values is: (i) < -5.0 then the compound is inactive, (ii) -5.0 ÷ 0.0 then the compound is moderately active and (iii) > 0, suggests the compound is active. From the results it can be concluded that most of the herbicides are active according to GPCRL and enzyme inhibitor parameters. All herbicides are inactive according to the ion channel modulator parameter.

Keywords: Lipinski's rule, bioactivity score, ADME parameters, herbicides

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OBPC P-34

Brain or Intestinal Estimated Permeation Predictive Model of Herbicides

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The assessment of absorption, distribution, metabolism, and excretion (ADME) properties is a necessary and responsible approach to bioactive compounds design.

SwissADME is a web tool designed for predicting pharmacokinetics parameters[1]. The physicochemical descriptors-based method part of SwissADME, termed the BOILED-Egg method, permits a clear and informative graphical representation of the potential for gastrointestinal absorption and brain-blood barrier permeation of bioactive compounds.

Herbicides are very poorly characterized with respect to their intestinal and brain passage in humans (in contrast to drugs). For a very limited number of them, intestinal absorption has been characterized from pharmacokinetics studies performed with human volunteers[3]. The intestinal and brain permeations of herbicides (and other pesticides) are nevertheless important to evaluate, in order to fully apprehend their potential toxicity.

The present study was therefore designed to evaluate in silico the intestinal absorption and brain permeation of 75 herbicides, using the SwissADME web tool. The investigated set consists of herbicides with different structural characteristics.

None of the tested herbicides belong to the yellow region; 28% of the herbicides belong to the white area, and the remaining herbicides are outside of the boundaries of the egg.

Keywords: Lipinski's rule, bioactivity score, ADME parameters, herbicides

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OBPC P-35

The Influence of Synthesized Ni(II)-Dithiocarbamato Complex on the Phytopathogenic Fungus *Botrytis Cinerea*

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Dithiocarbamates are a class of fungicides extensively used in agroculture worldwide due to their high efficiency in controlling plant pathogenic fungi and relatively low mammalian acute toxicity. *Botrytis cinerea* is a phytopathogenic fungus known in agriculture as "gray mold". This pathogen is able to survive at temperatures just above freezing, and poses a threat to agricultural products before and after harvesting (during storage and transport).

In this study, ammonium dithiocarbamate ($(NH_4)_3$idadtc) and the corresponding nickel complex Ni(H_2idadtc)$_2$ were synthesized according to a previously published procedure[1]. Antifungal properties of them against the plant pathogenic fungus *Botrytis cinerea* were investigated at five different concentrations ranging from 0,01 to 0,18 %. The Ziram, a commercial dithiocarbamato fungicide, was used as a control. Obtained results on the efficacy of the sythesized compounds compared and analysed based on the LSD test.

Compounds have inhibition effect towards fungal mycelium with all five concentrations applied in the experiment. The Ni- dithiocarbamate complex had enhanced antifungal activity compared with ligand precursor ($(NH_4)_3$idadtc). Especially good efficiency was observed with the first concentration of the Ni-complex, which was at the level of a commercial fungicide (about 68%).

Keywords: dithiocarbamates, Ni-complex, antifungal, *Botrytis cinerea*

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OBPC P-36

Investigating the Methods for Obtaining Extracts from Two Types of Herbal Substances from Elderberry, *Sambucus Nigra* L.

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Besides the most abundant flavonols (quercetin and apigenin) in the flowers, sambunigrin is mostly represented in the leaves. Some triterpenes, sterols, amino acids (glutamic acid, aspartic acid, and alanine), as well as lectins, have also been reported in the leaves and branches of elderberry, Sambucus nigra L[1].

We investigated two different methods of extraction: Soxhlet extraction (SOX) and Ultrasound-Assisted Extraction (UAE), against the conventional method for obtaining herbal infusions from two types of herbal substances: elderberry flower and elderberry herb (leaf with branches). SOX and UAE were performed with ethanol, while infusions were prepared with water. We noticed an important difference in the extraction yields from different herbal parts. Water is an ideal extraction solvent for elderberry flowers, but it has a very weak potential for extracting bioactive compounds from leaves and barks. Ethanolic Soxhlet extraction, performed as a 4-hour continuous extraction at a temperature of 60-65 ºC, was the most potent method for this aim. SOX extract absorbances measured at 550 nm were almost 10 times higher for the herb than for the flowers, with an A = 1.032 and 0.136, respectively.

In conclusion, although elderberry flowers are commonly known for their phyto-therapeutic properties, these preliminary findings suggest that there are different groups of hydrophobic bioactive substances represented in the leaves and barks of elderberry. These parts, traditionally used in the treatment of skin burns or wounds, should be analyzed in detail so their benefits can be fully realized.

Keywords: elderberry, extracts, ethanol, water, yield.

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OBPC P-37

Optimization of a Method for the Isolation of Theobromine from Cocoa

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Theobromine is a xanthine alkaloid that is consumed by millions of people every day in the form of hot or cold drinks, cocoa, tea, energy drinks and chocolate. Due to its enormous consumption, research on theobromine is constantly evolving to discover its potential pharmacological and health aspects. Recent studies have highlighted the potential of theobromine as a central nervous system stimulant, antitumor agent, anti-inflammatory and bronchodilator. [1]

The aim of this research is to optimise the process of isolating pure theobromine from commercially available cocoa powder by using different extraction methods. The choice of extraction solvents (70 % ethanol, 96 % ethanol, chloroform and dichloromethane) and the tannin removal agent (magnesium oxide and lead acetate) were varied to optimise the experimental conditions. It was also tested whether the steps of removing the carbohydrates and plant fibers and remove lipids the sample by Soxhlet extraction influence the isolation of theobromine. The purity of the theobromine obtained was confirmed by HPLC and TLC.

The best results for the isolation of pure theobromine were obtained by removing the tannins with MgO and extracting with 70 % ethanol for 3 hours. When the sample was extracted with 96% ethanol and refluxed for 1 hour, a higher yield of theobromine was obtained, but the presence of caffeine was also detected. Extraction with other organic solvents yielded a mixture of theobromine and caffeine.

Keywords: theobromine, caffeine, HPLC, extraction methods

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OBPC P-38

Ultrasound-Assisted Extraction of Silymarin from Milk Thistle Seeds (*Silybum marianum L.*)

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Milk thistle (Silybum marianum L.) is one of the oldest highly beneficial herbal medicines. Its seeds contain high levels of silymarin, a complex mixture of flavonolignan and flavonoid polyphenolic compounds.1 This work aimed to optimize the ultrasound assisted extraction (UAE) of silymarin from milk thistle seeds.

The UAE was carried out at a constant frequency of 37 kHz and 500 W ultrasound power by changing the operational parameters: time (10, 20, 30, 40, 50, and 60 min), temperature (30, 40, 50, 60, 70, and 80ºC), water to ethanol solvent ratio (100:0, 25:75, 50:50, 75:25, 0:100 v/v) and solid to liquid ratio (1:100, 5:100, 1:10, and 2:10 g/mL). An RP-HPLC method for the quantification of silymarin was applied. The chromatographic separation was conducted on a LiChrospher®100 C-18 column (150 mm length x 4.6 mm i.d., 5 µm particle size) using a mixture of phosphoric acid, methanol, and water (0.5:35:65 v/v) as mobile phase at 25ºC column temperature with 0.8 mL/min isocratic flow rate of the mobile phase.

The highest quantity of silymarin (20.3 mg/g dry weight) was determined in the extract obtained at followed extraction conditions: temperature 40ºC, time 60 min, 5:100 g/L solid to liquid ratio, and solvent composition water and ethanol in a ratio of 50:50 v/v.

Keywords: milk thistle seed, silymarin, ultrasound-assisted extraction, optimization

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OBPC P-39

Synthesis and Characterization of Novel Fluorescent Quinacridone Derivatives

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Fluorescent compounds (fluorophores) are often used as coupling agents for specific biomolecules (DNA, RNA, saccharides, etc.) investigated by different instrumental fluorescence techniques. However, biomolecules exhibit autofluorescence in the blue region of the electromagnetic spectrum, which causes interference, when the fluorescent-based techniques rely on blue-emitting fluorophores. This problem can generally be solved by using higher wavelength emitting fluorophores, or by choosing a technique that does not employ colour to discern the signal from the background.

The derivatives of quinacridone and its precursors are especially interesting, as they are promising in terms of both criteria mentioned before. Through variation of the substituents in the quinacridone derivatives, the emission spectra are tuned and at the same time, the fluorophores retain their chemical properties. This enables the application of multiple derivatives simultaneously in a single biological system, allowing for the imaging of various types of biomolecules at the same time. This study focuses on the synthesis of several derivatives of quinacridone and its precursors, their characterization, and the dependence of the emission on the substituents and substitution pattern.

The synthesis is conducted with diethyl succinate as a starting material, while the specific derivatives are introduced through the reaction of diethyl succinyl succinate with an appropriate arylamine. All synthetic steps were optimized, and the reaction was monitored by TLC. The derivatives are characterized using X-ray powder diffraction (XRPD), UV-VIS, and vibrational spectroscopy (IR and Raman). Fluorescence of the compounds was observed under UV light.

Keywords: quinacridone, fluorescence, XRPD, vibrational spectroscopy

OBPC P-40

Fungicidal Activity of The Zn(II) Complexes with Ethylenediamine and Dithiocarbamato Ligands on Phytopathogenic Fungus *Phomopsis Viticola*

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Dithiocarbamates (DTC) are a versatile class of easily preparable monoanionic 1,1-dithioligands.[1] DTC ligands exhibit significant potential due to their interaction with transition metal ions, reducing metal toxicity and enhancing biological properties such as antibacterial, antifungal, antiviral, inhibitory, etc.

For the purpose of this study, influence of Zn(II) complexes with ethylenediamine (en) and ammonium-iminodiacetate-dithiocarbamate ($(NH_4)_3$idadtc) as ligands: NH_4[Zn(idadtc)(en)] and NH_4[Zn(idadtc)$(en)_2$] on the inhibition of the pathogenic fungal mycelium *Phomopsis viticola* was analyzed. This phytopathogenic fungus causes by Phomopsis cane and leaf spot, a very significant vine disease that is common in Montenegrin vineyards.

The ligand and complexes, in five different concentrations were tested for fungus in laboratory conditions on PDA nutrient media. Complex NH_4[Zn(idadtc)$(en)_2$] showed a statistically insignificant inhibition of mycelial growth, while the ligand did not show antifungal effect at all. The highest tested concentration of NH4[Zn(idadtc)(en)] showed the highest statistically significant effectiveness in inhibiting the tested fungus, but it is still significantly less effective compared to the tested commercial active substance ziram. The results indicate that the coordination of $(NH_4)_3$idadtc with Zn(II) enhances the antifungal activity against the studied fungus.

Keywords: dithiocarbamate, antifungal, complexes, inhibition

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OBPC P-41

DNA Interactions of Palladium (II) Complex Containing a Thioamide-Type Ligand

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Thioamides and their derivatives are an interesting group of compounds because of their structural variations and also because of the combination of hard and soft donor atoms (S and N) that potentially allow coordination – in a variety of binding modes – to a wide range of metal centers, and also because of their biological significance.

In our previous studies, we have synthesized a palladium(II) complex with a thioamide-type ligand of the formula $[PdL_2Cl_2]$ (L= ethyl 4-[1-amino-2-cyano-3-(methylamino)-3-thioxo-1-propen-1-yl]-1-piperazine-1-carboxylate), whose ability to interact with HSA was investigated fluorometrically.[1] In this work, research was continued toward the study of interactions with calf thymus DNA in the presence of EB (ethidium bromide) or HOE (Hoescht 33258), with the aim of determining the binding affinity, binding strength and the binding mode. The results obtained showed that this complex binds moderately to the DNA via the minor groove, and that the quenching mechanism is static (Table 1).

Table 1. The Stern–Volmer constants (K_{sv}) and binding constants (K_b) for Pd(II) complex from CT DNA-EB and CT DNA-HOE fluorescence.

Complex	$K_{SV(EB)}$ [M^{-1}]	$K_{b(EB)}$ [M^{-1}]	$K_{SV(HOE)}$ [M^{-1}]	$K_{b(HOE)}$ [M^{-1}]
$[PdL_2Cl_2]$	2.58×10^4	6.59×10^3	3.77×10^4	2.76×10^5

Keywords: Palladium(II) complex; thioamides; DNA interaction; minor groove.

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OBPC P-42

Volatile Profile of Limonium Narbonense Mill. from Croatia

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Halophytes are plants that live in conditions with a high salt concentration. This is a large part of the earth's surface. Such areas are found on the shores of the sea, on inland lakes, in salt marshes and in inland deserts. In Croatia, halophytes grow not only by the sea, but also on the coast in the spray zone and in some places further away from the sea, where the salinity is pronounced due to strong winds and the soil is therefore salty. Plants that live in these areas have special adaptation mechanisms. These include a complex network of biochemical mechanisms and a number of bioactive molecules. Inadequate adaptation leads to osmotic and oxidative stress and increased expression of enzymes and phytohormones involved in stress responses. Halophytic medicinal plants have been used since ancient times to treat various diseases. This indicates the richness of biologically active compounds. In the Mediterranean, rural communities use halophytes both as food and as a source of health promotion. The aim of this study was to determine the volatile profile of *Limonium narbonense* Mill. from the Pantan Reserve, Croatia. The volatile compounds (VOC) were isolated directly from the plant material after heating, from the essential oil obtained by hydrodistillation and from the hydrolate remaining after isolation of the essential oil. The chemical composition of the VOC isolated from the air-dried plant material was identified by the coupled technique of gas chromatography-mass spectrometry (GC-MS) using the HP-5MS column. Headspace solid phase microextraction (HS-SPME) was used to isolate the VOC from the plant material and the hydrolate. The main VOC of the essential oil were *cis*-3-hexenol, nonacosane, heptacosane, *α*-thujone and camphor, the main VOC of the hydrolate were *cis*-3-hexenol, camphor, *α*-thujone and *trans*-2-hexenal, while the VOC isolated from the plant material were hexanal, benzaldehyde and camphor.

Keywords: Halophytes, *Limonium narbonense* Mill., volatile compounds, GC-MS.

OBPC P-43

The Antioxidant Capacity of Ammonium-Iminodiacetatedithiocarbamate and Its Transition Metal Complexes

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Dithiocarbamates (DTC) are chelating ligands that form stable complexes with all transition metals. DTC derivatives have been identified in a number of biologically active molecules[1], however the reports on their antioxidative potential are scarcer.

This research investigates for the first time the antioxidant activity of ammonium-iminodiacetatesdithiocarbamate ($(NH_4)_3$idadtc) and its complexes: $[Zn(idadtc)(en)]^-$ (en – ethylenediamine), $[Zn(idadtc)(en)_2]^-$, $[Cu(idadtc)]^{4-}$ and $[Ni(idadtc)]^{4-}$ by CUPRAC method. Experiments were performed with Cu(II)-neocuproine (Nc) as CUPRAC reagent and Trolox as a standard. The method is based on the absorbance measurement of Cu(I)-neocuproine (Nc) chelate at 450 nm.

The prepared samples were allowed to stand at room temperature prior to absorbance measurements which were performed after 30 and 60 minutes. After 60 min, the antioxidant capacities were slightly higher than that after 30 min. The ligand, $(NH_4)_3$idadtc, exhibited the highest antioxidant capacity compared to the complexes. Among them, only $[Zn(idadtc)(en)]^-$ did not show antioxidant activity, while all other compounds show satisfactory values and mutually similar antioxidant potential. These findings indicate that $(NH_4)_3$idadtc and its complexes have potential to be used as antioxidants, and are worthy of further investigation.

Keywords: CUPRAC, antioxidant capacity, complex, trolox

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OBPC P-44

Effective Caffeine Extraction from Cosmetics Containing Surface-Active Substances: An Optimization Study

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The extraction of caffeine from cosmetic products is essential for various applications, including quality control, product formulation and analytical studies. As there are no regulations for caffeine in the cosmetics industry, the source and content of caffeine in products are usually not specified. The aim of this research is to develop a method for the quantitative determination of caffeine in commercial cosmetic products, preceded by appropriate sample preparation for analysis.

In this study, various methods for the extraction of caffeine from different cosmetic matrices are evaluated. The principles, advantages, limitations and applications of each method are discussed. The focus is on optimizing the efficiency of liquid-liquid extraction and ensuring the purity of the extracted caffeine. The main challenge in the effective extraction of caffeine from cosmetic products was the presence of surfactants and the formulation of the emulsion. By using different solvent mixtures, including chloroform, dichloromethane, acetone and ethyl acetate in varying ratios, the optimal combination that effectively prevented emulsion formation was found to be a 1:1 ratio of chloroform to acetone. This solvent combination led to a recovery rate of around 97%.

The simple, rapid and reliable RP-HPLC method for the quantitative determination of caffeine in various cosmetics containing surfactants was developed. The best separation was achieved on a C-18 column (150 mm × 4.6 mm, particle size 5 μm) using an isocratic elution with methanol: water, 50:50. The developed method shows excellent linearity in the concentration range from 0.5 to 100 μg/mL The obtained concentration of caffeine in analyzed cosmetic products was in the range of 0.05 to 0.6%.

Keywords: Caffeine, Cosmetics, Liquid-liquid extraction, HPLC

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OBPC P-45

Thermal Decomposition of the Ferrocene Adsorbed on Boehmite

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NOT PRESENTED

OBPC P-46

Propane Dehydrogenation with Carbon Dioxide over the $VSbO/Al_2O_3$ Oxide Catalysts

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NOT PRESENTED

OBPC P-47

Synthesis of Acyclic and Cyclic C5-Curcuminoids and Comparison of Their Structurl and Spectroscopic Properties

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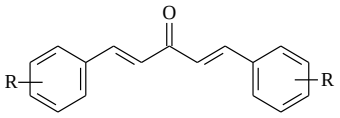
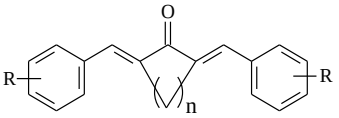
Despite its broad range of activity of curcumin, it is difficult to use it as a medication because of its low oral bioavailability. One way to circumvent this is to replace the beta-diketo moiety with monoketone to give so-called C5-curcuminoids. The goal of this study centered on the synthesis and characterization of acyclic and cyclic C5-curcuminoids and comparison of their spectroscopic and structural properties. The acyclic derivatives were based on the (1*E*,4*E*)-1,5-bis(2-methoxyphenyl) penta-1,4-dien-3-one moiety, while the cyclic analogs were based on cyclopentanone, cyclohexanone, cycloheptanone and 4-piperidone central core.



R = H, CH_3, OCH_3, F, Br, CF_3

vs.



n = 2 (cyclopentanone); n = 3 (cyclohexanone)
n = 3 (CH_2NHCH_2); n = 4 (cycloheptanone)

These C5-curcuminoids were synthesized by Claisen-Schmidt condensation. Structural elucidation was performed using mass spectrometry, UV-Vis and IR spectroscopy and mass spectrometry. Comparative analysis of the structural and spectroscopic properties of these curcuminoids revealed subtle differences between the acyclic and cyclic forms, stressing the impact of structural modification on their chemical and other behavior. These findings contribute to the understanding of C5-curcuminoid chemistry and may aid the development of novel bioactive compounds with potential applications in medicine and other fields.

Keywords: Curcumin, Acyclic and Cyclic C5-Curcuminoids, Claisen-Schmidt condensation, Structure, spectroscopic properties

OBPC P-48

Spectrophotometric Assessment of Reactivity of Symmetrical Monocarbonyl Analogs of Curcumin Containing a 2-Fluorobenzylidene Moiety with *N*-Acetylcysteine

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The rapid excretion and poor pharmacokinetics of curcumin limit its clinical use, prompting the development of novel monocarbonyl analogs of curcumin (MACs) with improved properties. These MACs contain an electrophilic α,β-unsaturated carbonyl moiety as a Michael acceptor, influencing key biological processes through thiol alkylation involving glutathione, cysteine, and cysteine-containing peptide residues. It is known that MAC, EF24, [(3*E*,5*E*)-3,5-bis(2-fluorobenzylidene)-4-piperidone] reacts with glutathione to give bis adduct and also with other biologically relevant thiols. One biologicialy useful thiol is *N*-acetylcysteine (NAC), which by itself is a potent antioxidant and has therapeutic uses. In this study the reactivity of symmetrical MACs containing a 2-fluorobenzylidene moiety with NAC was investigated using UV-Vis spectroscopy in 80:20 acetonitrile/water solution at 25 °C. The reaction progress was monitored for 6 to 12 hours with excess of NAC added. All the MACs used showed a λ_{max} above 280 nm and NAC offered suitable spectral window.

The relative reactivity compared to EF24 of these MACs towards NAC was assessed and preliminary kinetic data was obtained. The developed method is simple, can be extended to assess the reactivity of other MACs and can be utilized to probe the reversibility of the Michael addition.

Keywords: Curcumin, monocarbonyl analogs of curcumin, Michael acceptor, reaction kinetics, *N*-acetyl cysteine, fluorinated MACs, UV-Vis spectroscopy.

OBPC P-49

Application of Sucrose octaacetate and *Rosa damascena* Hydrosol in a Cosmetic Hand Gel

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Sucrose esters, known also as sucroesters found enormous application as odorless, nontoxic, and biodegradable nonionic surfactants, solubilizators and detergents in pharmacy and cosmetic with anti-fungal and anti-bacterial properties. The aim of this research was to obtain sucrose octaacetates by microwave irradiation and to apply them in a cosmetic gel. Sucrose ocatacetates was synthesized by microwave-assisted esterification of sucrose with acetic anhydride for 10 min. The physicochemical characterization demonstrated that this ester showed promising foaming stability properties. The antimicrobial potential of this compound was tested against seven microorganisms (Gram-positive and Gram-negative bacteria, yeasts and fungi). It inhibited the growth only of *Bacillus subtilis* 6633, and *Escherichia coli* ATCC 8739, while against *Listeria monocytogenes*, *Staphylococus aureus* 745, *Salmonella typhy* 745, *Candida albicans* 8673 and *Aspergillus niger* was inactive. A transparent cosmetic hand sanitizer gel was prepared with 0.1 % sucrose octaacetate, ethanol, 0.1 % rose hydrosol and hydroxypropyl cellulose. The rheological properties and sensory evaluation of the product were performed. The hand gel is transparent viscous liquid with flower rose odor with pH 7.7. Rheological characterization of the obtained gels demonstrated non-Newtonian behavior. The surveyed women clearly highlight the preference to cleansing hand gel in comparison to men.

Keywords: Sucrose esters, rheological properties, gel

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OBPC P-50

Biological Effects and Chemical Composition of African Frankincense Oil

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Frankincense oil is produced from the Boswellia genus. It finds extensive use in perfumery and aromatherapy and is increasingly applied for medicinal purposes, such as alleviating joint and muscle inflammation and arthritis. The aim of this study is to investigate the chemical composition and antibacterial activity of essential oil obtained from the resin of the African tree *Boswellia dalzielii*.

The oil was obtained through steam distillation and analyzed using gas chromatography-mass spectrometry. A microbiological analysis was conducted on 15 types of gram-positive and gram-negative microorganisms.

The gas chromatogram revealed 28 compounds, with the highest concentrations being α-pinene at 41.29 %, β-pinene at 27.15 %, limonene at 10.26 %, and p-cymene at 10.01 %. The oil showed the greatest inhibitory effect against the following microorganisms and fungi: *Saccharomyces cerevisiae* ATCC 9763 (13 ± 0.71 mm), *Penicillium chrysogenum* (11 ± 0 mm), and *Candida albicans* NBIMCC 74 (10 ± 0 mm).

Studies on the oil's solubility in Krebs solution were also conducted to explore its potential application through suitable nanoformulations (functionalization or encapsulation in nanostructures).

Keywords: Frankincense oil, chemical properties, antimicrobial activity

Acknowledgment

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POLYMERS AND POLYMER MATERIALS

PPM O-1

Enhancement of Triboelectric Nanogenerators with Nylon/Graphene Nanocomposite Films

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Triboelectric nanogenerators (TENGs) harness mechanical energy from various sources, offering the potential for self-powered devices. Challenges in TENG development include material wear, limited efficiency, and scalability issues. Innovative materials, such as durable nanocomposites and advanced polymers, are crucial for overcoming these obstacles and advancing TENG technology for diverse energy harvesting applications.This study investigates the development of TENGs utilizing nanocomposite films composed of nylon and graphene layers, fabricated through innovative spray coating. This research aims to enhance the triboelectric performance, mechanical flexibility, and durability of TENGs, addressing the current challenges in energy harvesting technologies. The nylon-graphene nanocomposite films exhibit excellent mechanical properties, combining the flexibility of nylon with the high conductivity of graphene[1] .The synergistic effect between these materials is expected to enhance the triboelectric performance of the TENGs.

In conclusion, this research contributes to the advancement of TENG technology by presenting a systematic exploration of nylon and graphene layer nanocomposite films fabricated through the spray coating method. Integrating these materials enhances mechanical properties and improves the overall performance of TENGs. The results hold promise for applications in wearable electronics, sensor networks, and self-powered systems, addressing the growing demand for efficient and versatile energy harvesting solutions.

Keywords: nylon, grafen layer, triboelectric nanogenerator, nanocomposite films

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PPM O-2

Semicrystalline Waterborne Coatings via Thiol-ene Polymerization in Dispersed Media

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Oxygen and humidity barrier waterborne coatings for food packaging represent a highly open market in terms of innovations. Driven by the growing awareness of ecological issues, the vinylidene chloride copolymer coating (PVDC), currently used industrially and presenting outstanding barrier properties, tends to be replaced by halogen-free and more sustainable options. To expand the range of products commercially available, we propose an approach that unites thiol-ene step-growth radical process and photopolymerization in dispersed media to obtain high sulfur content polymers that can be used as waterborne coatings. Herein, we report the synthesis of a 30% solid content poly(thioether) latex based on the monomers diallyl terephtalate (DATP) and glycol dimercaptoacetate (GDMA) forming a consistent film for the intended application[1]. Additionally, controlling the ordering of crystalline domains could yield smarter coatings presenting passive barrier to oxygen and water, and could be a good option to replace PVDC. For that aim, we present here self-nucleation processes to accelerate the crystallization kinetics[2] of as-synthesized films to potentially improve barrier properties and add value to films produced from thiol-ene chemistry.

Keywords: Miniemulsion polymerization, waterborne coating, crystallization

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PPM O-3

Electrospun (Dynamic) Composite Membranes for Water Desalination

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The aim of this research is to obtain electrospun smart dynamic composite membranes intended for water desalination with antifouling properties and high productivity. The performance and efficacy of the desalination membranes largely depend on their structure, topology, and surface chemistry. One common drawback of these membranes is their proneness to accumulation of scale referred to as fouling, which results in decreased mass transfer and reduced selectivity[1,2].

Electrospun membranes possess some appropriate advantages, including high hydrophobicity (higher than their bulk), high porosity, adjustable pore size, and membrane thickness, which makes them attractive candidates as membranes for membrane distillation (MD) systems. In order to obtain antifouling membranes with high productivity and rejection ability, the following approach is chosen: obtainment of composite membranes consisted of electrospun hydrophobic polymer matrix with embedded dynamic materials, so-called thermosalient (TS) crystals[1,2]. TS crystals are a newly established class of dynamic crystalline materials that are capable of sudden expansion or motion under thermal stimulation, thereby rapidly transforming thermal energy into mechanical work.

The results from the Direct Contact Membrane Distillation testing showed that the membranes are suitable for MD due to the rejection being high enough, comparable to commercial membranes, which encourages further research in this regard.

Keywords: electrospinning, thermossalient crystals, membrane distillation systems

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PPM O-4

Chrysin Loaded Iron Oxide Nanoparticles Coated with Chitosan and Cross-linked Chitosan: A Structural Study

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Iron oxide nanoparticles (Fe_3O_4 NPs) have gathered significant attention for various biomedical applications, such as hyperthermia, drug delivery, and magnetic resonance imaging (MRI). In these applications, control over particle size, size distribution, shape, and surface modification are crucial for the effective use of Fe_3O_4 NPs.

Unmodified Fe_3O_4 NPs possess high surface energy, leading to instability in physiological environments and a tendency to agglomerate due to strong magnetic dipole-dipole interactions[1]. This agglomeration causes recognition and clearance by the reticuloendothelial system (RES), reducing circulation time. Polymer coatings, such as chitosan, provide a cost-effective and straightforward approach to stabilizing these nanoparticles. Additionally, the temperature and pH-sensitive properties of polymer coatings enable controlled drug release, particularly in targeted drug delivery systems. This study investigates the structural properties of chrysin (5,7-dihydroxyflavone) loaded Fe_3O_4 NPs coated with chitosan and cross-linked chitosan. Fe_3O_4 NPs were synthesized via chemical co-precipitation. Chitosan and cross-linked chitosan coatings were applied to modify the surface morphology and structural characteristics of the nanoparticles, potentially enhancing drug loading efficiency.

Characterization techniques, including X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and Ultraviolet (UV) spectroscopy, were employed to analyze the structural properties and drug loading efficiency of the samples. The study highlights the feasibility of using polymer-coated Fe_3O_4 NPs in targeted drug delivery systems, offering a promising approach to enhance the anticancer efficiency of chrysin.

Keywords: iron oxide nanoparticles, chitosan, cross-linked chitosan, drug loading

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PPM O-5

CO_2 Adsorption of Nitrogen-Containing Porous Organic Materials: A Computationally Assisted Approach

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Developing new materials for the selective capture of carbon dioxide (CO_2) directly from the combustion products of fossil fuels is one way to minimize its negative impact on the environment. Covalent organic polymers have shown wide applicability for CO_2 adsorption. A computationally assisted approach can significantly help us reduce the dimensionality of the search space and guide the synthesis of CO_2 adsorption materials.[1] Along with the common azo bond, we studied two other types of nitrogen-nitrogen linkages, azoxy and azodioxy bonds, for assembling porous organic polymers from trigonal building units, such as trisubstituted triphenylbenzene, triphenylpyridine, triphenyltriazine and triphenylamine. Periodic density functional theory (DFT) calculations enabled us to investigate different topologies and stacking modes. Electrostatic potential (ESP) maps assisted us in identifying the most probable binding sites between the framework and CO_2 molecules. Adsorption isotherms were simulated by grand canonical Monte Carlo simulations (GCMC).[2] Recently, we have extended our investigation to include tetrafunctionalized tetraphenylethylene and porphyrin building units. Prior to synthesis, we employed a combined computational chemistry approach to study their structural and CO_2 adsorption properties.

This work has been fully supported by the Croatian Science Foundation (IP-2020-02-4467).

Keywords: gas adsorption, porous organic polymers, periodic DFT

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PPM P-1

Biopolymer-based hydrogels with microcapsuled vitamin E

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The increasing awareness of consumers about a healthy lifestyle, which implies the use of cosmetic and pharmaceutical products obtained from natural raw materials and with natural additives, requires the improvement of existing and the development of new products from the field of cosmetics and pharmacy. As a biodegradable natural polymer, chitosan attracts a lot of attention and presenting great potential for pharmaceutical and cosmetic applications due to its biocompatibility, high charge density, nontoxicity and mucoadhesion.[1] Nowadays, hyaluronic acid has become one of the most crucial ingredients in cosmetics as well as nutricosmetic products. Almost all products for mature skin that exhibit moisturizing, skin protective, and anti-aging properties contain hyaluronic acid.[2] Due to the favorable properties of both chitosan and hyaluronic acid on skin the goal of this work was the preparation of chitosan and hyaluronic acid based hydrogels with and without microencapsulated vitamin E for possible application in cosmetic products. First, the zeta potential of the mixture of chitosan and hyaluronic acid was measured in order to select the most suitable mass ratio for the preparation of hydrogels, and then the hydrogels were characterized (organoleptic, SEM, rheological properties, pH values, swelling and stability). The results showed that the examined hydrogels can be successfully used as carriers of active substances in the pharmaceutical and cosmetic industry.

Keywords: hydrogels, chitosan, hyaluronic acid, vitamin E

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PPM P-2

Microencapsulation of coenzyme Q10 in HPMC/SDS system

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Microencapsulation of bioactive components has attracted much attention in the last few decades, especially in the food, pharmaceutical and cosmetic industries. The most common goal of microencapsulation is to protect and preserve the bioactive compounds in the core covered with a shell, or dispersed in a matrix. The choice of a shell material affects to a various effect of the active substance delivery system, among which are often prolonged and targeted action. The biopolymer/surfactant systems, such as cellulose derivatives/low molar mass surfactants, were widely investigated for use as the shell or matrix materials in microencapsulation processes[1]. Coenzyme Q10 is one of the strongest liposoluble antioxidants, which has been proven to work in the prevention and treatment of many diseases caused by oxidative stress. As a cosmetic ingredient, coenzyme Q10 mainly acts as an antioxidant to protect skin cells from photo aging and damages caused by free radicals[2]. The objective of this work was to study the possibility to obtain coenzyme Q10 microcapsules using the coacervation method by depositing HPMC or HPMC/SDS complex on the oil/water interface and their separation by spray-drying. Physico-chemical properties of the emulsions and the microcapsules obtained from them (moister content, particle size and encapsulation efficiency) were determined. The results analysis indicates that HPMC/SDS complex is suitable for application as the wall material for microencapsulation of coenzyme Q10.

Keywords: microencapsulation, coenzyme Q10, HPMC/SDS complex

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PPM P-3

Characterization Of Poly(Vinylbutyrolactam) Based Hydrogels: Morphology, Thermal Properties And Swelling Behavior

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The poly(vinylbutyrolactam-*co*-acetoxyethene), p(VB/AE), copolymers have been utilized to produce transparent, flexible, oxygen-permeable films which adhere to plastics, glass and metals. They are used in various personal care products (e.g. for hair, skin, nails). They are characterized by their chemical stability, biocompatibility, and non-toxicity. This study aimed to characterize chemically copolymerized hydrogels based on vinylbutyrolactam monomer with 5mol% of acetoxyethene comonomer and varying crosslinker content using the free radical polymerization method. Micrographs obtained by scanning electron microscopy (SEM) revealed crosslinked, amorphous-crystalline and macroporous structures of p(VB/AE) copolymers, with an average pore diameter in the swollen state ranging from about 50 μm to 100 μm. Thermal phase transitions of the p(VB/AE) copolymers were detected using the DSC method, confirming their structure, good miscibility of comonomers and thermal stability. The obtained copolymers p(VB/AE) samples demonstrated glass transitions in the range of 130.61°C-140.39°C and maxima of wide melting regions in the range of 155.46°C-172.61°C. Thermosensitive crosslinked p(VB/AE) hydrogels are also pH sensitive, swelling intensively in alkaline solvents and very low in acidic solvents at 20°C. According obtained results, copolymers poly(vinylbutyrolactam-co-acetoxyethene) could be convenient for potential application as a carrier for various active substances.

Keywords: DSC, vinylbutyrolactam, acetoxyethene, swelling, morphology

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PPM P-4

Biodgeradable Triblock Copolymers Based on Poly(E-Caprolactone) and Different Poly(Alkylene Carboxylate)S

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Biodegradable polyesters are established as one of the most promising class of synthetic polymers to be used for environmental protection and in biomedicine. In order to broaden the application window for biodegradable polyesters different approaches are used to obtain new materials with desired properties. The most versatile approach is copolymerization to yield random, block, star, etc. copolymers with new properties. The aim of present research was the synthesis of triblock copolyesters based on blocks from different biodegradable polyesters, in order to establish correlation between their macromolecular structure and properties. As a central block two different condensation polyesters of a fixed molecular weight were used, poly(butylene succinate), PBS in the first series and poly(butylene adipate), PBA in the second, while lateral blocks were of poly(ε-caprolactone), PCL with varying length in the series. The structure of obtained polyesters was confirmed by ^{1}H and ^{13}C NMR, while GPC analysis confirmed unimodal molecular weight distribution. Thermal properties and degrees of crystallinity were determined by DSC and WAXS. Mechanical properties and transition temperatures were evaluated by dynamic-mechanical analysis and correlated with macromolecular structure. In the hydrolytic degradation tests during 4 weeks weight losses were lower in PBS series and higher in PBA series compared to homopolymer PCL, indicating possibility of tailoring biodegradation kinetics by copolyesters' composition. The changes in molecular weights during the course of degradation revealed surface erosion mechanism for the both series.

Keywords: biodegradable, aliphatic polyesters, block copolymers, biodegradability

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PPM P-5

Composites Based on Biodegradable Aliphatic Polyesters and Copper Enriched Zeolites with Antibacterial Activity

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Aliphatic biodegradable polyesters poly(ε-caprolactone), PCL and poly(lactic acid), PLA with their favorable mechanical and thermal properties could be environmentally friendly replacement for bio-resistant thermoplastics currently used for disposable packaging. It would be of interest for packaging purposes to introduce some "active" properties, such as antibacterial activity, into these materials. This can be achieved by the addition of different fillers, with further benefit of increasing mechanical properties of matrix. Special interest is in the use of fillers of natural origin, such as clays, sepiolites or zeolites. In this study composites of PLA and PCL with copper-enriched natural zeolite (CuZ) were prepared, with the aim to obtain materials with antibacterial activity. Thermal and mechanical properties of composites were characterized by DSC, TG and DMA. Reinforcing effect of CuZ was achieved, while thermal properties were not decreased. Antibacterial activity of all composites was investigated toward two bacterial strains, *Echerichia coli* DSM 498 and *Staphylococcus aureus* ATCC 25923. Composites showed good antibacterial activity toward *S. aureus*. From the analysis of the amount of released copper it was concluded that antibacterial activity was achieved not only through the action of the released metal ion, but also by direct contact with composite. Biodegradability of composites was followed in accelerated hydrolysis tests in alkaline medium, through evaluation of weight loss and decrease in thickness of exposed composite films. It was shown that CuZ presence and its amount in composite had an accelerating effect on degradation.

Keywords: biodegradable, polyesters, natural zeolite, composite, antibacterial

Acknowledgement: This work was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Contract No.451-03-65/2024-3/200135)

PPM P-6

Optimizing Starch/Alginate Aerogels: Impact of Formulation and Processing on Material Properties

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Starch aerogels are important due to their biodegradable nature, lightweight structure, and excellent thermal insulation properties, making them highly valuable for various applications. Combining starch with sodium alginate provides the opportunity for these aerogels to improve their mechanical strength, biocompatibility, and gel-forming capabilities, resulting in superior performance and broader application potential in fields such as biomedical engineering and environmental remediation.[1] Focus of this research was on the synthesis and characterization of starch/alginate aerogels, exploring various formulations and processing conditions to understand their impact on the aerogel properties. With that in mind, mechanical properties, swelling behavior, and porous structure of prepared aerogels were examined.

The study demonstrated that the properties of starch/alginate aerogels can be finely tuned by adjusting the alginate content, employing cross-linkers like calcium chloride, and optimizing the solvent exchange process.

Keywords: aerogels; starch; sodium alginate; characterization

Acknowledgment: This work was supported by the Ministry of Science, Technological Development, and Innovation of the Republic of Serbia (Contract No. 451-03-65/2024-03/200135 and 451-03-66/2024-03/200287).

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PPM P-7

Green Polysaccharide Hydrogels for Wastewater Remediation

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In light of environmental protection and water remediation as important topics nowadays, research in the field of polysaccharide hydrogels as wastewater pollutant sorbents attracts the attention of scientists. Polysaccharides, such as sodium carboxymethylcellulose (CMC) and sodium alginate (SA) are sustainable, biocompatible, biodegradable, non-toxic, and low-cost materials. Despite excellent assets, these polysaccharides have some drawbacks, such as the brittleness of SA hydrogels and the inability of neat CMC to maintain a stable structure in an aqueous environment. An effective method to overcome these drawbacks and improve the performance and physical properties of CMC/SA hydrogels is the mixing of polysaccharides and dual crosslinking[1].

The topic of this work is the synthesis of green and sustainable CMC/SA hydrogels and their sorption of pollutants from wastewater. Tannic acid together with $ZnCl_2$ is used in a two-step crosslinking process for green CMC/SA hydrogel production. The influence of the CMC/SA ratio and additional crosslinking on hydrogel properties was investigated. Moreover, the CMC/SA hydrogel sorption of various dyes in multiple-dye systems was studied. The eco-friendly green CMC/SA hydrogels obtained by two-step synthesis have excellent sorption properties of the toxic anionic dyes regardless of the presence of other pollutants in the wastewater.

Keywords: hydrogel, wastewater remediation, CMC, SA, sorption

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PPM P-8

Synthesis of Organic and Inorganic Geopolymers from Different Precursors

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Geopolymers, as a new group of binding materials of aluminosilicate origin, are created by the reaction of precursors of aluminosilicate materials with solutions of alkaline activators. Precursors can be of different types and origins. Recently, there has been a growing interest in mixing two different systems, organic and inorganic. In this work, the change in the structure of two different systems was monitored. Samples based on metakaolin with the addition of organic phase PVA and samples based on fly ash with the addition of eggshell were synthesized. The first step of the synthesis is the production of the solid phase. The second step is alkaline activation of the solid phase using an alkaline activator (mixture of NaOH and Na_2SiO_3). The concentration of used NaOH was 12 mol dm^{-3}. The structural and phase characterization of the samples was analyzed using X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR). New phases were detected in samples with added PVA. XRD determined an amorphous halo with the presence of quartz as the crystalline phase in the samples with the addition of eggshell. These results were confirmed by DRIFT analysis. The morphology of all samples was analyzed using a scanning electron microscope with energy dispersive spectroscopy (SEM/EDS). Efflorescence was observed and identified in samples with added PVA.

Keywords: geopolymer, hybrid, PVA, metakaolin, eggshell

PPM P-9

Antimicrobial activity of AB-Polybenzimidazole /plant-synthesized TiO_2 hybrid membranes

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The AB-Polybenzimidazole/TiO_2 nanocomposite membranes with 100 μm thickness were synthesized by film casting approach with subsequent anti-solvent inversion in order to obtain porous composites. Modified Eaton's reagent (methansulfonic acid/P_2O_5) was used as both reaction media for microwave assisted synthesis of AB-PBI and as efficient dispersant of partially agglomerated titania powders. The maximum content of achieved TiO_2 filler was 20 wt.%. The TiO_2 particles were obtained by green synthesis using Mentha Spicata aqueous extract.

The antibacterial effect of thus obtained composites was evaluated by the ASTM Standard Test Method E 2149–10 of dynamic contact, adapted for a 24-well sterile plate. For the photocatalytic antibacterial test, UV-irradiation of titania powders was applied for 30 minutes with constant stirring of the suspension. The combination of membrane and titanium dioxide nanoparticles demonstrated weak antibacterial activity, which appeared after prolonged contact of the bacterial suspension - over 48 hours. This effect is amplified after exposure to UV rays and the time to achieve it is shortened to a few hours.

Keywords: Antimicrobial activity, AB-Polybenzimidazole, membranes

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PPM P-10

First Steps Towards Synthesis of Molecularly Imprinted Polymers via Ionic Bonding for Future Sensing Application

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Molecularly imprinted polymers (MIPs) are polymer systems, engineered in a way best described as a "lock and key" structures[1], which gives them the ability to specifically bind to a certain template or pattern molecule. This unique capability, combined with their high selectivity, makes them a perfect candidate for applications that demand high-precision sensing. In this study, the advantages of the ionic bonds are employed to facilitate easy manipulation of the pattern molecule, by controlling the pH of the system. The ionic bonds are established by incorporating zwitterionic monomers (ZMs). One of the many potential uses of the MIPs is focused on the development pesticide-sensing devices, enabling customers to ensure the quality of the food products they use on a daily basis.

This work focuses on development of a methodology for fabrication of MIP, based on crosslinked butyl methacrylate/methyl methacrylate (BMA/MMA) polymer particles copolimerized with 3wt% zwitterionic monomer 3-[(3-Acrylamidopropyl)dimethyl ammonio] propane-1-sulfonate (DAPS) ZM. The procedure is multistep, covering:(i) polymer particles aqueous dispersions synthesis by emulsion polymerization;(ii) addition of template molecules, in this case 2,4-dimethylbenzoic acid (DMBA) under controlled pH to ensure deprotonated carboxylic acid group from DMBA and formation of ionic bonding with polymer particles;(iii) film formation in which the ionic bonded template molecules are homogeneously dispersed within the film; and (iv) removing of template molecules. This work presents early results related to the synthesis of the polymer particles and their surface modification by template molecules towards development of novel MIPs able to selectively adsorb pesticide molecules even at low concentration of the same.

Keywords: Molecularly imprinted polymers, template molecules, sensing application, pesticides

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PPM P-11

Evaluation of Some Properties Of Recycled Poly(Ethylene)/Lignin Composites

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Macedonia faces a significant issue with plastic waste, which is typically handled by disposing of it in landfills, and only a small portion is recycled. Recycled plastic has inferior qualities to newly synthesized plastic, thus stabilizers and fillers must be added to improve the recyclate's qualities and raise its value. In this research poly(ethylene) (PE)/lignin composites were prepared. Lignin is a natural polymer with good mechanical, thermal and antioxidative properties that makes it suitable for use as filler in synthetic polymer matrices.

The preparation process for the composites involved dissolving PE in a suitable solvent and adding different concentrations of lignin 1wt% and 3wt% with respect to the polymer. The incorporation of lignin resulted in a significant increase in visible light absorption as shown in the UV-Vis spectra. According to the results from contact angle and surface energy measurements, the addition of lignin leads to increased hydrophilicity and reduction of the surface energy values. A degradation study was performed by irradiating the samples with UV light of 254 nm at ambient conditions for 48 hours. The findings showed that lignin-containing samples did not alter their absorption properties when exposed. Absorption coefficients were calculated before and after exposure to UV light to eliminate the impact of sample thickness. The composite that contained 3wt% lignin demonstrated the greatest stability. To test the samples' water uptake ability, they were immersed in water for 48 hours and their weight was measured before and after a specified period. The percentage of weight change was calculated. Water uptake was observed to be higher in samples with higher concentrations of lignin.

Keywords: lignin, UV stability, PE, water uptake

PPM P-12

Effect of Lignin on Different Properties of Lignin/Polymer Composites

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Lignin is one of the most abundant natural polymers that is usually disregarded as a waste. Owning to its complex chemical structure, lignin has various properties as antioxidative, thermal stability, good mechanical properties, fire retardancy etc. Used as a filler in synthetic polymer matrix, lignin would contribute to the improvement of certain properties of the resulting composites.

In this research, lignin/polymer composites were synthesized by in-situ miniemulsion polymerization. Lignin was added to the polymer emulsion through continuous feeding for 40 minutes, with concentrations of 0.5 wt% and 1 wt% relative to the monomers. The monomer system was containing methyl methacrylate, butyl acrylate and acrylamide in weight ratio of 49.5:49.5:1.

The obtained composites were evaluated using different analysis methods. The scanning electron microscopy results showed that the incorporation of lignin leads to significant changes in the morphology of the composite. An improvement in yield strength, tensile strength, and strain at break for the composite containing 1 wt% lignin was confirmed through mechanical testing. Thermal gravimetric analysis revealed that the maximum decomposition temperature of the composites was shifted to higher values and residue after degradation increased. These results suggest that the incorporation of small amounts of lignin can improve the mechanical properties and thermal stability of the composites.

Keywords: lignin, polymer composites, in-situ miniemulsion polymerisation

PPM P-13

Morphological Peculiarities of Isotactic Polypropylene Nucleated with Alkaline Earth Metal Pimelates

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The α- and β-phases are technologically interesting crystalline forms of isotactic polypropylene (iPP). For homopolymers, the α-phase is most thermodynamically stable with a monoclinic crystal structure. In contrast, the β-phase is usually obtained by specific nucleation.[1] In this work morphological characteristics of iPP, crystalized with Ca-, Ba-, Sr- and Mg-pimelates, as nucleators, were studied by scanning probe microscopy (SPM). SPM showed that all samples are covered with micro-sized particles. The highest particle coverage was achieved using Ca-, while the lowest when using Mg-pimelate, as a nucleator, showing that Ca-pimelate exhibits the highest nucleation capacity. The particles and the background surface were probed with Raman spectroscopy, revealing identical spectra for all samples, hence suggesting that the nuclei are buried in the particles. Finaly, the XRD analysis showed that the dominance of β-phase correlates with the particles coverage which is observable when using Ca-, Ba- and Sr-pimelates as nucleators, while the α-phase dominates in the case of Mg-pimelate.[1]

Keywords: polypropylene, pimelates, morphology-structure correlations

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PHYSICAL, STRUCTURAL CHEMISTRY, SPECTROSCOPY AND ELECTROCHEMISTRY

PSSE O-1

Physical Properties of $Cd_xZn_{1-x}S$-Based Nanocomposite Materials Produced Via Sonochemical and SILAR Methods

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The study presents nanocomposite materials obtained in different compositions (different values of x) $Cd_xZn_{1-x}S$, synthesized as thin films and nanoparticles by two methods—sonochemical and SILAR methods. X-ray Diffraction (XRD), Ultraviolet-Visible (UV-Vis), and Scanning Electron Microscopy (SEM) were used to investigate structural, and optical properties and morphology. In the sonochemical method, samples were prepared with three different stabilizers for comparative analysis. Meanwhile, the SILAR method produced thin layers at different synthesis temperatures.

Under normal conditions, $Cd_xZn_{1-x}S$ were formed in the hexagonal phase by both synthesis methods. This indicates that less energy is spent to form the hexagonal phase. Annealing of PVA at a high temperature (65°C) resulted in the formation of the hexagonal phase of the CdZnS solid solution, as well as the formation of the hexagonal phase CdS compound as well as the cubic phase ZnS compound. This shows that a mixed phase was formed. A solid solution of CdZnS was formed, and due to the influence of temperature, Cd^{2+}, $Zn^{2+,}$ and S^{2-} ions, which are present in the sorption centers of PVA and are free, are formed separately into binary CdS and ZnS had enough energy. For the formation of the cubic phase, special reaction conditions - sufficiently high energy is required.

During the formation of particles, crystal structure, interphase interactions, and particle sizes are parameters that affect physical properties. Depending on the type of stabilizer used, the formation of an additional layer (double electrical layer) can lead to a change in properties. In general, band gap value and other physical properties of particles depend not only on their size, but also on the environment surrounding it, the characteristics of the environment, the dipole moment, and the interaction mechanism of the charge carriers in the particle with the environment. So, these changes in the Eg value of the particles can vary depending on the thickness of the double electrical layer formed at the boundary of the two environments, depending on the nanocomposite material. At the same time, as a result of the interaction of the particle with the environment, defective structures can be formed and thus affect the potential energy of charge carriers. This can affect its Eg value and other physical properties.

Keywords: $Cd_xZn_{1-x}S$, nanocomposite materials, SİLAR, sonochemical, physical properties

PSSE O-2

Influence of Gamma Irradiation and Thermal Annealing to the Graphene Oxide-Based Composite Materials

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Graphene oxide (GO) is a derivative of graphene that has garnered significant attention. This research involves producing GO using the Hummers method, generating a composite using GO and PVA, and analyzing these composites' structural and optical. The impact of thermal annealing and gamma irradiation on the structure and optical characteristics of GO/PVA materials at various concentrations were also investigated. The band gap value changed due to an increase in the concentration of GO in the composites in the PVA and the impact of thermal annealing. The band gap values were all found to be well controlled by varying thermal annealing temperature, influence of gamma irradiation and the concentration of GO in this case. To study the effect of temperature on the physical properties of GO/PVA nanocomposite materials with different percentages, all samples were thermal annealed at temperatures of 40°C, 70°C, and 110°C. It was determined that at temperatures of 40°C and 70°C, GO formed oriented orientations between PVA layers. Optical absorption increases with increasing GO concentration in nanocomposites. The band gap value diminishes when the thermal annealing temperature increases. The cause for this is that the polymer's mobility increases as the temperature of thermal annealing rises, making aggregation processes easier. As a result, the size of the particles increases, and the band gap value decreases. At the same time, it is important to study the effect of radiation on GO-based nanocomposite materials. Consequently, the diffraction peaks exhibited new features due to changes in bond configurations and the creation of a distinct polymer structure surrounding the GO sheets. It was observed that the band gap value decreased with an increase in the concentration of GO. Therefore, by adjusting the concentration of GO within the composite, control over the band gap value of the sample could be achieved.

Keywords: graphene oxides, gamma irradiation, thermal annealing, band gap value, structure

PSSE O-3

Deviations from the Beer-Lambert Approximation Investigated by 2D-Correlation IR Spectroscopy

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Two-dimensional correlation spectroscopy (2D-COS) is a highly sensitive method for uncovering nonlinear dependencies using asynchronous spectra[1]. In this study, we employ 2D-COS to investigate such nonlinearities in relation to the Beer-Lambert approximation. Contrary to the prevailing literature in molecular IR spectroscopy, which suggests a linear relationship between absorbance, molar concentration, and sample thickness, closer examination reveals that this relationship does not hold, even under ideal conditions, as demonstrated by electromagnetic theory. These nonlinearities introduce various patterns into asynchronous 2D-COS IR spectra. We explore examples such as the thickness dependence of absorbance for PMMA layers on CaF_2, Si, and gold, and the concentration dependence of absorbance in ideal liquid mixtures. Our findings show systematic changes not only in absorbance values but also in band shapes and peak positions. 2D-COS proves to be an excellent tool for uncovering and investigating these patterns.

Keywords: Infrared spectroscopy, wave optics, Beer-Lambert approximation

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PSSE O-4

The Influence of Aprotic Organic Solvents on the Kinetics and Mechanism of Electroreduction of Bi(III) Ions

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Electrochemical analysis is a key tool in chemical research, based on phenomena related to the flow of current through electrolyte solutions and electrode reactions[1]. Electrochemical methods such as voltammetry, potentiometry and conductometry are still irreplaceable techniques in the analysis of a variety of substances. The process of electroreduction of Bi(III) ions was accelerated by some organic substances, according to the cap-pair rule, in aqueous solutions of basic electrolytes[2]. However, data on the occurrence and nature of this phenomenon in non-aqueous solutions and mixed aqueous-organic solutions are lacking in the literature. Studies carried out using an HMDE electrode showed that the kinetic parameters of the electrode reactions strongly depend on the volume and adsorption of the organic solvent on the electrode surface[3]. It therefore seemed reasonable to translate these statements to the R-AgLAFE electrode. The aim of this study was to use aprotic organic solvents such as ethanol and methanol and to investigate their effects on the kinetics and mechanism of electrode processes. The theory was advanced that the use of these solvents could increase the solubility of the added organics, which in turn could lead to a greater catalytic effect. This work provides insights into the complexity of Bi(III) electroreduction process mechanisms and kinetics and points to the potential application of new tools in electrochemical analysis.

Keywords: electrochemistry, “cap-pair” effect, electroreduction, R-AgLAFE

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PSSE O-5

Combinatorial Screening of Structural Properties and Oxide Growth on a Co-Evaporated Al-Yb Thin-Film Library

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Studies of several Al - Rare Earth Element (Al-REE) compositions received a lot of scientific interest in recent years. A variety of electrochemical investigations of Al-REE thin film libraries were conducted on several elements in the past years. However, no studies with Yb as alloying element in such systems were carried out yet.

A thin film library of Al-Yb with a compositional gradient was produced, using a self-developed co evaporation system[1]. For the mapping of the Al-Yb library scanning energy-dispersive X-ray (SEDX) spectroscopy was used. Morphology studies with scanning electron microscopy (SEM) and X-ray diffraction (XRD) showed an amorphization of the compositions over the whole range. Scanning droplet cell microscopy (SDCM) using a 3D-printed cell with a tip diameter of 4 mm was employed for investigation of the electrochemical behaviour of the oxide film[1]. It was shown that the oxide formation factor exhibited a local minimum in the range of 7.2 to 7.5 at.% with 1.28 nm V^{-1}. The relative permittivity gave a similar behaviour, and showed a sudden increase to 40 in alloys containing 11 at% Yb and more. X-ray photoelectron spectroscopy (XPS) measurements of the oxide surface revealed a driving force of the formation of Yb_2O_3 over Al_2O_3 and gave a higher Yb content as expected from the EDX measurements. Analysis of the electrolyte using inductively coupled plasma optical emission spectroscopy (ICP-OES) indicated a 4 to 5 times higher dissolution of Yb than Al in the anodization process, indicating an increased protection of Al_2O_3.

Keywords: Aluminium; Ytterbium; thin-film; oxide formation

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PSSE P-1

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

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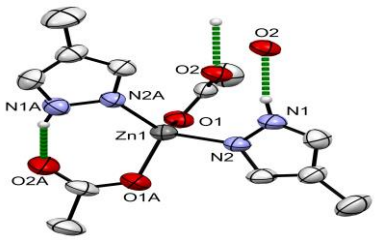

Ligands with multiple coordination sites are often used in the synthesis of the extended metallo-organic structures. Both pyrazolyl and acetato ligands can have a role of a "bridge" between the metallo-organic fragments[1]. As a part of the study of the coordination capabilities of pyrazole-based ligands we are reporting the molecular and crystal structure of the bis(acetato)-bis(4-methyl-1H-pyrazole)-zinc(II). The structure was solved using X-ray single crystal technique. 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 dimer.

Keywords: pyrazole complexes; fomepizole; Zn complex; structure

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PSSE P-2

Methanol Oxidation at Pt/Ni Electrode Prepared by a Galvanic Displacement Process

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One of the most promising alternative energy sources is direct methanol fuel cells (DMFCs) due to their non-toxic nature, reduced emissions of harmful pollutants and high energy density. Platinum (Pt) represents the best choice for both cathode and anode catalysts in DMFCs, but due to its costs, limited supplies and susceptibility to poisoning, full commercialization has not yet been achieved. Recent studies aim to reduce the amount of Pt and its susceptibility to poisoning species without affecting the activity and stability of the catalysts. These studies focus on methods for depositing noble metals through spontaneous deposition, also known as galvanic displacement.

In this research, Pt deposits were formed on a pure nickel (Ni) electrode substrate using a two-step process. Firstly, the Ni crystal was cleaned by annealing in a reductive atmosphere using induction heating, followed by spontaneous galvanic displacement with Pt from a drop of hexachloroplatinic acid ($PtCl_6^{2-}$) placed onto the Ni crystal in the second step. Surface characterization was performed using cyclic voltammetry, the CO stripping method, as well as atomic force microscopy (AFM). The influence of the thermal treatment of the initial catalyst on its structure and activity in the methanol oxidation reaction (MOR) was examined. Compared to the as-prepared catalyst, the annealed catalyst showed ~ 2.5-fold improvement in the methanol oxidation reaction.

Keywords: galvanic displacement, nickel, thermal treatment, methanol, electrooxidation

Acknowledgement: This work was financially supported by the Ministry of Science, Technological Development and Innovation of Republic of Serbia (contract no. 451-03-66/2024-03/200026) and the Science Fund of the Republic of Serbia under grant no. 7739802.

PSSE P-3

Ultra-thin-film Catalysts for Electrooxidation of Formic Acid

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Successful development of catalysts for formic acid electrooxidation (FAO) requires finding an optimal balance between catalytic performance (activity/stability/selectivity) and the material cost. Despite the disadvantages such as the price and the limited quantities platinum represents the best choice for the FAO catalyst. Another downside of using platinum is that it suffers from performance loss at low overpotentials due to poisoning with CO, which is one of the intermediates formed in the so-called indirect path of FAO.

In this work, we explored the synergistic effects of the supporting material and annealing temperature on the performance of ultra-thin film Pt@Ni catalyst, obtained through spontaneous galvanic exchange from a drop of hexachloroplatinic acid placed onto the Ni crystal. In an attempt to reduce the proneness of Pt to poisoning species i.e. CO and improve the catalytic performance of Pt@Ni at low potentials in the formic oxidation reaction, the as-prepared catalyst was modified using controlled thermal treatment. The catalyst was electrochemically characterized with cyclic voltammetry and oxidation of CO monolayer, while the influence of thermal treatment on the surface morphology was monitored using atomic force microscopy (AFM).

Thus by thoughtful choice of the supporting material and the annealing conditions, we were able to create an ultra-thin film catalyst with improved activity and stability, with a minimal amount of platinum used.

Keywords: galvanic displacement, nickel, thermal treatment, formic acid

Acknowledgement: This work was financially supported by the Ministry of Science, Technological Development and Innovation of Republic of Serbia (contract no. 451-03-66/2024-03/200026) and the Science Fund of the Republic of Serbia under grant no. 7739802.

PSSE P-4

Application of Electrode Mechanisms of Surface Active Systems in Drug Analysis

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Voltammetric analysis, a specialized electrochemical method, is tailored for probing the intricate electrode mechanisms of surface-active systems. This technique not only facilitates the development of precise analytical methods but also enables the extraction of essential parameters necessary for the quantitative determination of numerous drugs.[1,2] If there are interactions between two defined drugs, by using theoretical methods, kinetic and thermodynamic parameters can be determined that correlate with the kinetics of interactions.[1,3] The results of theoretical and experimental analyzes are useful in designing new electrochemical methods in drug analysis.[1,2,3]

Experimental Results: The kinetic parameters of the interactions between some studied systems are given in table 1.

	Type of electrode mechanism	Calculated values of chemical reaction rate constants k_f and k_b (or k_c for EC' mechanism)	Calculated values of chemical equilibrium constants - K_{eq}
Ascorbic acid	EC mechanism	k_b = 0.0505 $mol^{-1}Ls^{-1}$; k_f = 0.0075 $mol^{-1}Ls^{-1}$	K_{eq} = 0.15
H_2O_2	EC'mechanism	k_c = 55 $mol^{-1}Ls^{-1}$	
$KMnO_4$	EC'mechanism	k_c = 140 $mol^{-1}Ls^{-1}$	
Ketoprofen	No interactions		

Keywords: voltammetry, kinetics, thermodynamics, drug-drug interactions.

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PSSE P-5

The Structural Insights into the Myelin Model Membranes

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The lipid composition changes of the multilamellar myelin membrane responsible for the successful conduction of nerve impulses were detected in patients with autoimmune diseases such as multiple sclerosis (MS).[1] The larger amount of phosphoethanolamine (PE) lipids and cholesterol (Chol) influence adhesive action of myelin basic protein (MBP), an intrinsically disordered protein, whose performance is found to be altered in MS patients.[2] The background of the structural and morphological changes in the lipid bilayers of myelin in a pathological state needs to be investigated in a more detailed physicochemical sense. Therefore, the multilamellar liposomes with different ratios of lipid components (physiological/pathological conditions) in the presence/absence of MBP were used as myelin models. The multi-component myelin model membranes were measured with calorimetric (DSC), spectroscopic (FTIR, UV-Vis, CD) and structural (SAXS) techniques to characterize the properties of MBP and lipids in a changed composition, as well as at different temperatures where lipid phases are changed. All measurement data will be analyzed with the appropriate chemometric tools.[3]

Keywords: myelin, lipids, FTIR, SAXS

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PSSE P-6

Structural Properties of Synthesized Domestic Carbon from Almond Shells for Carbon Paste Electrode

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To obtain eco-friendly electrochemical sensors this study investigated the performance of bioresource material synthesized from almond shells for carbon paste electrode preparation (CPE). Collected almond shells were carbonized in an inert atmosphere at 800 °C in two batches, where the second batch was enriched with a Sm-Bi_2O_3 composite to improve the electrocatalytic properties of the material. The crystal phase structure and presence of functional groups were determined using X-ray diffraction (XRD) and Diffuse Reflectance Infrared Fourier Spectroscopy (FTIR-DRIFT), while electrochemical properties were examined by cyclic voltammetry. The obtained XRD diffractograms confirmed the amorphous phase of both samples with few low-intensity peaks of Sm-Bi_2O_3, at the same time DRIFT analysis indicated the presence of various functional groups: O-H (hydroxyl group), C-O (phenol group), C=O (carboxylic group) and C=C (alkene group) characteristic for this type of material. Cyclic voltammetry was recorded in a three-electrode system, where a carbon paste electrode made from the synthesized materials was used as the working electrode. For this proposal, it was prepared four different pastes: bare almonds carbon (carb_ad), hand mixture carb_ad with Sm-Bi_2O_3, sonicated carb_ad with Sm-Bi_2O_3, and carb_ad/Sm-Bi_2O_3 from the second batch. Cyclic voltammograms indicated that the paste from the second batch provided clear reversible peaks and the anodic and cathodic current peaks had the highest values. As a result, it was determined that future studies will concentrate on creating an electrochemical sensor using this substance. In addition, the prepared homemade carbon samples possess great potential for application as environmentally friendly carbon materials for CPE electrodes.

Keywords: Almond shell, Domestic carbon, Electrochemical sensors, XRD analysis, FTIR-DRIFT Spectroscopy

PSSE P-7

Ultrasound-Mediated Control of the Optical Properties of Silver-Based Nanoplasmonic Surfaces

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Plasmonic surfaces of close-packed Ag@Ag_2O core-shell nanoparticles (NPs) on glass substrates with tunable optical properties are prepared using an ultrasound-assisted bottom-up approach. Ultrasonic irradiation modifies the reaction mechanism, allowing precise control of the nanoparticles' composition, size and morphology and their packing on the substrate surface. The acoustic cavitation as well as primary and secondary sonochemical effects, provide formation of highly-reactive species, such as hydroperoxyl radical, $HO_2^{\cdot}$, which is the most relevant species for creation of Ag_2O shell on the silver core surface. The core-shell nanoparticles have spherical shape with narrow size dispersion in contrast to two populations of silver nanoparticles, obtained under sonoless conditions. The higher degree of structural ordering of nanostructured phase obtained by the ultrasound-assisted route, as well as the flatter surface (confirmed by AFM) are a consequence of the type of relevant interactions between nanostructure entities (i.e. hydrogen bonding).

The sonication provides modification of the plasmonic properties of prepared surfaces. The observed trends in the localized surface plasmon resonance (LSPR) absorptions in the case of bare Ag plasmonic surfaces are dominated by the particle size, inhomogeneous broadening induced by the nanoparticles' size dispersion, interparticle plasmon coupling as well as nanocrystal-substrate interaction. The notable red shift of the LSPR absorption maximum between two boundaries of the visible part of the spectrum for 1.3 eV in contrast to the shift of 0.2 eV under sonoless conditions is governed by the influence of the dielectric shell. In addition, the sonication provides control of silver core nanoarchitecture and formation of single crystal domains which is very important having in mind that metal nanoparticles usually have a tendency for creation of singly or multiply twinned crystal domains. AFM results show that the obtained Ag NPs are dominantly composed by singly twinned domains.

Keywords: metal NPs, core-shell NPs, plasmonics, thin films, sonication, localized surface plasmon resonance, LSPR.

PSSE P-8

Study on the Electrochemical Behaviour of Macrolides on Carbon and Platinum Electrodes

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Macrolide antibiotics Erythromycin (ERT), Clarithromycin (CLA) and Azithromycin (AZT) are widely used for the treatment of various infections. Therefor it is important their identification and quantification by more convenient methods, such as electrochemical ones [1]. In this work the voltammetric behaviour of macrolides in platinum and carbon electrodes was investigated. Other organic compounds were tested trying to clarify electro-active groups of macrolides. Cyclic voltammograms of each molecule in each electrode were recorded and similar electrochemical behaviour of macrolides was observed for all carbon based electrodes, which gave more defined current intensity peaks than platinum [2]. The three compounds gave current peaks during a cyclic voltammetry scan, AZT producing a stronger signal. The electrochemical signal of the three compounds was the strongest at pH 10. The slope of the line log(ip) vs log(v) was 0.77, which indicates that the oxidation of macrolides occurs through an adsorption step prior to the electron transfer.

Keywords: Macrolides, electrochemical, voltammetry, signal, electrodes

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PSSE P-9

Study of the Nucleophilic Reaction Between Dopamine and Glutathione and the Effect on Dopamine Oxidation

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Dopamine, a neurotransmitter crucial for neural signaling, and glutathione, a tripeptide pivotal for antioxidant defense, are among the many molecules that are essential for the homeostasis of the human organism. Due to their enormous importance, extensive research have been conducted on these two biomolecules. Of recent note is the investigation into what's known as the Michael's reaction, where these two molecules, when being nearby, particularly at basic *p*H values, undergo a reaction yielding an addition product [1].

This scientific study reveals the results obtained studying the Michael's addition reaction between dopamine and glutathione as a nucleophile. The reaction was examined by the mean of both electrochemistry in acetate buffer with *p*H = 5.02, so that the autoxidation of dopamine was excluded, alongside experiments conducted at various basic *p*H values. Cyclic and square-wave voltammetry techniques were employed utilizing a glassy carbon electrode as the working electrode to characterize electrochemical behavior. Simultaneously, spectrophotometric analyses were conducted in phosphate buffer in several basic *p*H values, using UV–Vis spectrophotometer scanning the wavelength area from 190 to 900 nm. Moreover, studying the reaction and the effect of glutathione on the oxidation mechanism of dopamine, which in acidic *p*H values is EC, it was discerned that not only glutathione acts as a nucleophile, but also influencing the overall oxidation mechanism of dopamine.

Keywords: dopamine, glutathione, voltammetry, spectroscopy.

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PSSE P-10

Asymmetric Phospholipid Vesicles as Cell Membrane Models

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Biological membranes are complex compositions with hundreds of different lipids and proteins. A common feature of eukaryotic cell membrane is the non-random distribution of lipid species in the inner and outer leaflets of the lipid bilayer, which is called lipid asymmetry.[1] In mammalian plasma membranes aminophospholipids phosphatidylserine (PS) and phosphatidylethanolamine (PE) are predominantly exposed on the cytosolic leaflet, whereas phosphatidylcholine (PC) and sphingomyelin (SM) are predominantly located on the outer leaflet.[2] Commonly used symmetric model membrane vesicles cannot provide control of lipid distribution between inner and outer leaflets. Asymmetric vesicles are better biological mimetics as compared with their symmetric counterparts that have dominated membrane biophysical studies.[3] In this research we were focused on preparation of various systems of asymmetric model membranes, giant unilamellar vesicles (GUVs) and large unilamellar vesicles (LUVs) and their characterization using fluorescent spectroscopy and microscopy.

Keywords: model membranes, asymmetric vesicles, fluorescent spectroscopy, microscopy

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PSSE P-11

Rosemary (Rosmarinus Officinalis) as a Natural Corrosion Inhibitor

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NOT PRESENTED

PSSE P-12

On the Structure and Stability of Pillar[5]Arene-Water Complexes: a DFT Study

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In recent decades, macrocyclic hosts (e.g., crown ethers, cyclodextrins, cucurbiturils, and calixarenes) have attracted considerable attention due to their remarkable conformational and physicochemical properties. Pillar[n]arenes, originally discovered in 2008, became the fifth classical macrocycle. Although the composition of pillararenes is similar to that of calixarenes (phenolic-based repeating units connected by methylene bridges), they have different structural features - the repeating units of the pillar[n]arene are connected by a methylene bridge in para position, which forms a unique symmetric pillar architecture. The distinctive characteristics of pillararenes, which have hollow-column shapes, and the feasibility of chemical modifications based on versatile aromatic hydroxyl groups have inspired supramolecular chemists to synthesize diverse channel-like tubular architectures.

Our computational (at Density Functional Theory level) study is focused on the nature of the interactions in the inclusion complexes formed by unsubstituted pillar[5]arene and simple confined molecule such as water, and on the thermodynamics of the formation processes of the corresponding pillar[5]arene-water complexes.

Keywords: pillar[5]arene, water, host-guest complex, DFT, thermodynamics

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PSSE P-13

Exploring the Electrochemistry of Surface-Active Redox Systems in Voltametric Analysis of Drug-Drug Interactions

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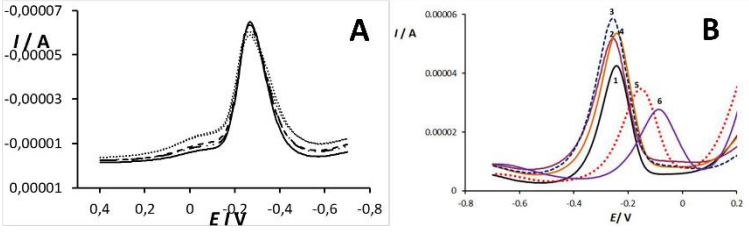
Methylene blue is a model-like surface-active redox system, suitable to study various effects related to chemical interactions involved in voltammetry of surface electrode mechanisms. The redox transformation of methylene blue (MB) described by $2e^-/2H^+$, whereby MB switches between the oxidized form (blue-MB) to a reduced form called leuko-methylene blue (MBH_2).[1] The voltammetric patterns of methylene blue can be analyzed in a way to get access to thermodynamics and kinetics of eventual interactions between MB/MBH_2 and a defined drug. By applying suitable theoretical models developed under square-wave voltammetry, it is possible to evaluate the mechanism, and also kinetic and thermodynamic parameters of interaction between given drug and the electroactive molecules of MB. In experimental protocol, all parameters are kept constant and only concentration of the drug changes.[2]

Experimental Results: (A) Net SW voltammograms of methylene blue recorded in absence and in presence of ibuprofen, (B) Net-SW voltammograms of methylene blue recorded in absence of vitamin and in presence of vitamin C.



Keywords: voltammetry, kinetics, thermodynamics, drug-drug interactions.

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PSSE P-14

Synthesis, Characterization and Electrocatalytic Properties of $GdMn_{0.5}M_{0.5}O_3$ (M = Cr, Fe, Co) Perovskites

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Complex perovskite materials incorporating manganese have attracted significant attention due to their interesting properties and versatile applications. Here, the research related to the synthesis and characterization of new complex perovskites with the general formula $GdMn_{0.5}M_{0.5}O_3$ (M = Cr, Fe, Co), is presented.

The solution combustion method was chosen for the synthesis of these compounds, using glycine as fuel. The obtained perovskites were investigated by X-ray powder diffraction (XRPD), scanning electron microscopy (SEM) with energy dispersive X-ray spectroscopy (EDX), infrared (IR) spectroscopy and cyclic voltammetry. Besides their purity, the XRPD patterns showed that the compounds within the series are isostructural to each other. The recorded SEM images of the perovskites revealed a porous morphology and the EDX analysis confirmed the 2:1:1 ratio of Gd:Mn:M. These perovskites were also studied by IR spectroscopy. The recorded spectra in the far IR region, show the characteristic bands arising from the stretching and bending vibrational modes of the Mn/M–O and Gd–O moieties. The influence of the M cation on the corresponding band shifts is in line with the predictions. The electrocatalytic properties of obtained perovskites were studied by cyclic voltammetry, using paraffin impregnated graphite electrode (PIGE) modified with investigated perovskites. The obtained results confirm their electrocatalytic ability towards oxidation of OH^- ions and of H_2O_2 oxidation in phosphate buffer.

Keywords: complex perovskites, PXRD, SEM, IR spectroscopy, cyclic voltammetry.

PSSE P-15

Synthesis, Characterization and Voltammetric Study of Dimethylammonium Lead Halide Perovskites

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During the past decade, hybrid organic-inorganic perovskites (HOIPs) have attracted significant attention for their optoelectronic properties and potential application in photovoltaics, leading to ongoing exploration and detailed study of both new and existing HOIPs. This research focuses on the synthesis, comprehensive characterization, and cyclic voltammetric study of hybrid lead halide perovskites with the formula $[(CH_3)_2NH_2]PbX_3$, ($DMAPbX_3$), where X represents I^-, Cl^-, or Br^-. A slightly modified synthesis method from literature was employed, using stoichiometric amounts of lead halides (PbX_2) and dimethylammonium halides (DMAX) dissolved in acetonitrile or *N,N*-dimethylformamide. Controlled evaporation yielded $DMAPbI_3$ as yellow crystals, $DMAPbCl_3$ and $DMAPbBr_3$ as colourless needle-like crystals. X-ray powder diffraction (XRPD) confirmed distinct perovskite structures with distinctive lattice parameters for each halide, while scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM-EDX) revealed well-defined morphologies and homogeneous elemental distribution. Cyclic voltammetry (CV) studies of $DMAPbX_3$ perovskites performed in dichloromethane (DCM) with tetrabutylammonium chloride (TBAC) or tetrabutylammonium perchlorate (TBAPC) as electrolytes, using a paraffin-impregnated graphite electrode (PIGE), demonstrated significant variations in redox behavior due to different halides. The results showed that $DMAPbX_3$ perovskites are electrochemically active, with oxidation (and reduction) currents decreasing in subsequent scans, indicating partial degradation of the perovskite structure.

Keywords: dimethylammonium lead halide perovskite, cyclic voltammetry, PXRD, SEM-EDX.

PSSE P-16

Chronoamperometric Studies in the Electrodeposition of Bi_2Se_3 Thin Films

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NOT PRESENTED

PSSE P-17

Construction of a Predictive Model for the Characterization of Layered Perovskite Structures

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The advent of perovskites as materials with a wide variety of potential applications due to their flexible structure and unique properties, has led to vast synthesis and investigation of new types of perovskites, such as hybrid organic-inorganic perovskites (HOIPs) and different classes of so-called layered perovskites, which consist of one or more perovskite-like layers with additional species inserted between them. As small changes in their elemental composition can affect their structure and, consequently, their physicochemical properties, while still retaining the characteristic perovskite motif, the possibility of modeling their composition and structure to tune their properties arises. This is especially true for layered perovskite structures, where the physicochemical properties are further influenced by the nature of the intruding layers.

This work aims to develop a predictive model for characterizing layered perovskites by correlating unit cell parameters with the dimensions of the constituents, anion electronegativity, and other relevant independent variables related to structure. To achieve this, crystal structure data from over 50 layered perovskites in space group $P2_1/c$ were utilized to calibrate the model. Subsequently, the model was validated against a separate test set of layered perovskites to evaluate its predictive accuracy and refine its effectiveness.

Keywords: Layered perovskites, multiple linear regression

PSSE P-18

Centrosymmetric or Non-Centrosymmetric Space Group for $Ca_2KH_7(PO_4)_4 \cdot 2H_2O$ and $Ca_2(NH_4)H_7(PO_4)_4 \cdot 2H_2O$: Infrared and Raman Spectroscopy Study

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The main purpose of this study is to examine the infrared and Raman spectra of $Ca_2KH_7(PO_4)_4 \cdot 2H_2O$ and $Ca_2(NH_4)H_7(PO_4)_4 \cdot 2H_2O$ to obtain useful information about the space groups for these compounds. These spectra were reported for the first time and interpreted by factor group analysis. The recorded infrared spectra are obtained at both room temperature (RT) and the boiling temperature of liquid nitrogen (LNT) along with room temperature Raman spectra. The scientific interest towards these little-known phosphate salts was greatly influenced by their potential proton conductivity properties. As expected, the infrared spectra of these examined compounds revealed bands resembling the characteristic ABC trio (around 2800 cm^{-1}, 2400 cm^{-1}, and 1700 cm^{-1}), indicative of strong OHO hydrogen bonds, aligning well with their structural data. Through a thorough examination of band frequency, intensity, and shape in both the IR and Raman spectra, coupled with a consideration of temperature effects in the IR spectra, we propose the most probable assignment of the vibrational bands. A thorough spectra-structural correlation analysis suggests that, from a spectroscopic point of view, a probable space group is $P\bar{1}$ rather than $P1$, as initially proposed using neutron diffraction for the potassium salt[1].

Keywords: structural data, spectroscopic analysis, space group.

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TEXTILE ENGINEERING

TE O-1

When Biomass Waste Becomes a Valuable Bioproduct

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Energy culture Giant Reed (*Arundo donax* L.) is a wild-growing plant already quite represented in the Croatian Mediterranean climate. Initially, it was used to produce biofuel, but through the cooperation of agronomic and textile experts, new procedures were developed and patented, which isolates first the valuable textile cellulose fibers[1]. In the next step, the solid and liquid residues from this production are completely utilized to produce solid biofuels[2]. In this way both requirements of closing the loop and creating zero waste are met. By applying this newly developed process, quality fibers with a length in the range 2.65-3.20 mm and density in the range 1.57-1.65 g/cm^3 are obtained. Isolated fibers are suitable for usage in various industries, primarily in the paper and textile industry, but their most significant application is expected in the field of technical textiles. The use of isolated bast fibers to reinforce biopolymer matrices ensures a high-quality bioproduct that meets all today's functionality and biodegradability requirements. The patented procedure to produce pellets from ligno-cellulosic residues after fiber production, gives the bioproduct of high energy value which has HHV (Higher heating value) within the range 17.10-17.63 MJ/kg and LHV (Lower heating value) within the range 16.10-16.53 MJ/kg. Those results are in the same range with the products already on the market. The newly developed pellets are not made from wood biomass and therefore their availability is much higher. Applied biomass is widely available and CO_2 neutral, so consequently, developed bioproducts are sustainable and circular. Furthermore, their competitiveness on the increasingly demanding global market has been increased.

Keywords: biomass, energy culture, *Arundo donax* L. fibers, pellets

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TE O-2

The Ecological Impact of Protective Clothing Washing

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The properties of materials used in the production of protective clothing are usually viewed through purpose and degree of protection, often ignoring sustainability[1]. In order to gain a complete insight into their life cycle, the effects of the maintenance (washing) process should be taken into account[2]. This research includes the analysis of materials for less demanding firefighting suits and the composition of washing wastewater, with a focus on the fragments that are released in the process. The influence of the, blue dyed fabric and the integrated retroreflective (RR) stripe was investigated through material spectral and morphological characteristic and by analysing effluent from washing cycles.

The wastewater collected after 5 and 10 washing cycles was analysed using physico-chemical parameters: pH, conductivity, turbidity, particle volume distribution, total suspended solids, total dissolved solids and total solids using gravimetric, potentiometric and laser diffraction methods.

The obtained results show a change in the material spectral properties and intolerable damage to the RR stripe. The wastewater was overloaded with fragments that were released during the washing cycles.

Keywords: protective clothing, washing, sustainability, spectral and morphological properties

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TE P-1

Characterization of Chokeberry Pomace Extract and its Utilization for Dyeing and Functionalization of Fabrics

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Berry pomaces, which are waste products from the food industry, contain a significant amount of colored bioactive polyphenolic compounds. These compounds are known for their excellent antioxidant and antimicrobial activities. Given these properties, bioactive compounds from chokeberry pomace (CBP) extract were utilized for the simultaneous dyeing and functionalization of fabrics of different chemical compositions. After the preparion, CBP extract was characterized[1] from the aspect of total polyphenolic content (204.61 mg/g of CBP), total flavonols and flavonones content (14.74 mg/g of CBP), and total anthocyanin content (14.62 mg/g of CBP). The antioxidant activity of the extract, determined by the DPPH and ABTS assays, was found to be 66.44% and 99.70%, respectively. This characterized extract was then used for dyeing and functionalizing of fabrics of different chemical compositions brought together in a multifiber fabrics. The carried out experiments indicated that cotton and viscose exhibited excellent antioxidant activity (99.99%) and antibacterial efficacy against *Escherichia coli* and *Staphylococcus aureus*. Colorimetric measurements showed that the fabric color strength values ranged from 2.06 to 18.93. These results suggest that the treated fabrics are suitable for the production of protective textiles.

Keywords: chokeberry pomace extract; fabric; dyeing; functionalization; antioxidant and antimicrobial activity

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TE P-2

Examination of CIELAB coordinate values for samples painted red by three different manufacturers

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In this work, the metric program "Super MATCH 6 supplement" was used, in which the instrumental method is used spectrophotometry.[1]

Six different samples were obtained by dyeing polyester knitwear in red solutions from different manufacturers, the reflection spectra of which were recorded in the visible range of the spectrum. Folowing colors were used: „DISPERZNIJ KRASNIJ ALIJ Z", „TERASIL ROT W-4BS" and „BEMACRON RUBIN SE-RDL". For each of the colors used, two samples were obtained, in a lower (1.00%) and higher (4.00%) concentration. The CIELAB coordinates were obtained for each of the six samples colored in red color solutions for all three types of light: D65 - DAYLIGHT, A - bulb light AND TL84 - fluorescent light.

The sample colored with „DISPERSION RED ALIUM Z" showed the maximum values for the brightness maximum (L), saturation (C) as well as the maximum values according to the red-green (A) and blue-yellow (B) coordinates in both concentrations (1.00% and 4 .00%). The maximum tone value (H) had the sample colored with „TERASIL ROT W-4BS", in both concentrations.

Keywords: CIELAB, DISPERZNIJ KRASNIJ ALIJ Z, TERASIL ROT W-4BS, BEMACRON RUBIN SE-RDL

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