Book of Abstracts NeXT-Chem

INNOVATIVE CROSS-SECTORAL TECHNOLOGIES

Exploratory Workshops Series

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Bucharest, ROMANIA

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FOREWORD

Welcome to the latest edition of the Exploratory Workshop "INNOVATIVE CROSS-SECTORAL TECHNOLOGIES - NeXT-Chem", a forum that has established itself as a beacon for young scientists to showcase their groundbreaking achievements in inter- and trans-disciplinary research. With each passing year, this workshop continues to foster collaboration, inspire new ideas, and shape the future of scientific exploration.

At its sixth edition, the NeXT-Chem workshop remains dedicated to providing a platform for young researchers, M.Sc. and Ph.D. students, to present their latest discoveries and gain invaluable insights through invited lectures. As usual, participation in this enriching experience is completely free, ensuring equal access for all passionate minds.

The overall number of participant registrations careered to previous editions and amounted to 43, seconded by additional registered participants who have requested video proceedings of the scientific event due to scheduling conflicts. All enrolled scientific papers abstracts have undergone the scrutinity of the reviewers' panel as per the inter pares evaluation methodology applicable.

In Workshop Section 1- Multifunctional materials, nanocomposites, innovative technologies and cultural heritage preservation, 28 oral presentations for scientific contributions were delivered. Their topics were alligned with top directions of research in organic chemistry, inorganic chemistry and polymer chemistry. The new materials have potential applications in areas of great socio-economic interest: Biomedical, Cultural Heritage Protection, Electronics Engineering, Agriculture and Environment, Energy, Industrial products development.

In Workshop Section 2- Bioresources, biotechnologies and biorefining, 15 oral presentations and scientific contributions were delivered. Their topics consisted of research in the field of biotechnology, biochemistry and biophysics. New technologies and materials have applications in many fields of great socio-economic importance: Food industry, Agriculture, Industrial applications, Biomedical, Environment and Construction.

Oral communications enrolled in the predefined sections were delivered by 20 young researchers affiliated with NIRDCP-ICECHIM and 23 young researchers affiliated with other universities and research institutes in Romania and abroad:

- United States of America, Georgia Institute of Technology, 950 Atlantic Dr. NW, Atlanta;

- India, Dr. B. R. Ambedkar National Institute of Technology, Punjab / Babasaheb Bhimrao Ambedkar University, Uttar Pradesh/ Government SSP College Waraseoni, Balaghat/ Christ Church College, Kanpur/ Institute of Nuclear Medicine and Allied Sciences, Delhi/ University of Delhi;

- Mexico, Autonomous University of Puebla;

- Pakistan Abdul Wali khan University Mardan / Shaheed Benazir Bhutto Women University/ COMSATS University Islamabad;

- France, UMRt INRAE 1158 BioEcoAgro, Université de Lille
- Republic of Moldova, Nicolae Testemitanu State University of Medicine and Pharmacy

- Greece, National Hellenic Research Foundation Athens

The coordinators of this edition extend their gratitude to all the participants, speakers, and contributors who have made this workshop possible. May this edition of NeXT-Chem be a catalyst for transformative breakthroughs and an inspiration for future generations of scientists.

INVITED LECTURES

Thursday, March 21st, 2024

1. Prof. Paula Celeste DA SILVA FERREIRA, Ph.D., Coordinator Researcher - CICECO, University of Aveiro, Portugal

"SEARCHING FOR SUSTAINABLE BIOBASED FUNCTIONAL COMPOSITE MATERIALS"

2. Assist. Prof. Nefeli LAGOPATI, Department of Biology, School of Medicine of the National & Kapodistrian University of Athens

"ANTICANCER EFFECT OF PHOTOCATALYTIC NANOPARTICLES"

3. Prof. Dr. Habil. Anton FICAI, Department of Science and Engineering of Oxide Materials and Nanomaterials, Faculty of Applied Chemistry and Materials Science, University POLITEHNICA of Bucharest

"COLL/HA COMPOSITE MATERIALS FOR BONE TISSUE ENGINEERING"

Friday, March 22nd, 2024

5. Prof Corina BRADU, Faculty of Biology, University of Bucharest *"NON-CONVENTIONAL WATER TREATMENT PROCESSES FOR SUSTAINABLE USE OF WATER RESOURCES "*

6. Naomi TRITEAN, ICECHIM Bucharest

"PLANT BIOSTIMULANT EFFECTS OF RICE HUSK NANOBIOSILICA EMBEDDED IN A FILM-FORMING FORMULATION AND APPLIED AS SEED COATING "

7. Grigore PŞENOVSCHI, ICECHIM Bucharest

"SCIENCE-INSPIRED APPS AND GAMES"

8. Andrei SÂRBU, Romanian Chemical Society

"EuChems- SChR COOPERATION FOR A SUSTAINABLE CHEMISTRY"

SEARCHING FOR SUSTAINABLE BIOBASED FUNCTIONAL COMPOSITE MATERIALS

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Keywords: Chitosan; Graphene-like material; Magnetic nanoparticles; Hyperthermia; Electrical conductivity

Introduction: Flexible biobased composite materials are interesting for a wide range of applications from electronics, to smart packaging and healthcare. Biodegradable biopolymers, namely polysaccharides, are sustainable alternatives to be used as matrices. The development of eco-friendly strategies using non-toxic precursors, energy- and time- saving methods is necessary to reduce costs, mitigate the environmental impact, and facilitate the industrial production. In this regard, the development of fabrication strategies, characterization methodologies and investigation of potential applications is fundamental.

Materials and methods: Polysaccharides are exploited to develop functional composites through the integration of different fillers, such as clays, metal oxide particles and graphene derivatives, and studied for different applications.

Results: This presentation will show an overview of some work performed at CICECO – Aveiro Institute of Materials at the University of Aveiro in Portugal mainly on the development of appropriate fillers and composites for electrical conductive, adsorbent, elect and magnetic responsive materials. [1-4]

Conclusions: The biocomposites may be designed to display suitable properties for the desired application.

Acknowledgements: This work was developed within the scope of the project CICECO - Aveiro Institute of Materials, UIDB/50011/2020, UIDP/50011/2020 & LA/P/0006/2020, financed by national funds through the FCT/MEC (PIDDAC). Cost action CA20126 – NETPORE is also acknowledge.

- [1]. Barra et al., Compos Sci Technol, 173 (2019) 53.
- [2]. Barra et al., Carbon 218 (2024) 118767.
- [3]. Alves et al. J Mol Sci, 22 (2021) 9943
- [4]. Barra et al. Adv. Healthcare Mater. (2023) 2303861

ANTICANCER EFFECT OF PHOTOCATALYTIC NANOPARTICLES

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Keywords: Ag-TiO₂; cancer; photodynamic therapy; cytotoxicity, nanomedicine

Introduction: Titanium dioxide nanoparticles (TiO₂ NPs) have a great spectrum of photocatalytic antibacterial and anticancer applications ^[1]. The chemical modification of TiO₂ optimizes its photocatalytic bioactive behavior ^[2] thus sometimes chemically modified TiO₂ is preferable, minimizing either the required concentration or the irradiation time ^[3]. This study focused on the development of silver modified NPs (Ag/TiO₂ NPs) with anticancer potential.

Materials and methods: Ag/TiO₂ NPs were prepared through the sol-gel method and then characterized through DLS, XRD, micro-Raman spectroscopy, XPS, UV-vis spectroscopy, and SEM microscopy, and tested *in vitro* on breast cancer epithelial cells (MCF-7 and MDA-MB-468). MTT colorimetric assay was applied to estimate cellular viability. Western blot analysis of protein expression that are related to cell apoptosis along with a DNA-laddering assay were employed to ensure about the type of cell death ^[4].

Results: We showed that photo-activated Ag/TiO_2 NPs exhibited significant cytotoxicity on the highly malignant MDA-MB-468 cancer cells, decreasing the proliferation rate, and inducing apoptosis that is related to PARP cleavage and DNA fragmentation. MCF-7 (non-metastatic cells) were unaffected under the same conditions.



Figure 1. a) SEM images from Ag-TiO₂ NPs, b) Effect of Ag/TiO₂ NPs and Photo-excited Ag/TiO₂ NPs on the viability of MCF-7 (low metastatic potential) and MDA-MB-468 (human breast adenocarcinoma, highly invasive) breast cancer epithelial cells. *p<0.05 vs. negative control, based on the Kruskal-Wallis test. MTT assay was employed to determine cell viability.

Conclusions: Our promising results showed that photoexcited Ag/TiO_2 might be considered as an anticancer agent. Hence, an alternative approach based on the use of nanomaterials might be very intriguing, if we consider that multidrug-resistance of tumor cells is a common major obstacle to the success of a chemotherapy in addition to undesirable side effects ^[5].

Acknowledgements: IKY scholarships program (action "Reinforcement of Postdoctoral Researchers" MIS5001552

- Lagopati N., Evangelou K., Falaras P., Tsilibary EC., Vasileiou PVS., Havaki S., Angelopoulou A., Pavlatou EA. and Gorgoulis VG.:Nanomedicine: Photo-activated nanostructured titanium dioxide, as a promising anticancer agent. Pharmacol Ther. 2020; 222: 107795.
- [2]. Turcu, E., Coromelci, CG., Harabagiu, V., Ignat, M. Enhancing the Photocatalytic Activity of TiO2 for the Degradation of Congo Red Dye by Adjusting the Ultrasonication Regime Applied in Its Synthesis Procedure. Catalysts 2023, 13, 345.
- [3]. Li R., Li T., Zhou Q. Impact of Titanium Dioxide (TiO2) Modification on Its Application to Pollution Treatment—A Review. Catalysts. 2020; 10(7):804.
- [4]. Lagopati N., Kotsinas A., Veroutis D., Evangelou K., Papaspyropoulos A., Arfanis M., Falaras P., Kitsiou PV., Pateras I., Bergonzini A., Frisan T., Kyriazis S., Tsoukleris DS., Tsilibary EC., Gazouli M., Pavlatou EA., Gorgoulis, VG. Biological Effect of Silver-modified Nanostructured Titanium Dioxide in Cancer. Cancer Genomics Proteomics. 2021;18(3 Suppl):425-439.
- [5]. Mir SA., Hamid L., Bader GN., Shoaib A., Rahamathulla M., Alshahrani MY., Alam P., Shakeel F. Role of Nanotechnology in Overcoming the Multidrug Resistance in Cancer Therapy: A Review. Molecules, 2020, 27(19), 6608.

COLL/HA COMPOSITE MATERIALS FOR BONE TISSUE ENGINEERING

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Keywords: bone grafts; composite materials; collagen; hydroxyapatite; active agents; drug delivery, bone related diseases: osteoporosis, infections, cancer.

Abstract: Bone is a remarkable composite material based on Hydroxyapatite (HA) and Collagen (COLL). The high need of bone grafts (almost 50% of the total amount of grafts needed worldwide is related to bone) is only surpassed by the need of blood while the need of the other grafts is much lower (9-11% for skin, blood vessel and nerve grafts). The availability of the auto-, alo- and xenografts is limited and also there are some risks with their use (need of second surgical intervention, risks of infections and rejections, etc.) and this is why, synthetic grafts are needed and thus many researchers and companies are focusing their research and development programs in this field. This presentation will be mainly focused on presenting some relevant data about bone, the evolution of the materials in the field of bone grafting and repair, some examples of preparation of COLL/HA composite materials and some drug delivery systems developed for specific applications. A special attention will be paid to the design and processing of COLL/HA composite materials paying attention to the composition and morphology and their impact on regeneration and delivery profile.

PLANT BIOSTIMULANT EFFECTS OF RICE HUSK NANOBIOSILICA EMBEDDED IN A FILM-FORMING FORMULATION AND APPLIED AS SEED COATING

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Keywords: mixture design; alginate-glycerol-sorbitol; Wurster process; salt stress; reactive oxygen species;

Introduction: Ensuring a favorable environment for seed growth and development in order to improve crop quality and yield is critical in the context of climate change which intensifies the harmful effects of abiotic stresses such as salt stress [1]. Rice husk (RH) is a well-known significant source of biosilica [2]. Silicon has been shown to have biostimulant effects on plants, with both physiological and mechanical functions. The biopolymer alginate is known for its biostimulant activity as well as for its excellent film-forming properties. Mitigation solutions to reduce the negative effects of climate change in agriculture are needed, the aim of this study being focused on an alginate-glycerol-sorbitol (AGS) formulation with embedded silica nanoparticles (SiNPs) from rice husk (RH) which exhibits plant biostimulant effects when applied as seed coating.

Materials and methods: Synthesis of biogenic SiNPs was carried out by dilute acid hydrolysis of RH in a temperature-controlled hermetic reactor followed by calcination. The physical-chemical properties of the native RH, the intermediates, and SiNPs, as well as the release of soluble silicon (Si) from SiNPs were investigated. Mixture design with three factors was used in order to optimize the seed coating, based on traction tests that were conducted with Dynamic Mechanical Analysis (DMA). All the activities performed on Mung bean seedlings were determined both in the presence and in the absence of salt stress. Seedling growth and development was investigated by measuring radicle and hypocotyl length, alpha-amylase activity and photosynthetic pigment content. The metabolic activity was determined by investigating proton pump and mitochondrial enzyme activity. Reactive oxygen species (ROS) metabolism was assessed by determining the content of hydrogen peroxide, lipid peroxides, L-proline, nitric oxide (NO) and by analyzing the activity of several key-enzymes involved in ROS scavenging, i.e., superoxide dismutase (SOD), catalase (CAT), guaiacol peroxidase (G-POX), glutathione reductase (GR). The amount of ROS in the leaves was determined by fluorescence microscopy image analysis. Inductively Coupled Plasma-Optical Emission Spectrometry (ICP-OES) was used for the determination of Si accumulation in Mung bean seedlings.

Results: Amorphous SiNPs of about 50 nm were biosynthesized from RH and embedded in an AGS film optimized by mixture-design. Using the Wurster process we obtained a homogeneous AGS film with or without embedding biogenic SiNPs. The formulation of nanobiosilica in an AGS seed coating resulted in the alleviation of salt stress on Mung seedlings by decreasing the level of ROS and products of peroxidation reactions that occur at cellular level, compensating the necessary L-proline content, and increasing the photosynthetic pigments and NO content, as well as the specific extracellular H⁺ level into the medium. A complex behavior of the analyzed antioxidant enzymes was observed.

Conclusions: Recovery of biogenic SiNPs from RH and the effective application in an alginate-based beneficial seed coating as plant biostimulants that mitigate salt stress from the early stages of plant development represent an important approach not only scientifically but also socio-economically.

Acknowledgements: This work was carried out through the PN 23.06 Core Program - ChemNewDeal within the National Plan for Research, Development and Innovation 2022-2027, developed with the support of Ministry of Research, Innovation, and Digitization, project no. PN 23.06.02.01 InteGral. We also acknowledge project 15PFE NeXT-BExcel.

- [1]. Tolisano, C. and D. Del Buono. Biobased: Biostimulants and biogenic nanoparticles enter the scene. Sci. Total Environ. 2023; 885: p. 163912.
- [2]. Chen, H., et al. Extraction of lignocellulose and synthesis of porous silica nanoparticles from rice husks: a comprehensive utilization of rice husk biomass. ACS SCE. 2012; 1: p. 254-259.

SCIENCE-INSPIRED APPS AND GAMES

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Keywords: games, science, apps, influence, society

Introduction: In today's digital age, science-based apps and games are revolutionizing the landscape of education and exploration. This abstract delves into the profound influence of these innovative tools on advancing scientific knowledge and fostering curiosity. Science-based apps and games serve as dynamic platforms that engage users in immersive learning experiences. Through simulations, puzzles, and quests, users are encouraged to experiment, analyze data, and problem-solve, thereby enhancing critical thinking skills and deepening their understanding of scientific principles. With the convenience of smartphones and tablets, individuals from diverse backgrounds can embark on scientific journeys from anywhere in the world. This inclusivity not only expands the pool of aspiring scientists but also encourages collaboration and knowledge-sharing on a global scale.

Conclusions: the emergence of science-based apps and games marks a significant paradigm shift in how we engage with and perceive scientific knowledge. These digital tools have transcended traditional boundaries, democratizing access to education and research while fostering a culture of curiosity and collaboration. By gamifying complex concepts and leveraging the power of crowdsourcing, they not only enhance learning outcomes but also contribute to scientific discovery on a global scale.

Session 1 - Multifunctional materials, nanocomposites, innovative technologies and cultural heritage preservation

NEW ADSORBENTS BASED ON CHITOSAN AND INORGANIC-ORGANIC COMPOSITES FOR EFFICIENT REMEDIATION OF WASTEWATER CHARGED WITH HEAVY METALS

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Keywords: chitosan, inorganic-organic composite, polymeric bead, heavy metals retention

Introduction: In general terms, pollution is defined as the process of introducing toxic substances into the environment, causing devastating effects on ecosystems, and leading to destabilization and illness of wildlife and further to serious problems for humans. Heavy metals are some of the most dangerous pollutants because they bioaccumulate and have a long half-life. The most widely used techniques for the removal of heavy metals from water are ion exchange, membrane processes, electrochemical and biological treatments, and adsorption. Among these, adsorption using adsorbent materials is the most efficient and simple process ^{[1][2]}. The need for new environmentally friendly adsorbent materials with minimal production costs is increasing. Nowadays, the most widely used adsorbents are carbon nanotubes, activated carbon, or graphene oxide. However, natural adsorbents from waste materials such as chitosan, eggshells, fruit peels, ash, etc. can be used^[3].

Materials and methods: New adsorbents based on different types of chitosan (commercial, commercial chitin derived-chitosan and chitosan synthesized from shrimp shell waste) and inorganic-organic composites were synthesized to determine the adsorption capacity for copper ions from wastewater. The technique for obtaining adsorbates is relatively simple and does not require special working conditions.

Results: The study of the synthesis efficiency to obtain new adsorbent materials was evaluated from a physicochemical and morpho-structural point of view by Fourier-Transform Infrared Spectroscopy (FTIR), X-Ray Diffraction (XRD), porosimetry (N_2 adsorption) and Scanning Electron Microscopy (SEM) analysis. The adsorption kinetics of the materials were evaluated using several adsorption models to identify the behavior during the adsorption process.

Conclusions: The newly synthesized adsorbents have remarkable Cu(II) ion retention capabilities and are feasible for industrial applications.

Acknowledgements: This work was supported by the Ministry of Research, Innovation and Digitization through Program 1 - Development of the national research and development system, Subprogram 1.2 - Institutional performance- Projects to finance excellence in RDI, Contract no. 15PFE / 2021, PN-III-Human Resources Programme-YOUNG RESEARCH TEAMS-PN-III-P1-1.1-TE-2021-0915, grant no. 135/2022 - I-ON-MEM. The authors also acknowledge the opportunity given by the Ministry of Research, Innovation, and Digitalization, for supporting the research on this theme, through ctr. nr. 2N/03.01.2023 (PN 23.06.01.01. AQUAMAT).

- Vardhan KH. A Review on Heavy Metal Pollution, Toxicity and Remedial Measures: Current Trends and Future Perspectives. J. Mol. Liq. 2019, 290
- [2]. Singh A. Heavy Metal Contamination of Water and Their Toxic Effect on Living Organisms. In The Toxicity of Environmental Pollutants; IntechOpen: London, UK, 2022; ISBN 978-1-80355-580-5.
- [3]. Renu. Removal from Wastewater Using Various Adsorbents: A Review. J. Water Reuse Desalination 2017, 7, 387-419.

MIP- MODIFIED SCREEN PRINDED SENSING TOOLS FOR SELECTIVE LIPOPOLYSACCHARIDES DETECTION

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Keywords: molecularly imprinted particles, LPS detection, selective recognition, LOD, SPCE

Introduction: Mutations and worldwide spreading of pathogenic bacteria has pushed forwards the research regarding detection of bacterial endotoxins, such as lipopolysaccharides (LPS), which is crucial in addressing both environmental and healthcare challenges^[1]. Nowadays, LPSs are accountable for various infections, including septic shock and lately it's considered to be one of the contributors to the development of Parkinson's disease^[2]. Traditional methods used for LPS detection in research and medical field include enzyme-linked immunosorbent assay (ELISA) and the Limulus amebocyte lysate (LAL) assay^[3]. However, these aged methods have enough limitations in the era of rapid technological development such as low sensitivity and complex time-consuming procedures. Hence, there is an up growing need for the development of new, low-cost, affordable advanced approaches, particularly in the environmental and medical realms.

Regarding the latest concerns, this work describes the development of a MIP-modified sensing tool capable of selectively recognizing a specific targeted type of LPS (i.e., LPS from *Pseudomonas aeruginosa*) from different bacterial strains. To maintain the goal of obtaining a cheap, sensitive, and easy-to-handle device, a regeneration process was prepared to preserve the electrochemical properties of the final sensing product.

Materials and methods: The development of the LPS-sensing platform consisted in the drop-casting deposition of a lab made MIP-carbon paste (containing electroactive ZnO particles, a polyether-based binder, and a compatible solvent) on a commercial ceramic electrode.,

Results: Modern techniques, including structural and morphological analyses, were employed to characterize the obtained MIPs modified sensing tools, which demonstrated the successful entrapment of MIP particles into the drop casted paste. The electrochemical analyses (Cyclic voltammetry and Differential pulse voltammetry) of the obtained MIP- modified SPCEs along with the static and selective adsorption analysis were used to determine the imprinting factor, sensitivity and selectivity for the targeted LPS.

Conclusions: As a result, the obtained MIP-modified SPCEs proved to be effective in detecting lipopolysaccharide from *Pseudomonas aeruginosa*. These novel tools are advantageous due to their practical size, low manufacturing cost, and the minimal amount of resources needed for the fabrication and detection process.

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- [1]. Laxminarayan, R. et al. Antibiotic resistance—the need for global solutions. The Lancet Infectious Diseases, 2013, 13, 1057-1098
- [2]. Brown, G.C.; Camacho, M.; Williams-Gray, C.H. The Endotoxin Hypothesis of Parkinson's Disease. Movement Disor-ders 2023, 38, 1143–1155
- [3]. Mackenzie, A.M.; Lebel, P.; Orrbine, E.; Rowe, P.C.; Hyde, L.; Chan, F.; Johnson, W.; McLaine, P.N. Sensitivities and Specificities of Premier E. Coli O157 and Premier EHEC Enzyme Immunoassays for Diagnosis of Infection with Verotxin (Shiga-like Toxin)-Producing Escherichia Coli. The SYNSORB Pk Study Investigators. J Clin Microbiol 1998, 36, 1608– 1611

THE CHEMICAL MODIFICATION OF NANOCELLULOSE WITH A NATURAL ALDEHYDE TO INCREASE ITS SURFACE HYDROPHOBICITY

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Keywords: nanocellulose; chemical modification; hydrophobicity

Introduction: Cellulose, the most ubiquitous biopolymer on Earth, is a material with a long history used since ancient times in the construction of shelters, paper manufacturing, production of textiles and fabrics, craftsmanship, and medical applications, that played a pivotal role in the evolution of mankind ^[1]. Despite the prevailing belief that all knowledge concerning cellulose had been uncovered, in the last thirty years, cellulose has experienced an amazing renaissance, emerging in more and more applications, in its nano form, generically called "nanocellulose". Nanocellulose (NC), a material isolated from cellulose through chemical, enzymatic and/or mechanical treatments, has gained the attention of researchers around the world due to its exceptional properties such as its excellent mechanical strength, light weight, biocompatibility, biodegradability, high specific surface area, and the multitude of hydroxy (-OH) groups from its surface which open plenty of possibilities for physical and chemical modification. Nevertheless, the innate hydrophilic nature of NC and tendency to agglomerate in hydrophobic media makes NC's processing difficult and severely limits its wide application in drug delivery systems, packaging, as reinforcement agent in polymeric composites, stabilizer for oil/water systems, material for the removal of contaminants from the environment, etc ^[2]. In this work, cellulose nanofibers (CNFs) obtained from microcrystalline cellulose (MCC) by mechanical defibrillation were chemically modified with a natural aromatic compound from the flavonoids class to increase their surface hydrophobicity, and the changes in the CNFs' properties following the surface modification reaction were comprehensively evaluated and discussed.

Materials and methods: CNFs were isolated from MCC by mechanical defibrillation in a microfluidizer and chemically modified by reaction with cinnamic aldehyde. The changes in the chemical structure and thermal stability of CNFs after the chemical modification were assessed by Fourier-transform infrared spectroscopy (FTIR), Raman spectroscopy and thermogravimetric analysis (TGA), while the changes in the surface morphology and hydrophobicity of CNFs after functionalization were assessed by scanning electron microscopy (SEM) and contact angle measurements.

Results: The FTIR and Raman spectroscopies confirmed that the surface modification of CNFs with cinnamic aldehyde took place successfully, while the TGA revealed an increase in the thermal stability of CNFs post modification. The SEM images showed that CNFs maintained their nano diameter following the chemical modification reaction.

Conclusions: In this work, an innovative, inexpensive, and facile route for increasing the surface hydrophobicity of CNFs by chemical modification, which has the prospect to expand the range of applications of CNFs has been proposed, and the resulted product was thoroughly characterized in terms of chemical structure, thermal stability, and morphology.

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- [1]. Culica ME, Chibac-Scutaru A-L, Mohan T, Coseri S. Cellulose-based biogenic supports, remarkably friendly biomaterials for proteins and biomolecules. Biosens. Bioelectron. 2021;182.
- [2]. Usurelu CD, Badila S, Frone AN, Panaitescu DM. Poly(3-hydroxybutyrate) Nanocomposites with Cellulose Nanocrystals. Polymers 2022;14.

INVESTIGATING THE BEHAVIOUR OF TEA TREE AND BERGAMOT ESSENTIAL OILS LOADED PLURONIC MICELLES

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Keywords: micellar system; Pluronic; encapsulation; essential oil

Introduction: Currently, essential oils are used as natural therapeutic agents because of their biological activity, however, they are highly lipophilic and easily degradable, thus, encapsulating them in drug delivery systems such as polymeric micelles is an efficient solution for this downside ^[1].

Materials and methods: Micellar systems of Pluronic block-copolymers with different molecular weights and HLBs (F127, P123 and P84) have been studied, and the influence of encapsulating various commercial volatile oils has been evaluated. Tea tree oil and bergamot oil have been selected as volatile oils for the study due to their wide range of therapeutic uses ^{[2], [3]}. Polymeric micelles were prepared at a very low polymer concentration (1%), which has been reported in the literature to have minimal toxic effects on normal cells ^[4]. The micellar systems were characterized in terms of the average size of the aggregates, size distribution, zeta potential, and flow properties.

Results: For the vast majority of systems, an increase in micelle size was observed upon encapsulating increasing amounts of essential oils, without deforming the initially considered spherical aggregates. Analysis via DLS (Dynamic Light Scattering) and viscosity variation for the Pluronic P123 system with tea tree oil may lead to the assumption that for moderate amounts of encapsulated oil, both an increase in micelle size and a transition to elongated morphology occur.

Conclusions: Encapsulation of essential oils does not, in most cases, affect the stability of micelles, as evidenced by small variations in the zeta potential. The sizes of the micelles undergo a slight increase, and their distribution generally remains monodisperse. Investigating these systems further in order to highlight the shape of the aggregates remains an ongoing subject of interest, enabling the explanation of theoretical aspects of changes in the self-assembly process of Pluronic molecules in the presence of complex mixtures such as volatile oils.

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- Shetta, A., Kegere, J., Mamdouh, W., Comparative study of encapsulated peppermint and green tea essential oils in chitosan nanoparticles: Encapsulation, thermal stability, in-vitro release, antioxidant and antibacterial activities. Int J Biol Macromol. 2019;126:731–742
- [2]. Usachev, E. V., Pyankov, O. V., Usacheva, O. V., Agranovski, I.E., Antiviral activity of tea tree and eucalyptus oil aerosol and vapour. J Aerosol Sci. 2013;59:22–30.
- [3]. Celia, C., Trapasso, E., Locatelli, M., Navarra, M., Ventura, C.A., Wolfram, J., et al., Anticancer activity of liposomal bergamot essential oil (BEO) on human neuroblastoma cells. Colloids Surf B Biointerfaces. 2013;112:548–553.
- [4]. Ganguly, R., Kumar, S., Tripathi, A., Basu, M., Verma, G., Sarma, H.D., *et al.*, Structural and therapeutic properties of Pluronic® P123/F127 micellar systems and their modulation by salt and essential oil. J Mol Liq. 2020;310

APPLICATION OF SILVER MODIFIED ZnAI-LDH's IN CONSERVATION OF STONE MASONRY

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Keywords: LDH's, conservation, stone masonry

Introduction: Silver is a well-known antimicrobial agent extensively used in many applications such as biomedicine or conservation of cultural heritage elements prone to biodeterioration. In the recent years, a lot of interest has been placed on the silver (nano)particles incorporated or supported on 2D inorganic materials [1]. Among 2D compounds layered double hydroxides (LDHs) are interesting materials for developing 0D/2D nanostructured architecture. The use of LDH surface as a substrate or support for the antimicrobial component allow combination of the LDH biocompatibility and ion exchange properties with the bacteriostatic properties of silver. To our knowledge, materials such as these were not previously studied as conservation or consolidation agents. In this work, a material developed by us, with good antimicrobial properties ZnAl-(Ag) -LDH and a pure ZnAl-LDH were investigated for their preservation/conservation activity in heritage applications with the main goal to develop a material able to long-term protect the stone monuments from environmental and microbiologic factors.

Materials and methods: The LDH materials were synthesized via a coprecipitation method, modified from [2] and [3]. Their structure was confirmed by powder x-ray diffraction. In order to investigate their properties as consolidants, the kinetic stabilities of the material dispersion in water and water-ethanol mixtures were determined from the variation of absorbance over time by UV-VIS spectrometry. KS was calculated using the formula:

$$KS\% = 1 - \left[\frac{A_0 - A_t}{A_0}\right] \times 100 \tag{1}$$

where: A_0 represents the absorbance at 0 min, and A_t is the absorbance at time t.

Some mortar test bricks 4x4x4 cm were used as test specimen to investigate the effect of the LDH dispersion on the properties of the mortar: aesthetic, compressive strength and peeling test.

Results: Both materials tested form relatively stable dispersions, especially in water:ethanol (80:20) mixtures Ks= 49% for silver containing LDH and respective 68% after 180 minutes, it is also noteworthy that the dispersions stability strongly depend on the solvent compositions. For the treated samples, chromatic parameters are not visibly changed ($\Delta E^*=0.6$ for bricks brushed with ZnAl-LDH and $\Delta E^*=2.1$ for samples brushed with the silver modified material). The peeling test also showed an improvement of the surface stability of around 20% for the samples brushed with ZnAl-LDH while the samples treated with ZnAl(Ag)-LDH showed no notable changes, the changes in compressive strength of the treated samples were also negligible.

Conclusions: Both materials shows good stability in water:ethanol (80:20) mixtures as well as distilled water (30% and 59% for the pure LDH) the silver modified material showing a lower stability compared to the pure LDH. The change in aesthetic parameters ΔE^* is lower than the observable limit of the naked eye and the stability of the surface after brushing with ZnAl-LDH is improved. We are currently performing further studies on these materials.

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- [1] M. Nocchetti, A. Donnadio, V. Ambrogi, P. Andreani, M. Bastianini, D. Pietrella, L. Latterini, Ag/AgCl nanoparticle decorated layered double hydroxides: Synthesis, characterization and antimicrobial properties, Journal of Materials Chemistry B. 1 (2013) 2383–2393. https://doi.org/10.1039/c3tb00561e.
- [2] J. Shen, A. Shi, M. Wu, H. Zhang, Z. Jiang, Efficient degradation of bisphenol A over facilely optimized ternary Ag/ZnO/ZnAl–LDH composite with enhanced photocatalytic performance under visible light irradiation, Solid State Sciences. 132 (2022) 106992. https://doi.org/10.1016/j.solidstatesciences.2022.106992.
- [3] C.E. Rizescu, D.A. Vasile, D.A. Minea, R.-M. Stirbescu, L. Marin, I. Atkinson, L. Predoana, R.-M. Ion, Layered Double Hydroxides as Consolidants and Anion Absorbents for Heritage Conservation, Proceedings. 57 (2020) 84. https://doi.org/10.3390/proceedings2020057084.

SYNTHESIS & CHARACTERIZATION OF GRAPHITE FROM *TERMINALIA ARJUNA* AS PRECURSOR FOR BIOMATERIALS DEVELOPMENT IN BONE TISSUE ENGINEERING APPLICATIONS

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Keywords: T. arjuna; Graphite; Biomaterials; Tissue Engineering, Sintering

Introduction: The development of novel biomaterials for bone tissue engineering is one of the most significant domains of research in nanomedicine. The promising characteristics of graphite open their practical applications in tissue engineering. The biomaterials developed from graphite such as graphene oxide (GO), reduced graphene oxide (rGO), etc can play a crucial role in supporting cell-biomaterial interactions and facilitating bone tissue regeneration.

Materials and methods: In the present research, method for the synthesis of graphite from *Terminalia arjuna* (*T. arjuna*), performed with heat treatments without using additional chemicals. The research focuses on valorizing dried whole fruit (WF), seed (SD), and pericarp (PC) of *T. arjuna* to produce graphite, thus utilizing non-edible plant resources. For heat treatment, a muffle furnace was employed to subject the dried fruits to various temperature ranges (250° C - 900° C) for 45 min to obtain graphite. The morphological analysis, elemental composition, and trace elements were analyzed using FESEM-EDS. XRD confirmed the synthesis of crystalline graphite, while FT-IR analysis revealed functional groups for graphite present. ^[1]

Results: According to the experimental results, it was determined that the ideal temperature range for SD and PC is between 350°C and 550°C, while for WF, the ideal temperature ranges are 650°C to 850°C, whereas 700°C WF is the best resulting diffraction pattern closely matched the peaks found in the JCPDS database for a particular crystalline phase.^[1]



Figure 1. Optimal graphite yield from dried T. arjuna fruit components achieved at 700°C.

Conclusions: This study shown an efficient, feasible, and reproducible approach for the synthesis of graphite from hydrocarbon-rich fruit waste to synthesis graphene oxide and reduce graphene oxide for developing bioactive scaffolds in bone tissue engineering applications.

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References:

[1]. Dan S, Sah MK. Terminalia arjuna fruit-derived graphite: a versatile biomaterial precursor for bone tissue engineering applications. Biomass Conv. Bioref. 2023

THERMO-RESPONSIVE HYBRID NANOSTRUCTURES OF CHITOSAN AND POLY(N-ISOPROPYLACRYLAMIDE)

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Keywords: polysaccharides; hybrids; complexation; thermal response; nanostructures

Introduction: Polysaccharides have attracted attention in recent decades due to their excellent biocompatibility and high availability. From chitin, the second most common natural material, chitosan is produced by deacetylation^{[1][2]}. Chitosan's antibacterial properties, biocompatibility, biodegradability, and lack of toxicity make it suitable for a wide range of applications, such as food additives, cosmetics products, drug administration, tissue regeneration, and wound healing^[3].

Materials and methods: The aim of this study was to investigate the electrostatic interaction between water-soluble chitosan (M_w =1,500 g/mol, Chi) and a poly(*N*-isopropylacrylamide) (M_w =3,000 g/mol, PNIPAM) with a carboxylic end group prepared by RAFT polymerization. The obtained complexes were characterized in solution by dynamic and electrophoretic light scattering (DLS and ELS). Also, the thermal response was investigated by DLS at different temperatures, between 25 and 45 °C.



Figure 1. Size distributions of (a) the initial polymers and the obtained complexes, and (b) the Complex 4/1 at different temperatures

Results: Size distributions (Figure 1a) exhibit the presence of two different populations of particles in the case of Chi, PNIPAM and the complexes, respectively. The different observed populations most probably correspond to complexes comprising of varying total numbers of chains. The corresponding size distributions for Complex 4/1 at different temperatures are shown in Figure 1b. It is evident that, above 35 °C, only one population is present, indicating the production of compact structures, which is likely caused by the increased hydrophobicity of the PNIPAM chains present in the complexes. However, after cooling, the system returns to its original state.

Conclusions: PNIPAM homopolymer with a carboxylate end group was successfully bound by electrostatic interactions to a low molecular weight chitosan biopolymer. This resulted in the formation of thermoresponsive hybrid nanostructures which exhibited properties related to the ratio of the two macromolecular components.

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- [1]. Karayianni M, Sentoukas T, Skandalis A, Pippa N, Pispas S. Chitosan-Based Nanoparticles for Nucleic Acid Delivery: Technological Aspects, Applications, and Future Perspectives. Pharmaceutics 2023; 15:1849.
- [2]. Hisham F, Maziati Akmal MH, Ahmad F, Ahmad K, Samat N. Biopolymer chitosan: Potential sources, extraction methods, and emerging applications. Ain Shams Eng. J. 2023; 102424.
- [3]. Abourehab MAS, Pramanik S, Abdelgawad MA, Abualsoud BM, Kadi A, Ansari MJ, Deepak A. Recent Advances of Chitosan Formulations in Biomedical Applications. Int. J. Mol. Sci. 2022; 23:10975.

DRESSINGS BASED ON POLY (3-HYDROXYBUTYRATE-CO 3-HYDROXYVALERATE), NANOCELLULOSE, AND A PHENOLIC NATURAL PRODUCT

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Keywords: nanocellulose, poly(3-hydroxybutyrate-co-3-hydroxyvalerate), wound dressing

Introduction: Cellulose is one of the most abundant polysaccharides on Earth, with multiple uses in tissue engineering, wound dressing, and drug delivery, bringing to the table its low toxicity, biodegradability, and biocompatibility^[1]. Nanocellulose (NC) is obtained from cellulose sources by combined mechanical, chemical, or enzymatic treatments and opens new opportunities for biomedical applications because of its nano dimension. Due to the hydroxyl groups from its surface and porous nature, NC has a great ability to absorb and release active compounds, which is mandatory for wound dressings^[2]. Poly(3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV) is a polyhydroxyalkanoate that exhibits valuable properties such as high crystallinity and stiffness, good biocompatibility, and biodegradability, which recommend it for biomedical applications. Moreover, it is easily processed by melt compounding, extrusion, and injection in various forms like films, single-use bottles and cutleries, plates, and others. Pairing NC with PHBV is difficult because of their different nature, NC being highly hydrophilic and PHBV hydrophobic. However, plasma treatment of PHBV films drastically changes its surface properties, turning it into a highly hydrophilic material, which becomes compatible with NC. In this work, NC and PHBV were paired to obtain a dressing with antibacterial activity provided by curcumin, a phenolic natural compound with a known bactericidal effect.

Materials and methods: NC was obtained from microcrystalline cellulose by microfluidization and was afterward immersed in a curcumin ethanolic extract (CE) in different ratios for 24 h. A part from each of these mixtures (NC/CE) was lyophilized for further investigations while the rest was kept for ulterior preparation of dressings using a PHBV commercial film with a thickness of 10 microns. The morphostructural characteristics, thermal, and surface properties were investigated by Fourier-transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), thermogravimetric analysis (TGA), and contact angle. An in vitro study to assess the antibacterial activity and cytotoxicity of selected samples was carried out as well.

Results: The presence of curcumin in the NC/CE mixtures was attested by the specific IR vibrations and the changes in the morphological aspects observed by SEM. Curcumin also led to an increase in the thermal stability of the NC/CE samples with about 20 °C. Dressing obtained by the uniform spraying of NC/CE mixtures on the plasma-treated PHBV films showed a change in the surface properties of the films as observed by contact angle measurements, a slight antibacterial effect, and a lack of cytotoxicity, similar to the unmodified films.

Conclusions: The results emphasized the effect of the plasma treatment and NC/CE covering on the hydrophilicity, thermal, biological, and morphological characteristics of the PHBV films. Plasma treatment at room temperature together with the addition of a phenolic natural compound led to the obtaining of wound dressings with interesting properties for medical application.

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- [1]. Oprică GM, Panaitescu DM, Usurelu CD, Vlăsceanu GM, Stanescu PO, Lixandru BE, Vasile V, Gabor AR, Nicolae C-A, Ghiurea M, et al. Nanocellulose Sponges Containing Antibacterial Basil Extract. Int. J. Mol. Sci. 2023; 24(14):11871.
- [2]. Oprică GM, Panaitescu DM, Lixandru BE, Uşurelu CD, Gabor AR, Nicolae C-A, Fierascu RC, Frone AN. Plant-Derived Nanocellulose with Antibacterial Activity for Wound Healing Dressing. Pharmaceutics. 2023; 15(12):2672.

INFLUENCE OF TREATED ASH WASTE ON THE PROPERTIES OF GLASS FIBER REINFORCED POLYAMIDE 6 AND POLYAMIDE 6/POLYAMIDE10.10 HYBRID COMPOSITES

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Keywords: polyamide 10.10; polyamide 6; glass fiber; ash powder; nanoindentation

Introduction: Polyamide 6 (PA6) reinforced with glass fiber (GF) is a polymer composite that offers exceptional strength, durability, and stiffness ^[1]. Bio-based polyamide 10.10 (PA10.10) can be fully obtained from bio-based products while its industrial-scale applicability is still under development ^[2]. Ash waste is also seeing development in its applications being mainly used in mortar mixtures but also in epoxy compositions ^[3]. The objective of this study is to investigate the influence of ash waste treated with 3 different dispersion agents on the thermal, dynamic-mechanical and nanomechanical properties of glass fiber PA6 and PA6/PA10.10 hybrid composites. The effect of replacing 5 wt.% of GF with treated ash waste on the required properties of these composite materials in industrial applications will be analyzed.

Materials and methods: Ash waste (C) was treated with 3 dispersion agents (P, S and G) by melt compounding. GF reinforced PA6 (PA6-F) and PA6-F/PA 10.10 hybrid (PA6/PA10) were used as the polymer matrix. In the obtained samples 5 wt. % GF was replaced with treated ash so that all composites have a 30 wt.% concentration of GF and ash. These composites were prepared in dynamic conditions through extrusion and injection molding for dynamic-mechanical (DMA), thermal (TGA, DSC) and tribological characterization (nanoindentation and nanoscratching) of properties.

Results: From a nanomechanical point of view, Figure 1 (a) and (b) showed an increase in reduced modulus for treated fly ash composites compared to PA6-F (with 30 wt.%) ranging from approx. 10 to 23% for the PA6 series and approx. 9 to 41% for the PA6/PA10 series. Nanoscratching indicated an increase of coefficient of friction for the treated ash composites compared to PA6-F. The introduction of treated ash waste in the composites provided small changes in thermal stability and melting and crystallization temperatures for both series compared to PA6-F. DMA showed a decrease in stiffness and elastic behavior evaluated by the storage modulus for the ash treated composites compared to PA6-F but an increase in viscous property and weight of the elastic and viscous phase as evaluated by loss modulus and tan delta. This shows an improvement of the viscous properties due to a strong polymer matrix-ash adhesion.



Figure 1. Hardness and reduced modulus for samples with 30% reinforcing agent/treated ash; (a) PA6 series; (b) PA6/PA10 series

Conclusions: For composites with 30% wt. glass fiber and ash waste, a significant improvement in nanomechanical properties was observed and the best results were obtained for PA6-F-CS in series PA6 and PA6-PA10-F-CG in series PA6/PA10. Based on these results, the final composites can have 5 wt.% glass fiber removed and replaced with ash waste without compromising the general properties of materials. *Acknowledgements: The authors gratefully acknowledge the support of the Ministry of Research, Innovation and Digitization through Program 1 - Development of the national research-development system, Subprogram 1.2-Institutional performance-Projects to finance excellence in RDI, Contract no. 15PFE/2021.*

- Petraşcu, O.-L.; Pascu, A.-M. Comparative study of polyamide 6 (PA6) and polyamide 6 reinforced with 30% of glass fiber (PA6GF30). Materials Today: Proceedings 2023, 93, 625-629.
- [2]. Pagacz, J.; Raftopoulos, K.N.; Leszczyńska, A.; Pielichowski, K. Bio-polyamides based on renewable raw materials. J. Therm. Anal. Calorim. 2016, 123, 1225–1237
- [3]. Kasar, A.K.; Gupta, N.; Rohatgi, P.K.; Menezes, P.L. A Brief Review of Fly Ash as Reinforcement for Composites with Improved Mechanical and Tribological Properties. JOM 2020, 72, 2340-2351.

References:

SYNTHESIS OF MULTIFUNCTIONAL SEMI-INTERPENETRATING HYDROGELS BASED ON QUATERNARY AMMONIUM SALTS AND CHEMICALLY MODIFIED NANOCELLULOSE WITH POTENTIAL ANTIBACTERIAL AND ANTIFUNGAL PROPERTIES

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Keywords: hydrogels, bacteria, nanocellulose, semi-interpenetrated materials, antifungal properties

Introduction: The development of advanced wound dressings with efficient antimicrobial properties tailored to specific wound needs presents an intriguing challenge for researchers. However, the requirements for these dressings are stringent, necessitating a delicate balance between inhibiting bacterial growth and compatibility with host tissues. In this context, nanocellulose has garnered attention for its potential in various biomedical applications, although its current limitations diminish its utility as a wound dressing. While initially exploited as a reinforcing agent for various polymer matrices, nanocellulose has rapidly penetrated other applications such as biomedicine, water purification, pharmaceuticals, cosmetics, and food industries^[1]. Despite its attractiveness due to its renewable origin, ability to retain wound exudates, biodegradability, and excellent mechanical strength, nanocellulose remains deficient when applied as a wound dressing due to the absence of antimicrobial and hemostatic activities. On the other hand, interpenetrating and semi-interpenetrating hydrogels (IPN, semi-IPN) are considered promising alternatives for wound care due to their ability to maintain a conducive moist environment for healing and provide structural support. Additionally, IPN hydrogels represent a special category of materials, with enhanced potential due to the unique combination of properties of the constituent polymers. Research in this direction aims to optimize material properties and develop innovative strategies to improve wound care and combat bacterial infections in the current context of increased antibiotic resistance ^{[2][3]}.

Materials and methods: The series of simple and semi-IPN hydrogels based on vinyl benzyl trimethylammonium chloride (VBTAC) and polyethyleneglycol diacrylate (PEGDA700) has been synthesized through radical polymerization process in the presence of nanocellulose that has been chemically modified with various antibacterial agents such as cinnamaldehyde, citric acid and TEMPO catalyzer (2,2,6,6-tetramethypiperidin-1-oxyl).

Results and conclusions: The new semi-IPN materials based on quaternary ammonium salts and modified nanocellulose have been characterized using different techniques such as FTIR, TGA/DTG and SEM. The influence of different modification agents was observed alongside a significant decrease in swelling degree due to higher PEGDA700 crosslinking agent concentration for enhanced mechanical strength. Hydrogels containing NC modified with TEMPO showed maximum swelling of approximately 27%, attributed to interactions between carboxyl groups and the aqueous environment. FTIR spectroscopic analyses revealed characteristic peaks of monomer and crosslinker, but due to their intensity and low NC concentration, specific NC peaks couldn't be differentiated. SEM morphologies depicted irregular porous structures for unmodified NC and evenly porous structures for NC-CINAM, correlating with swelling degree values. NC-Citric samples exhibited potential interaction between carboxyl groups on NC and quaternary ammonium salt groups, resulting in additional crosslinking and a denser final hydrogel structure. By integrating modified NC into the semi-IPN 3D structure, the antibacterial/antifungal potential of the final hydrogels was improved, combining the known properties of the component materials from literature. Efficient antimicrobial activity of the tested products was observed after incubation, evidenced by the presence of growth inhibition zones, both at the contact zone and in the form of a halo around the sample.

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- [1]. Cao, L. Nanocellulose-A Sustainable and Efficient Nanofiller for Rubber Nanocomposites: From Reinforcement to Smart Soft Materials. Polymer Reviews 2022, 62, 549–584.
- [2]. Pradeep, H.K., Role of Nanocellulose in Industrial and Pharmaceutical Sectors A Review. Int J Biol Macromol 2022, 207, 1038–1047.
- [3]. O-chongpian, P., Composite Nanocellulose Fibers-Based Hydrogels Loading Clindamycin HCl with Ca2+ and Citric Acid as Crosslinking Agents for Pharmaceutical Applications. Polymers 2021, 13, 4423.

BIOTOXICOLOGICAL MONITORING OF MICRO- AND NANOPLASTICS IN AQUATIC MODEL DAPHNIA MAGNA

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Keywords: Nanoplastics; Elutriate; Daphnia magna; Polyvinyl chloride; Toxicology

Introduction: During the last decade, the presence of microplastics (MPs) has been reported across the globe, predominantly in water bodies ^{[1][2]}. MPs are particles or fragments whose sizes range from 5 mm (0.19685 in) to 0.1 μ m ^[3]. Below this measured size, it is defined as nanoplastic (NP). Premanufactured MP and NP exposure has been previously recorded in diverse animal models ^[4]. The main objective in this study is to observe and quantify the biotoxicological effects of micro- and nanoplastics in aquatic model *Daphnia magna*.

Materials and methods: Aquatic animal model *Daphnia magna* was exposed to an elutriate containing micro- (5 μ m, 1.9%) and nanoparticles (182 nm, 98.1%), obtained from the grinding process of a Polyvinyl chloride (PVC) sample purchased from a non- regulated mexican market. Ten days old Daphnia groups, were subjected 24 h to a concentration of 570 mg/L.

Results: After trial individuals were monitored, noting a visible lack of energy. Heartbeats and thoracic rhythm observed in exposed groups were much slower than those in the control groups, 77.4% and 71.8% respectively. Afterwards, subjects were subjected to histological studies, where evidence of morphological deformation was discovered. The digestive track of exposed groups presented a lack of microvilli and notable inflammation, being 71.6% more inflamed than the control groups.

Conclusions: The negative effects observed in the acute exposure to an elutriate of micro- and nanoplastics of PVC indicate severe malformations, metabolic alterations, and a disruption of the animal's life cycle. Considering that *Daphnia magna* lays at the base of the food chain, the negative impacts it may suffer could greatly affect its depredators and the overall health of its ecosystem.

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- [1]. Van Sebille E., Wilcox C., Lebreton L., Maximenko N., *et al. A global inventory of small floating plastic debris*. Environ. Res. Lett. 2015;10. DOI:10.1088/1748-9326/10/12/124006.
- [2]. Álvarez-Zeferino J. C., Ojeda-Benítez S., Cruz-Salas A.A, Martínez-Salvador C and Vázquez-Morillas A. *Microplastics in Mexican beaches, Resources. conservation and recycling.* Rev. Int. Contam. Ambie. 2020;155:1-8. DOI: https://doi.org/10.1016/j.resconrec.2019.104633.
- [3]. Yuan Z., Nag R. and Cummins E. Human health concerns regarding microplastics in the aquatic environment-from marine to food systems. Sci. Total Environ. 2022;153730.
- [4]. Kögel T., Bjorøy O., Toto B., *et al. Micro- and nanoplastic toxicity on aquatic life: Determining factors*. Science of the Total Environment, Elservier. 2019; 709:1-16. DOI: https://doi.org/10.1016/j.scitotenv.2019.136050.

HARNESSING IMMOBILIZED LACCASE FOR SUSTAINABLE WATER REMEDIATION

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Keywords: laccase, enzyme immobilization, composite materials, biocatalysis, water cleaning

Introduction: The development of efficient, cost-effective and sustainable water treatment methods is of paramount importance in mitigating the water pollution that became a global concern in the recent years. The use of immobilized enzymes in such application has gained increasing interest due to the biochemical characteristics of enzymes, which make them ideal candidates for greener processes^[1]. Enzymes are proteins of natural origin, are highly efficient in converting specific substrates and are able to successfully reduce the toxicity of polluted water samples by catalyzing the degradation of different classes of pollutants. Moreover, by using immobilized enzymes, an increased economic feasibility can be reached by facilitating their reuse on multiple reaction cycles. In this study, we investigate the catalytic degradation of a synthetic dye using immobilized laccase for potential application in water purification systems.

Materials and methods: The fabrication of the support composite microparticles was achieved by the layer-by-layer deposition of poly(ethylene imine), poly(acrylic acid) or poly(methacrylic acid) on silica microparticles (Daiso Co., Japan), followed by a stabilization/ flexibilization treatment. The dried composite microparticles were used as support for the physical immobilization of laccase and the biocatalysts obtained were employed in water cleaning tests, using indigo carmine (IC) as a model pollutant, in different process conditions.



Figure 1. IC discoloration profile using the immobilized laccase composite

Results: The immobilization of laccase on the core-shell microparticles led to the fabrication of stable composite biocatalysts that could successfully be used in dye degradation tests. The laccase-based composites were able to lead to complete discoloration of an IC-polluted water sample, in about 60 minutes, as observed in Figure 1. Moreover, the laccase-based composite microparticles could be successfully used in 4 water treatment cycles, maintaining more than 95% discoloration efficacy.

Conclusions: The immobilization of laccase onto a suitable support matrix offered several advantages in the usage of the biocatalyst in water cleaning applications, including enhanced stability, reusability, and ease of separation from the reaction medium. Herein, we present some results on the immobilization of laccase on composites based on polyelectrolytes, aiming to optimize the enzymes catalytic performance in dye degradation. The tests performed assessed a very good efficacy of the biocatalyst in dye degradation, corroborated with a satisfactory stability and reusability of the biocatalyst obtained.

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References:

[1] Petrila LM, Grădinaru R., Bucatariu F, Mihai M. Polymer/enzyme composite materials – versatile catalysts with multiple applications. Chemistry2022; 4:1312-133

WELL DISPERSED Ni-Au NANOPARTICLES ON MIXED OXIDE DERIVED-ZnAI LDH AS EFFICIENT CATALYSTS FOR PHOTODEGRADATION OF BISPHENOL A

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Introduction: Nowadays, hazardous contaminants represent a serious environmental and health concern that needs to be resolved urgently. Layered double hydroxides (LDHs) are an important class of lamellar solids, chemically expressed by the general formula $[M^{2+}_{1-x}M^{3+}_{x}(OH)_{2}]^{x+}$ (A^{n-})_{x/n}·mH₂O, where M^{2+} and M^{3+} are divalent and trivalent metal cations, A^{n-} is an anion and $2 \le (1-x)/x \le 4$ ^[1]. These compounds are very attractive due to their outstanding physicochemical properties, as well as their environment-friendly preparation and cost–effectiveness. An interesting way to obtain mixed oxides catalysts is through the use of LDHs as precursors ^[2]. Indeed, after a calcination treatment, mixed oxides with unique properties such as high specific surface area, good stability and homogeneity of cations are obtained. (A promising way to increase) One promising route to boost the photocatalytic activity of LDHs-derived mixed oxides is to decorate its surface with well-controlled nanoparticles (NPs). This study focuses on the development of LDH-derived mixed oxide supported NPs and their detailed characterization. The synthesized materials were investigated as efficient catalysts for the photocatalytic degradation of Bisphenol A (BPA) as a model pollutant molecule.

Materials and methods: First, mono- (Ni, Au) and bimetallic (Ni-Au) NPs protected by PVP (polyvinylpyrrolidone) were prepared by the alkaline polyol method. The precursors used for the synthesis of NPs were Ni(NO₃)₂*6H₂O (2*10⁻²M) and HAuCl₄*2H₂O and PVP (M.W. 8000 0.2M). The preparation protocol is described in detail in a previous publication [3]. ZnAl-LDH was prepared by coprecipitation method at constant pH (9.5), using the corresponding metal nitrates in a ratio of $M^{2+}/M^{3+} = 3/1$ and an aqueous precipitation solution of NaOH (1 M) and Na₂CO₃ (0.2 M). The precipitate was stirred and aged at 75 °C for 12 h. The obtained solid was further washed with deionized water until pH 7 was reached and dried at 110 °C for 12 h before the calcination at 650 °C for 6 h in an air atmosphere. Well-dispersed nanoparticles (NPs) deposited on ZnAl oxides issued from LDH precursors were obtained by dispersing the colloidal nanoparticles on the ZnAlO_x-support. The catalytic materials were dried at 100°C for 4 h and then calcined at 400°C for 1 h to burn off the PVP protective polymer.

Results: The obtained materials were characterized by X-ray diffraction, UV-Vis, DRIFT-ATR spectroscopies and H_2 -TPR and CO chemisorption measurements. The photocatalytic ability of original ZnAlO_x and NPs –modified ZnAlOx was investigated for the photocatalytic degradation of BPA reaction The effect of immobilization of NPs was also investigated.

Conclusions: Mono- (Au, Ni) and bimetallic (Au-Ni) NPs-dispersed on ZnAl-mixed oxides derived-LDH precursors were successfully synthesized. The obtained materials were characterized and tested for the photocatalytic degradation of BPA from wastewater.

- Cavani F., Trifiro F., Vaccari A. Hydrotalcite-type anionic clays: Preparation, properties and applications. Catal. Today1991; 11: 173–301.
- [2]. Peng D., Zhang Y. Engineering of mixed metal oxides photocatalysts derived from transition-metal-based layered double hydroxide towards selective oxidation of cyclohexane under visible light. Appl Catal A 2023; 653: 119067.
- [3]. Papa F., Negrila C., Miyazaki M., Balint I., "Morphology and chemical state of PVP-protected Pt, Pt-Cu, and Pt-Ag nanoparticles prepared by alkaline polyol method" Journal of Nanoparticle Research: 13(10), 5057-5064,2010

SYNTHESIS OF PVC BIO-COMPOSITE MEMBRANE USING CHITOSAN FOR BLOOD BAG APPLICATION

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Keywords: PVC-bio composite; Chitosan; Blood Bag.

Introduction: Safe storage of blood is a big problem now a days.^[1] The composites have been developed by the addition of certain plasticizers to PVC.^[2] But a lot of problems were associated with the storage including chemical and bacterial contamination. So, there is need of blood bag having antibacterial properties.^[3]

Material and methods: In this research the objective is to find the effect of chitosan concentration on hemolysis of blood. Chitosan based PVC-THF bio composites with different concentration of chitosan was prepared and characterized by using tensile strength and hemolysis.

Results: There was remarkable increase in the force required to break composite and has high tensile strength. The hemolysis percentage was also found to be less, making this composite to be a suitable candidate for its application as blood bag.

Chitosan Concentration w/v (%)	Force Peak kN	Elongation Peak mm	Stress Peak N/mm2	Strain Peak (%)	Strain Break (%)	Width Width/mm	Thickness mm	Tensile Strength N/mm2
0.5	25.7	0.365	0.496	0.884	13.89	37.0	1.4	18.7
0.7	67.4	0.679	3.876	1.523	1.954	37.0	0.47	49.2
1	28.7	1.038	7.401	2.75	2.771	37.0	0.47	94

Table 1: Tensile Strength Test of PVC-THF-Chitosan Bio composite Membranes

Conclusion: The Chitosan-THF-PVC composite was tested by using tensile strength and hemolysis test. The tensile strength shown remarkable increase from 18.7 N/mm² to 94 N/mm² by increasing the concentration of chitosan. The hemolysis test also shows that by increasing chitosan concentration, the hemolytic activity decreases, making the composite a suitable candidate to be used as material for manufacture of blood bag

- [1]. Chiellini, E., S. D'Antone, and R. Solaro. *Biodegradable synthetic and semisynthetic polymers*. in *Macromolecular Symposia*. 1997. Wiley Online Library.
- [2]. Hacker, M.C., J. Krieghoff, and A.G. Mikos, *Synthetic polymers*, in *Principles of regenerative medicine*. 2019, Elsevier. p. 559-590.
- [3]. Saeki, Y. and T. Emura, *Technical progresses for PVC production*. Progress in polymer science, 2002. **27**(10): p. 2055-2131.

AMYLOPECTIN-GRAFT-POLY(N-ISOPROPYLACRYLAMIDE) COPOLYMER

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Keywords: Polysaccharides, Amylopectin, Thermoresponsive polymer, Poly(n-isopropylacrylamide)

Introduction: Amylopectin (AMP) is a highly branched polysaccharide linked by α -(1,4) and α -(1,6)-glycosidic bonds and is one of the major components found in starch granules (75–85%)^[1,2]. Amylopectin has higher molecular weight, is inexpensive and has excellent biocompatibility and biodegradability^[2,3]. Poly(N-isopropylacrylamide) (PNIPAM) is a thermoresponsive synthetic polymer with a low critical solution temperature (LCST) in the range of 31 - 33°C. The change of its hydrophilic interactions takes place between the room temperature and body temperature, making it a promising polymer for the medical field. Due to its low biodegradability and considerable biocompatibility PNIPAM is widely used with polysaccharides for the development of materials/hydrogels suitable for biomedical applications^[4,5].

Materials and methods: The amylopectin-*graft*-poly(N-isopropylacrylamide) copolymer (AMP-*g*-PNIPAM) has been synthesized by the "*grafting to*" technique which is based on the anchoring of synthetic homopolymer macromolecular chains to polysaccharides via coupling interactions where potassium persulphate was used as the radical initiator. Amylopectin was solubilized in two solvents, dimethylsulfoxide (DMSO) and (EtOH):NaOH 10%:H₂O (1:2:10). The obtained AMP-*g*-PNIPAMs were purified by dialysis and freeze-dried. FTIR and ¹H NMR spectroscopies were performed to confirm the structure of grafted copolymers.

Results: The stucture of the AMP–g–PNIPAM copolymers (Figure 1) was confirmed by both spectroscopic methods, FTIR and ¹H NMR. The degree of substitution of copolymers was determined by ¹H-NMR spectroscopy (31.69% for AMP solubilized in EtOH:NaOH10%:H₂O and 19.72% for AMP solubilized in DMSO).



Figure 1. Synthesis of Amylopectin-graft-poly(N-isopropylacrylamide) (AMP-g-PNIPAM)

Conclusions: The grafting of PNIPAM chains onto amylopectin was successfully achieved. The highest degree of substitution was obtained in the case of amylopectin solubilized in EtOH:NaOH 10%:H₂O (1:2:10).

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- [1]. Bergthaller W, Hollmann J, Starch. In: Kamerling, H(Editor), Comprehensive Glycoscience, 2007; pp. 579-612.
- [2]. Sarkar AK, Mandre NR, Pandac AB, Pal S. Amylopectin grafted with poly (acrylic acid): Development and application of a high performance flocculant. Carbohydrate Polymers. 2013; 95, 753–759.
- [3]. Bazoubandi B, Soares JBP. Amylopectin-graft-polyacrylamide for the flocculation and dewatering of oil sands tailings. Minerals Engineering. 2020; 148: 106.
- [4]. Fan Y, Boulif N, Picchioni F. Thermo-Responsive Starch-g-(PAM-co-PNIPAM): Controlled Synthesis and Effect of Molecular Components on Solution Rheology. Polymers. 2018; 10(1), 92.
- [5]. Conzatti G, Cavalie S, Combes C, Torrisani J, Carrere N, Tourrette A. PNIPAM grafted surfaces through ATRP and RAFT polymerization: chemistry and bioadhesion. Colloids and Surfaces B: Biointerfaces. 2017; 151 143–155.

A GREEN AND ECONOMIC APPROACH TO SYNTHESIZE MAGNETIC *LAGENARIA SICERARIA* BIOCHAR (γ-Fe₂O₃-LSB) FOR DYE REMOVAL FROM WASTEWATER

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Keywords: Magnetic Biochar, Wastewater remediation, Adsorption, Methylene Blue

Introduction: In the printing and textile industry, methylene blue (a cationic-azo dye) is commonly used. MB is a well-known carcinogen and another major issue is its high content in industrial discharge (Vigneshwaran et al. 2021). There are numerous removal methodologies have been employed to remove it from industrial discharge however, these current modalities have one or more limitations. Many textile companies in India use synthetic dyes, which are typically derived from petrochemicals. These dyes can contain toxic substances such as heavy metals, formaldehyde, and aromatic compounds, which threaten both human health and the environment. Toxic pollutants released into water bodies disrupt the balance of aquatic flora and fauna, which affects fishes, and marine organisms, and causes biodiversity loss as well (Kim et al. 2017). The goal of the current investigation was to obtain the maximum adsorption capacity of γ -Fe₂O₃-LSB. We also examined the kinetics of the sorption process, isotherms equilibrium, and thermodynamic factors to better understand equilibrium properties and the mechanism followed in the sorption process.

Materials and methods: The synthesized γ -Fe₂O₃-LSB was characterized using FTIR, X-ray diffraction, Raman, SEM-EDX, BET, and VSM. The batch adsorption process was performed to analyze the adsorptive removal of MB dye using γ -Fe₂O₃-LSB. The adsorption efficiency of γ -Fe₂O₃-LSB for MB was analyzed by varying parameters like initial concentration of adsorbate (MB), γ -Fe₂O₃-LSB dose, pH effect, contact time, and temperature (Hassaan et al. 2023)(Belcaid et al. 2022).

Results: The non-linear Langmuir model fitted the best to explain the adsorption isotherm mechanism and resulting adsorption capacity ($q_e = 54.55 \text{ mg/g}$). The thermodynamics study showed the spontaneous and endothermic nature and pseudo-second-order rate kinetics was followed during the adsorption process. Regeneration study showed that γ -Fe₂O₃-LSB can be used up to 4 cycles.



Fig:1 Graphical representation of the work.

Conclusions: The results obtained suggest that magnetic *Lagenaria siceraria* biochar, which is economical and efficient, can be used as a potential biochar material for industrial applications in the treatment of wastewater.

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- [1]. Belcaid A, Beakou BH, Bouhsina S, Anouar A (2022) Insight into adsorptive removal of methylene blue, malachite green, and rhodamine B dyes by cassava peel biochar (Manihot esculenta Crantz) in single, binary, and ternary systems: competitive adsorption study and theoretical calculations. Biomass Convers Biorefinery. <u>https://doi.org/10.1007/s13399-022-02928-w</u>
- [2]. Hassaan MA, Yılmaz M, Helal M, et al (2023) Isotherm and kinetic investigations of sawdust-based biochar modified by ammonia to remove methylene blue from water. Sci Rep 13:1–20. <u>https://doi.org/10.1038/s41598-023-39971-0</u>
- [3]. Kim H, Watthanaphanit A, Saito N (2017) Simple Solution Plasma Synthesis of Hierarchical Nanoporous MnO2 for Organic Dye Removal. ACS Sustain Chem Eng 5:5842–5851. <u>https://doi.org/10.1021/acssuschemeng.7b00560</u>
- [4]. Vigneshwaran S, Sirajudheen P, Karthikeyan P, Meenakshi S (2021) Fabrication of sulfur-doped biochar derived from tapioca peel waste with superior adsorption performance for the removal of Malachite green and Rhodamine B dyes. Surfaces and Interfaces 23:. <u>https://doi.org/10.1016/j.surfin.2020.100920</u>

PHARMACOLOGICAL AND POLAROGRAPHIC STUDY OF MODIFIED Cu-Atropine MOLECULE

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Keywords: Atropine, Polarography, DCP, DPP, anesthetic drug, in vivo study

Introduction: An analytical chemists solve their chemical analysis problems quantitatively and qualitatively by making use of some instrumentation techniques, like polarography, pH metering, spectroscopy etc. Past three decades have witnessed a wider use of electroanalytical techniques for the study of metal complexes in solution. For metal ligand system it is possible to determine the degree of formation, distribution and stability constants of all species

present. Polarography, finds an extensive use in the determination of various organic and inorganic depolarizers present even in micro to ultra micro quantity.

Materials and methods: All the chemical used were of Himedia/BDH/CDH grade. The sulphate of Cu²⁺ was used. Double distilled water was used to prepare all the solutions. Stock solution of 1M Borate buffer and .01M Atropine was prepared in double distilled water and alcohol.

Experimental sets were prepared by keeping overall metal ion and supporting electrolyte (borate buffer) concentrations fixed at 1.0mM and 1.0M respectively. The pH of the solution was adjusted to 8.2 ± 0.1 . Necessary amount of boric acid and sodium Hydroxide solution was used to adjust the pH of test solutions.

Results: Atropine and its complexes gave well-defined cathodic reduction wave at $pH = 8.2\pm0.1$ in 1M Borate buffer. The plots of i_d vs $\sqrt{h_{corr}}$ yielded straight lines in each case, passing through the origin confirming the diffusion controlled nature of the reduction process.

Conclusions: The observed analytical data clearly speaks the formation of complex form of the drug (Cu-Atropine) in 1:1 ratio in each case.

Results of pharmacological study on the anesthetic activities of above systems showed that the modified drug complex is found to be more potent than parent atropine drug.

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- [1]. Weinberg, G. L., Ramaraju, G. A., Garcia-Amaro, M. F., Cwik, M. J., "Pretreatment or resuscitation with a lipid infusion shifts the dose-response to bupivacaine-induced asystole in rats", Anesthesiology. 88: 1071-5,1998
- [2]. Picard, J., Meek, T., "Lipid emulsion to treat overdose of local anaesthetic: the gift of the glob", Anesthesia. 61:107-9, 2006
 [3]. Rang, H. P., Dale, M. M., Ritter, J. M., Flower, R. J., "Rang and Dale's Pharmacology", Elsevier Churchill Livingstone, 153, 2007
- [4]. Latifa, Rabi., Adnane, Moutaouakkil., Mohamed, Blaghen., "<u>Ionophoric properties of atropine: complexation and transport of Na⁺, K⁺, Mg²⁺ and Ca²⁺ ions across a liquid membrane", Natural Product Research: Formerly Natural Product Letters, 1478-6427, 22(6), 547–553,2008.</u>

BATCH AND COLUMN SORPTION STUDY OF HEAVY METAL IONS REMOVAL

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Keywords: batch study; fixed-bed column study; heavy metal removal; composite sorbent.

Introduction: Lead, as well as other heavy metals, became a common pollutant due to its extensive use in various industries. Even in small concentrations, lead causes extreme toxicity towards marine and fresh water organisms and has been linked with certain human cancers ^[1]. To diminish this threat and to retain this Pb²⁺ from wastewater, new innovative sorbents has been designed last years. A composite sorbent of a silica core (IS) and a polyelectrolyte coacervate shell have been proposed as an effective material for heavy metal ions immobilization ^[2]. Thus, the main objective of this study was to investigate the adsorption performances of the sorbent in industrial application mode by fixed-bed column experiments, and also in batch experiments.

Materials and methods: The sorbent was obtained by one-pot coacervate deposition approach, where polyethyleneimine (PEI) and polyacrylic acid (PAA) macromolecules have been in-situ precipitated onto the inorganic substrate (IS) as coacervate (PEI/PAA)_c. The in-situ precipitation of the coacervate was followed by a chemical cross-linking reaction in the presence of glutaraldehyde (GA) at a molar ratio $r = [CHO]:[NH_2] = 0.1$, and then the polyanion extraction in strong basic medium. After polyanion extraction more space is created inside the crosslinked shell, therefore the accessibility of active groups for sorption is increased ^[3]. The heavy metal ions sorption properties of IS/(PEI-PAA)_c composite microparticles were investigated through static and dynamic experiments. The Pb²⁺ sorbed amount at equilibrium (q, mg/g) was determined by using the following equation:

 $q = (C_0 - C_e) \cdot V/m$

where, C_0 and C_e are the initial and equilibrium concentrations of Pb²⁺ solution (mg/L), respectively; V = volume of supernatant or collected fraction (mL); m = amount of IS/(PEI/PAA)_c (mg). In dynamic column experiments, the initial and equilibrium concentrations were replaced by influent and effluent concentrations of Pb²⁺ solution, determined by atomic absorption spectroscopy (contrAA 800, Analytik Jena, Germany). The desorption experiments was carried out with HNO₃ (1 M). Before reusing the material in other sorption cycle, the activation of sorbent material has been carried out with NaOH (1 M) solution. **Results**: The results of the adsorption experiments show good sorption capacities for both methods, batch and fixed-bed column sorption. Nevertheless, the composite sorbent capacity for Pb²⁺ ions was four time higher for dynamic column experiments (21.87 mg/g) than for batch experiments (5.66 mg/g). This means that fixed-bed column experiments can provide applicability for real scenarios, addressing environmental concerns related to heavy metal contamination of industrial effluents. The breakthrough curve was plotted and analyzed for fixed-bed sorption column performance assessment and the Pb²⁺ ions concentration at equilibrium was fitted with Langmuir isotherm.

Conclusions: The successful immobilization of Pb^{2+} in IS/(PEI-PAA)_c composite microparticles was achieved for both batch and fixed-bed column methods. The fixed-bed column adsorption method presented as an effective alternative for the removal of heavy metals from aqueous solutions for real wastewater systems.

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- [1]. Michalczyk K., Kupnicka P., Witczak G., Toutsy P., Bosiacki M., Kurzawski M., Chlubek D., Cymbaluk-Ploska A. Assessment of Cadmium (Cd) and Lead (Pb) Blood Concentration on the Risk of Endometrial Cancer. Biol. 2023;12:717.
- [2]. Fighir D., Paduraru C., Ciobanu R., Bucatariu F., Plavan O., Gherghel A., Barjoveanu G., Mihai M., Teodosiu C. Removal of Diclofenac and Heavy Metal Ions from Aqueous Media Using Composite Sorbents in Dynamic Conditions. Nanomaterials. 2024;14:33.
- [3]. Morosanu I., Paduraru C., Bucatariu F., Fighir D., Mihai M., Teodosiu C. Shaping polyelectrolyte composites for heavy metals adsorption from wastewater: Experimental assessment and equilibrium studies. J. Environ. Manage. 2022;321:115999.

Co(II) AND Ni(II) COORDINATION COMPOUNDS WITH THIOUREIDE LIGANDS: SYNTHESIS, CHARACTERIZATION, AND BIOLOGICAL ACTIVITY

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Keywords: cobalt and nickel complexes, thioureide ligands, molecular structures, biological activity

Introduction: Heteroatom-containing compounds are biologically active, and they are building blocks for various drug molecules ^[1]. Due to the presence of heteroatoms (N, S and O) in the thioureide-type ligands, their corresponding complexes have a variety of biological functions and are largely used in the field of medicinal chemistry ^[2].

Materials and methods: The Co(II) and Ni(II) complexes with thioureide-type ligands from 2-thiophene carboxylic acid were synthesized. All the compounds were characterized spectrally and structurally in solid state. Molecular structures were determined by single-crystal X-ray diffraction with a Rigaku XtaLAB Synergy S diffractometer using SHELT-2018. The IR spectra were obtained in the range of 4000-400 cm⁻¹ on a Bruker Fourier Transformance Tensor V-37 spectrophotometer, using OPUS software and KBr as reference. The electronic spectra of the compounds in the solid-state were recorded using the UV-Vis-NIR Jasco V670 spectrophotometer, equipped with Spectra Manager software.

Results: In the present study, several compounds were obtained in the reaction of Co(II) and Ni(II) salts with the ligands derived from different thioureides. The ligands were synthesised previously by a multisteps process. All compounds were characterized in the solid state by spectroscopic techniques (IR, UV-Vis) and single crystal X-ray diffraction analysis. The molecular structures of ligands and their complexes were determined. The *in vitro* antimicrobial activity of the 2-thiophene carboxylic acid thioureides was evaluated through a qualitative screening of the susceptibility spectra of different microbial strains, Grampositive: Staphylococcus aureus, Bacillus subtilis, Gram-negative: Pseudomonas aeruginosa, Escherichia coli, Klebsiella pneumoniae, as well as Candida albicans and Aspergillus niger, using both reference and clinical, multidrug resistant strains. We are now in the process of evaluating the biological activity of the obtained complexes.

Conclusions: The influence of metal ion on the topology of the obtained coordination compounds with different ligands, as well as on the biological activity of these compounds are evaluated. The biological activity of all obtained compounds and a detailed comparison with ligands are under investigation.

- [1]. Singh, D.P.; Gangwar, M.; Kumar, D.; Nath, G.; Pratap, S. Synthesis, spectroscopic characterization, crystal structure, antimicrobial and in vitro hemolytic studies of some novel substituted thiourea derivatives. J. Chem. Crystallogr. 2013, 43, 610.
- [2]. Saeed, S.; Rashid, N.; Jones, P.G.; Ali, M.; Hussain, R. Synthesis, characterization, and biological evaluation of some thiourea derivatives bearing benzothiazole moiety as potential antimicrobial and anticancer agents. Eur. J. Med. Chem. 2010, 45, 1323

PHOSPHATIC NANOBIOMATERIALS WITH METAL-OXIDE HETEROJUNCTIONS -PHOTOCATALYSTS FOR WASTEWATER TREATMENT

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Keywords: phosphatic materials, photocatalysis, organic pollutants, dyes, depollution

Introduction: A widespread issue confronting the global scientific community is the persistent pollution of water resources due to ongoing industrial and agricultural expansion, alongside other human activities. The main goal of the study was to develop an innovative technology for the elimination of organic pollutants, especially dyes, coming from various effluent-generating industries, using a phosphatic nanobiomaterial with photocatalytic properties, obtained from natural resources, namely wastes mussel shells, through modifying its surface with different metal oxides.

Materials and methods: The specific objectives proposed for the implementation of the study were: 1) synthesis and characterization of the phosphate nanobiomaterials with the aim of using them as photocatalysts with metal-oxide heterojunctions. 2) optimization of the synthesis parameters and the photocatalytic process; 3) demonstration of the efficiency of the obtained nanobiomaterials in the treatment of waters contaminated with organic pollutants (especially dyes); 4) choosing the nanobiomaterial with the highest efficiency in the depollution process.



Figure 1. Schematic illustration of the proposed objectives of the study.

Results: The efficiency of the nanobiomaterials proposed for the depollution process was demonstrated, involving minimal resources, thus facilitating the development of the bioeconomy. Also, the study supported increasing the visibility of institutional research internationally, by publishing 2 papers in ISI indexed journals with factor ≥ 1 , participating in 5 international conferences, participating in invention fairs, submitting a patent application and developing a pHd thesis, thus capitalizing on the quality of the research results.

Conclusions: The study, covering a period of 12 months, provided great outcomes in terms of organic pollutants content removal from wastewater. Meanwhile, it led to the full achievement of the proposed targets, enhancing the value through the dissemination of the obtained research results.

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- Natural and Natural-Based Polymers: Recent Developments in Management of Emerging Pollutants. Fierascu, R.C., Fierascu, I., Matei, R.I., Manaila-Maximean, D. Polymers, 2023, 15(9), 2063
- [2]. Removal of phenol and non-steroidal anti-inflammatory drugs from water matrices using doped hydroxyapatite. Matei (Brazdis), R.I., Avramescu, S.M., Baroi, A.M., Fistos, T., Fierascu, I., Raduly, F.M., Fierascu, R.C., Scientific Bulletin Series B: Chimie şi Ştiinţa Materialelor (Submitted for publication)
- [3]. Patent application A-00444/2023 Organic/Inorganic composite material for the adsorption of heavy metals from aqueous solutions and procedure for obtaining it – Matei (Brazdiş), R.I., Fierăscu, R.C., Baroi, A.M., Fistoş, T., Fierăscu, I., Chican, I.E., Hosu, I.S.

SYNTHESIS AND CHARACTERIZATION OF NEW COPPER(II) SCHIFF BASE COMPLEXES WITH POTENTIAL ANTICANCER ACTIVITY

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Keywords: Schiff base ligands; copper complexes; synthesis and characterization; biological activity

Introduction: The fundamental role of copper and its complexes as bioactive compounds has sparked growing interest in using them as potential therapeutic drugs for various diseases [1]. Schiff base ligands are appealing to researchers because of their excellent coordination tendency with a wide range of metals and their significant applications in chemotherapy and antibacterial treatments. Copper(II) complexes with Schiff base ligands revealed promising potential for antibacterial, antifungal, antioxidant, and anticancer activity [2].

Materials and methods: Reagents and solvents used for the synthesis of the complexes were purchased from Sigma-Aldrich, being characterized by high purity. The compounds were characterized spectrally and structurally in solid state. The elemental analysis was performed using the Euro EA Elemental Analyzer (Euro Vector) and Callidus software. Molecular structures were determined by single-crystal X-ray diffraction with a Rigaku XtaLAB Synergy S diffractometer using SHELT-2018 and Diamond 3.2 software for calculations and graphical representations. IR spectra were recorded on a Bruker Fourier Transformance Tensor V-37 spectrophotometer, using OPUS software. Solid-state electronic spectra were recorded using the UV-Vis-NIR Jasco V670 spectrophotometer, equipped with Spectra Manager software.

Results: The salen-type Schiff bases are ligands obtained from salicylaldehyde or its derivatives and different diamines. They usually consist of rigid aromatic rings and flexible aliphatic chains. In this study, the Shiff base ligands were obtained from aromatic aldehydes, such as ortho-vanillin, salicylaldehyde and its halogenated derivatives, in reaction with 1,3-diaminopropane. Their corresponding Copper(II) complexes were obtained from different Copper(II) salts. The complexes were synthesized in a step-wise manner without the isolation of the Schiff base ligands. All compounds were characterized in their solid state by elemental analyses and spectroscopic techniques (IR, UV-Vis), as well as single crystal X-ray diffraction analysis. The crystal structures of the resulting compounds have been determined and the biological activity of the compounds is under investigation.

Conclusions: All the copper complexes with Schiff base ligands have been designed, synthesized and adequately characterized using various spectroscopic techniques. We anticipate that this work will provide new insight for potential applications of copper(II) complexes with Schiff base ligands as anticancer compounds.

- Osman, A., Hassan, A., Importance of the Applicability of O-Vanillin Schiff Base Complexes: Review. Advanced Journal of Chemistry-Section A. 2021, 4, 87.
- [2]. Keshavarzian, E., Asadi, Z., Kucerakova, M., Dusek, M., Rastegari, B., DNA interaction and BSA binding of O-vanillinbased new Schiff base Co(III) and Ni(II) complexes: Theoretical, experimental, antibacterial and anticancer studies, Polyhedron, Volume 223, 2022, 115987.

NITROGEN DOPED GRAPHENE: A REVIEW

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Keywords: Nanomaterial; graphene; doped graphene; futuristic material

Introduction: Graphene is a carbon nanomaterial known for its exceptional electrical and optical properties. After the successful exfoliation, it has been an highly researched topic ^[1]. Due to the 2-dimensional structure it provides a high surface area for further application in numerous fields. Graphene stands as a material of future and is highly potent nanomaterial. To further increase the potential of graphene, various compounds, molecules and atoms are added to it. This forms the doped graphene with improved set of properties and applications. Nitrogen doped graphene is formed by a similar addition and has been studied for its application in fuel cells, supercapacitors, sensors etc. ^[2]. Various strategies have been adopted for the mixing and production of N doped graphene ^[3]. The source of renewable energies such as solar cells, supercapacitors and batteries are the fields of doped graphene application ^{[4][5]}. This will also reduce our dependence on fossil fuels for energy production

Conclusions: As already stated, graphene holds the place in future due its exceptional properties. Further improvement in the properties of it, with the help of doping has increased its value in numerous fields. An easier pathway for obtaining good yield is required to boost the application of doped graphene. A review helps understand the future possibility of proposing a better pathway of synthesis and production.

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- [1]. Xu H, Nitrogen doped graphene: synthesis, characterisations and energy applications, Journal of Energy Chemistry, 2018,27 (1), 146-160.
- [2]. Vessel A, A review of strategies for the synthesis of N doped graphene like materials, Nanomaterials, 2020, 10(11)
- [3]. Ullah S. et al. Advances and Trends in chemically doped graphene, Advances Materials Interfaces, 2020, 7(24).
- [4]. Jun Lee S. et al., Heteroatom doped graphene-based materials for sustainable energy applications: A review, Renewable and sustainable Energy Reviews, 2021, 143.
- [5]. Bie C et. al. Design, Fabrication and Mechanism of Nitrogen Doped Graphene Based photocatalyst, Advanced Materials ,2021, 33(9).

REVIEW ON A NEW RANGE OF POLYMERS

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Keywords : Plastics; Nano polymers; Polymer Concrete; biomedical application; Specialty polymers; Liquid Crystal Polymers (LCPs);Hydrogels; Smart Polymers

Introduction: Plastics have become an indispensable part of our global society and are used in a wide variety of applications, including packaging, building/construction, transportation, consumer products, textiles, medicine, and electronics. They are strong, lightweight, durable, chemically resistant, mouldable, and low in cost and are used in thousands of products that add comfort, convenience, and safety to our everyday lives. Over the past two decades, global plastic production has more than doubled and the production rate in 2018 reached more than 400 million metric tons (MTs) per year. Single-use packaging accounts for approximately 40% of all plastics globally produced and contribute to 47% of the plastic waste produced. There is a wide range of Nano polymers and speciality polymers which can resolve the problems of increasing pollution. These special class of polymers are currently used in the diversified fields like medicine, space, manufacturing and infrastructure etc.

Materials and methods: As the presented paper is a review paper so the content was selected by the study of many research papers and websites.

Results: This review paper give us a brief introduction of different types of polymers like speciality polymers, dendritic polymers, Nano polymers and hydrogels etc. These polymers have multiple uses in daily use, space engineering and biomedical application.

Conclusion: This review presents the overall view for the reuse of polymer and also multiple fields where polymers can be used. Polymers are very important part of our livelihood so we cannot imagine our lives without them. We can only utilize them with consciousness and can protect our environment.

- Vega, Daniel and Villar, Marcel A., Thermogravimetric analysis of starch based biodegradable blends, Polymer Bulletin, 1996,37, 229-235.
- [2]. Chandra, R. and Rastogi, Renu , Biodegradable polymers, Progress in Polymer science, 1998, Vol 23, 1273-1335.
- [3]. Barikani,M. and Mohammadi ,M., Synthesis and characterization of starch modified polyurethane , Carbohydrate Polymers, 2007, 68 , 773-780 .
- [4]. Polymer, www.britannica.com, 2022.
- [5]. Polymer, https://en.m.wikipedia.org/wiki/Polymer ,2022.

NANOTEXTURED STAINLESS STEEL FOR ANTIFUNGAL APPLICATIONS

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Abstract: Drug-resistant fungal infections are a growing concern due to their increasing prevalence and the limited availability of effective antifungal treatments, posing a significant challenge in healthcare and public settings. Transmission of drug-resistant fungal infections through surface contact has resulted in 1.7 million deaths in 2022, particularly through surfaces such as stainless steel which is susceptible to the transmission of fungal infections. To address this issue, it is crucial to prevent fungal adhesion to a metallic surface and control its proliferation. However, conventional methods to inhibit the spread of fungal growth are manual disinfection of the areas in the facilities, which may produce chemical resistance in microorganisms, making them more resilient. Recently, the Centers for Disease Control and Prevention (CDC) reported a high transmission rate of drug-resistant Candida auris which caused a 21% in-hospital mortality rate in 2022. Therefore, a physical method of killing through surface contact could be advantageous against drug-resistant fungi. In our previous study, we demonstrated the application of nanotextured steel (nSS) for inhibiting bacterial adhesion and their cytocompatibility with mammalian cells. In this study, we are investigating the fabrication of nSS using an electrochemical etching technique and their application to eliminate fungal adhesion such as Candida albicans. The damage to the cell membranes of the fungus will be studied using microscopic observations such as scanning electron microscopy (SEM), atomic force microscopy (AFM), transmission electron microscopy (TEM), and confocal microscopy. Our preliminary results indicate the "spike-like" structure in nSS which may physically damage fungal cell membranes upon contact, generate reactive oxygen species (ROS) and hydrophobic behavior, contributing to the inhibition of fungal growth. Overall, nSS holds potential as a promising solution to various metallic surfaces such as stair and door frames encountered in daily life.

Drug-resistant fungal infections are a growing concern due to their increasing prevalence and the limited availability of effective antifungal treatments, posing a significant challenge in healthcare and public settings. Thus, it is crucial to prevent fungal adhesion to a metallic surface and control its proliferation. However, conventional methods are manual disinfection, which may produce chemical resistance in microorganisms. Therefore, a mechanical method to eliminate could be advantageous against drug-resistant fungi. Previously, we demonstrated the use of nanostextured steel with "spike-like" topology to damage bacterial cell membrane and prevent adhesion. Now we are investing the impact on fungi like *Candida albicans* and *Fusarium oxyporum*. The effects were studied using microscopies like scanning electron microscopy (SEM), atomic force microscopy (AFM), transmission electron microscopy (TEM), and confocal microscopy. Overall, nSS holds potential as a promising solution to various metallic surfaces such as stair and door frames encountered in daily life.

EXPLORING THE IMPACT OF SINTERING TREATMENTS ON THE CHARACTERISTICS OF SOL-GEL SYNTHESIZED WALSTROMITE

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Keywords: walstromite, factorial sintering experiment, crystalline phases, porosity, cell viability

Introduction: In the field of medical innovations biomaterials have emerged as groundbreaking tools with the potential to revolutionize healthcare. Within this realm, calcium silicates have attracted considerable attention due to their distinctive properties and wide-ranging applications^[1]. In this work, the main focus was on the study of walstromite compound which is a barium calcium silicate belonging to the cyclosilicate group with the structural unit consisting of simple rings of three tetrahedra of $[Si_3O_9]^{6-}$. Its chemical formula is BaCa₂Si₃O₉ and it has a triclinic crystal structure^[2]. The walstromite powder was obtained by sol-gel synthesis and after that the impact of sintering treatments on its characteristics (crystalline phases, microstructure, density, biological properties) were evaluated following the conditions of a factorial sintering experiment.

Materials and methods: In this study, $BaCa_2Si_3O_9$ walstromite powder was synthesized by sol-gel method using nitrate salts of barium and calcium and TEOS (tetraethyl orthosilicate) as raw materials. The walstromite powder underwent uniaxial hydraulic pressing into pellets, followed by sintering. To determine the optimal sintering conditions, a factorial sintering experiment was planned and conducted. Special attention was paid to the structural transformations or deformations and morphological properties of the material following these heat treatments, aiming to select the best sintering conditions for obtaining a material suitable for subsequent processes. Additionally, preliminary tests were performed to assess the biocompatibility of the sintered material under various temperature and time conditions.

Results: Following sintering, all pellets expanded and became highly porous, displaying a typical appearance of ceramic scaffolds. Based on the information provided by the factorial experiment, the optimal sintering conditions for the BaCa₂Si₃O₉ material were determined as follows: sintering temperature -1000°C, sintering time - 4 hours, sintering rate -10° C/min. SEM microscopy results revealed that a higher heating rate leads to increased porosity. Characterization of the samples by X-ray diffraction highlighted an increase in the number of secondary phases with the increase in sintering temperature. Additionally, at 1000°C, the presence of walstromite was identified alongside the major phase of Ba_{1.55}Ca_{0.45}SiO₄. In vitro tests demonstrated that HEK293T cells adhere to the analyzed materials, and cellular aggregates tend to incorporate fine particles detached from the biomaterials.

Conclusions: Using the sol-gel method, walstromite powder was obtained and subsequently examined to assess the influence of sintering treatments on its properties. The analysis results highlighted the optimal conditions for achieving the necessary properties of the compound in bone regeneration applications. Also, based on the biological test performed the analyzed materials exhibit biocompatibility and have potential for further development and improvement by reducing the alkalizing effect on the culture medium.

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References:

- Yin, H.; Yang, X.; Peng, L.; Xia, C.; Zhang, D.; Cui, F.; Huang, H.; Li, Z. Trends of Calcium Silicate Biomaterials in Medical Research and Applications: A Bibliometric Analysis from 1990 to 2020. Front Pharmacol 2022, 13, doi:10.3389/fphar.2022.991377.
- [2]. Krzątała, A.; Krüger, B.; Galuskina, I.; Vapnik, Y.; Galuskin, E. Walstromite, Baca2(Si3o9), from Rankinite Paralava within Gehlenite Hornfels of the Hatrurim Basin, Negev Desert, Israel. Minerals 2020, 10, doi:10.3390/min10050407.

Fig.1 SEM micrograph of the samples sintered at 1000°C



NANOCOMPOSITE MATERIAL WITH ANTIMICROBIAL EFFECT FOR PRESERVATION AND CONSERVATION OF WATERLOGGED WOOD CULTURAL HERITAGE OBJECTS

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Keywords: cultural heritage, hydroxyapatite, waterlogged wood, reinforcement nanomaterial

Introduction: Cultural heritage refers to the legacy of physical artefacts, traditions, practices and values that are passed down through generations in a particular society or community. It includes the tangible (immovable heritage, movable heritage, natural heritage) and intangibles aspects (traditions and rituals, the various forms of expression, knowledge and skills)^{[1][2}]. Wood is one of the organic materials most used by humans, since ancient times. By processing it, people built multiple kind of things such as: shelter, tools, ships, furniture, sculptures, musical instruments, objects used in rituals. Wood mostly consists of 3 components: cellulose, hemicellulose and lignin. Like any organic material, after it is cut, in the presence of water, oxygen and and different bacteria or fungi, it degrades. Wood is divided into two categories, hardwood (maple, beech, ash, walnut, oak) and softwood (spruce, fir, cedar, pine). Waterlogged wood refers to wood that has been saturated or soaked with water for an extended period of time. This saturation occurs when the wood is immersed in water or exposed to a constant high level of humidity and the water penetrates its entire structure, down to the smallest level (capillarity, microcapillary) and it reaches its saturation point^[3]. For preservation and consolidation of waterlogged wood, a nanocomposite material consisting of two components was obtained: an antimicrobial component (apatite material doped with various heavy metals) that provides the compound protection against biodeteriogens and a polymeric component that functions as a filling material, entering the cracks and crevices caused of wood water and improvement of mechanical properties (strengthening)^{[4][5]}.

Materials and methods: For the synthesis of the antimicrobial component (apatite material doped with heavy metals) the coprecipitation method was used and for the synthesis of the polyol 2 reactions were used successively: the glycolysis reaction and the esterification reaction. The final product, film-forming composite with antimicrobial effect intended to cover waterlogged wood, is made up of solvent, binder, apatitic material doped with heavy metals, catalyst and additives. The nanocomposite material was applied to different types of wood that were subjected to an aging process to simulate waterlogged wood objects. Different tests were performed on the treated wood samples (mechanical resistance, gloss, color, water adsorption) to establish the degree of efficiency of the composite nanomaterial

Results and Conclusions: The composite nanomaterial was successfully obtained and applied. It improved the mechanical properties of waterlogged wood; it filled the cracks and fissures caused by water and offers protection against bacteria and fungi. Based on these results, an invention patent application registered at OSIM ^[6] was developed and an ISI-listed article was sent for publication ^[7].

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- [1]. Rouhi J. Definition Of Cultural Heritage Properties And Their Valuesby The Past. AJST. 2017;08;7109-14
- [2]. Vecco M. A definition of cultural heritage: From the tangible to the intangible. J. Cult. Herit. 2010;11;321–4
- [3]. Broda M., Hill C.A.S. Conservation of Waterlogged Wood-Past, Present and Future Perspectives. Forests. 2021;12;1193
- [4]. Fistos T., Fierascu I., Doni M., Chican I.E., Fierascu R.C. A Short Overview of Recent Developments in the Application of Polymeric Materials for the Conservation of Stone Cultural Heritage Elements. Mater. 2022;15;6294.
- [5]. Gîfu I.C., Ianchiş R., Nistor C.L., Petcu C., Fierascu I., Fierascu R.C. Polyelectrolyte Coatings—A Viable Approach for Cultural Heritage Protection. Mater. 2023;16;2873
- [6]. Fistos T., Dolana S.V., Matei (Brazdis) R. I., Fierascu I., Raduly F.M., Nicolae C.A., Iordache T.V., Ficai A., Fierascu R.C. Composite Material With Antimicrobial Effect For The Preservation Of Waterlogged Wood Cultural Heritage Objects. UPB Sci. Bull. B: Chem. Mater. Sci.
- [7]. Fistos T., Dolana S.V., Fierascu R.C., Fierascu I., Baroi A.M., Brazdis (Matei) R. I., Sarbu A., Iordache T.V., Zaharia A. A-00070/2024 - Organic/Inorganic Composite Material With Antimicrobial Effect For Consolidating Archaeological Wood With Excess Of Moisture And Method Of Obtaining It.

COLORIMETRIC AND GLOSSMETER ANALYSIS FOR THE CHARACTERIZATION OF DIFFERENT TYPES OF GRANITES

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Keywords: Granite, Surface damage, Cultural heritage

Introduction: Historic buildings made of natural stones represent a significant part of the world's-built heritage, enclosing historical, aesthetic and material value (). Color is one of the most important visual properties of ornamental and monumental stone. Color changes caused by weathering and decay greatly influence the aesthetic value of stone. Measurement of granite aestethic parameters of granite is complicated by the lack of compositional homogenity present in these natural materials (spatially heterogeneous color), and different colors of the constituent minerals. There is great interest in measuring the color of granite because, amongst other reasons, granite is one of the most commonly used types of igneous rock owing to its abundance and great variety of color and textures, and because it is a major construction material in European historical buildings and monuments.

Materials and methods: The samples were cut to identical size, having the same thickness. In this experiment we have 3 types of granite whose origin is Italy (Rosa Aswan (RA), Gray Granite (GT) and Beige Granite (BG) and one sample from Romania (GR) In the present experiment we investigated the artificial weathering at different temperature and relative humidity (t=45C° and Rh=60%), in the climatic chamber, the sample being exposed to 20 cycles for six hours. These four types of samples were previously analyzed by visual and stereoscopic analysis with (Euromex Binocular Stereomicroscope) and chromatic analysis (with a Konica Minolta CR-410 Chromometer) and by Glossmetry (with Glossmeter HG268)

Results: Following the images obtained with the Stereomicroscope, some changes of the color have been observed, changes both due to the constituent components of which the samples are made up and due to the conditions to which they were subjected. Considering the set of samples, regardless of type of granite, the color difference between the initial and final value undergoes a small change. To check if granite undergoes changes, we analyzed the samples and from the point of view of the chromatic and gloss value parameters, these parameters suffered low changes between the initial measurements and the final measurements.

Fig 1. Stereomicroscopy granite, before and after the climatic chamber.



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References:

parameters.

- [1]. F.Vagnonet.all., Effects of thermal treatment on physical and mechanical properties of Valdieri Marble NW Italy, International Journal of Rock Mechanics and Mining Sciences, 2018;103:195-204
- [2]. I.O. Zaulet, R.M. Ion, Evaluation of Marble Alteration Processes. Scientific Bulletin of Valahia University Materials and Mechanisc.2022;18:29-32
- [3]. S. Siegesmund, et al., Physical weathering of marbles by anisotropic thermal expansion Int J Earth Sci. 2000:89-170-182.



Session 2 - Bioresources, biotechnologies and biorefinery

DEVELOPMENT OF MOISTURIZING CREAM FORMULATION BASED ON ROYAL JELLY, HYALURONIC ACID AND DAMASK ROSE WATER

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Keywords: royal-jelly, hyaluronic acid, rose water, moisturizing cream

Introduction: There is one main priority when it comes to beauty and personal care industry focusing on delaying skin aging processes by improving hydration. Hyaluronic acid (HA) represents a natural biopolymer used in cosmetic formulations due to its good skin benefits such as wrinkles reducing and water molecules binding capacity. Another active ingredient with outstanding properties is represented by Royal Jelly (RJ) extracted from honey bees and rich in proteins, polyphenols, peptides, fatty acids and vitamins. RJ is well-known for its anti-inflammatory and antioxidant properties and for enhancing collagen production^[1]. Rose water has also numerous benefits to the skin including anti-inflammatory, antioxidant and anti-microbiological activities^[2].

Materials and methods: The proposed study involves obtaining an o/w moisturizing formulation enriched with RJ, HA, vitamin E and Damask Rose water. The emulsifier and other oil-soluble components were dissolved in the oil phase (Part A) and heated up to 70° C. The water components were dissolved in the aqueous phase (Part B) and heated also to 70° C. After heating, the phase A was added to the phase B with continuous stirring. Then, the flask was introduced in a cool water bowl until a homogenous emulsion with glossy and uniform appearance was formed. When the composition has cooled to below 40° C, other ingredients such as HA, RJ, perfume and preservative were added and thoroughly mixed until smooth. A proper mixing between the water and oil phase ensures a fine texture and good stability for the final product. The physico-chemical properties of the moisturizing cream were investigated as follows: pH, colour, smell, texture, homogenity, consistency, visual appearance, touch, acid and saponification values, dilution and dye tests, FT-IR and rheological properties.

Results: In the first place, the moisturizing cream formulation was successfully obtained. Furthermore, its physico-chemical characteristics were studied intensively through various laboratory methods. The o/w emulsion was examinated under microscope. The FT-IR spectra of HA, RJ and dried cream were also analysed. Furthermore, the moisturizing cream was investigated by rheological measurements.



Figure 1 . A) Royal Jelly powder B) the formulated moisturizing cream

Conclusions: A novel, promising and hydrating cream with a light floral scent was obtained and characterized. The moisturizing formulation is stable at room temperature, creamy, homogeneous, fluid, without sediments or phase separations.

References:

[1]. Park H.M., Hwang E, Lee K.G., Han S.M., Cho Y., Kim SY., Royal jelly protects against ultraviolet B-induced photoaging in human skin fibroblasts via enhancing collagen production, *J Med Food.*, 2011, 14(9):899-906.

[2]. Mahboubi M., Rosa damascena as holy ancient herb with novel applications, *Journal of Traditional and Complementary Medicine*, 2016, 6(1):10-16.

EFFICIENCY OF MICROBIAL BIOMASS IN HEAVY METAL REMOVAL FROM CONTAMINATED ENVIRONMENTS

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Keywords: bioremediation, heavy metal, nanomaterials

Introduction: The remediation efficiency of biological agents against xenobiotic compounds has been the subject of numerous recent studies, as bioremediation is recognized as an environmentally-friendly, economical and sustainable method. Microorganisms can develop pollution-induced tolerance over time and can be further used in remediation strategies for long-term ecological restoration^[1]. The purpose of this study was to gain a better understanding on the removal efficiency of metal-tolerant bacteria and fungi isolated from heavy metal - contaminated soil for future bioremediation applications.

Materials and methods: Two metal-resistant microbial strains that displayed above moderate tolerance to high concentrations of Cr, Pb and Zn were used in the current study. The microbial strains have been previously identified by Biolog phenotypic tests^[2]. The bio-removal potential of the microbial strains was tested in broth culture media amended with a concentration of 100 mg/L of K₂Cr₂O₇, Pb (NO₃)₂, and ZnSO₄ individually. The microbial biomass was further characterized by SEM/EDX and FTIR analyses. The efficiency of the process was evaluated by comparing the differences in concentrations prior and after the bioremediation assay, by electrochemical determinations using nanomaterial-based sensor.

Results: Both strains, identified as *Bacillus marisflavi* and *Trichoderma longibrachiatum* displayed different degrees of efficiency in reducing the concentration of Cr, Pb and Zn from solution. The fungal strain was more efficient in reducing 90% of the concentration of Cr, respectively 70% of the concentration of Zn, whereas the bacterial strain was more efficient in removing Pb from solution. SEM/EDX images confirmed the accumulation of metal ions onto the surface of the cells as the primary uptake mechanism of *T. longibrachiatum*, whereas intracellular accumulation was observed predominantly in *B. marisflavi*. The removal process was proved to be mediated by numerous functional groups, as observed through FTIR spectra. The electrochemical sensors presented good accuracy in contaminants determination, assessing the performance of the microbial strains in heavy metal bio-removal.

Conclusions: Our results indicate a higher removal efficiency of fungi for Cr and Zn, while bacteria demonstrated the efficacy in removing Pb. The electrochemical sensors used in the present study represent a simple, affordable and fast method for monitoring heavy metal concentrations in different contaminated environments. Research will continue by studying the in-field bioremediation potential of the isolated microorganisms and by monitoring soil quality as part of a long-term management strategy for heavy metal contaminated environments.

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References:

[1]. Campillo-Cora C, González -Feijoo R, Arias- Estévez M, Fernández-Calvino D. Do heavy metals affect bacterial communities more in small repeated applications or in a single large application? J Environ Manage. 2023; 325:116494

[2]. Firincă C, Zamfir L-G, Constantin M, Răut I, Capră L, Popa D, Jinga M-L, Baroi AM, Fierăscu RC, Corneli NO, Postolache C, Doni M, Gurban AM, Jecu L, Şesan TE. Microbial Removal of Heavy Metals from Contaminated Environments Using Metal-Resistant Indigenous Strains. *Journal of Xenobiotics*. 2024; 14(1):51-78.

LIGNOCELLULOSIC WASTE DERIVED BIOCHAR – SYNTHESIS AND ACTIVATION FOR AGRICULTURAL APPLICATION

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Keywords: biochar; slow pyrolysis; lignocellulosic waste

Introduction: The aim of this work is to evaluate the characteristics of biochar derived from lignocellulosic waste, resulting from the slow pyrolysis of wheat straws, before and after subjecting the biochar samples to activation treatment. Biochar serves as a natural fertilizer and support material for controlled release of nutritive elements, having positive effects on the environment such as reduced eutrophication risk, atmospheric carbon capture, amendment for degraded soil, while also providing excellent adsorption capacity for environment contaminants ^{[1][2]}. The premise is that lignocellulosic wastes resulting from crops serve as feed to produce biochar which can be further used as soil amendment, returning to the place of origin for feedstocks these benefits.

Materials and methods: Experiments were carried out using wheat straws as feedstock, in a tubular slow pyrolysis reactor, using nitrogen as inert gas. Biochar samples were obtained through slow pyrolysis for 2h at 600 and 750°C, respectively, using a heating ramp of 3°C/min. The activation of obtained biochar samples was carried out in a 10% KOH solvent-aqueous mixture, using a solid to liquid ratio of 1:20, in a 1L Parr autoclave under 2.2 MPa, 200°C (heating ramp of 20°C/min) for 1h at 150 rpm.

Results: Biochar samples before and after being subjected to the activation process were characterized physicochemically through SEM analysis coupled with EDX using a Hitachi TM4000plus II microscope, as well as porosimetry analysis using a NOVA 2200e Gas Sorption Analyzer (Quantachrome). EDX analysis confirmed the loading of biochar samples with potassium, which is beneficial for agricultural applications of biochar such as fertilizers, while BET analysis highlighted the increase in specific surface and total pore volume for samples subjected to activation over control samples.



Fig 1. SEM analysis of biochar samples ($1 = 600^{\circ}$ C; $2 = 750^{\circ}$ C; A - after activation; B - before activation)

Conclusions: Activation procedure of biochar samples led to a significant improvement of physico-chemical characteristics, with both specific surface and total pore volume increasing, almost doubling in both cases, while the pore diameter decreased by less than 10%, and loading the activated samples with K. This activation procedure allows for a waste stream to be upgraded and valorized in the form of soil amendment and fertilizer.

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- [1]. Chen J., et al., Environmentally friendly fertilizers: A review of materials used and their effects on the environment. Science of the Total Environment, 2018;613-61:829–839.
- [2]. Amalina F., et al., Advanced techniques in the production of biochar from lignocellulosic biomass and environmental applications. Cleaner Materials, 2022;6.

COMPUTATIONAL APPROACHES REGARDING THE EFFECT OF CYCLIC AROMATIC HYDROCARBONS ON THE ENVIRONMENT AND HUMAN HEALTH

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Keywords: computational study, polycyclic aromatic hydrocarbons, toxicology, chemoinformatics, enviroment, health

Introduction:Rapid industrialization and urbanization have resulted in pollution from anthropogenic activity, which releases various into the environment, including polycyclic aromatic hydrocarbons (PAHs) Due to their inherent properties, persistent pollutant PAHs with a wide range of biological toxicity; remediation of PAHs from the environment has been a global concern. PAH pollutants are ubiquitous, found equally in aquatic and terrestrial ecosystems as well as in the atmosphere^[1]. Also, these compounds have harmful effects on human health ^[2]. The purpose of this work is to evaluate *in silico* the physicochemical properties, the pharmacokinetic and pharmacodynamic profile, the molecular targets as well as the mathematical correlation of the various properties.

Materials and methods: A set of 9 compounds from the class of polycyclic aromatic hydrocarbons were used in this study. The Pubchem database was used to extract the Simplified Molecular Imput Line Entry (SMILES) files and physicochemical properties of selected compounds. To study the absorption, distribution, metabolism, excretion and toxicity (ADMET) profiles in silico, we used the pkCSM database, ProTox II database and the web tool admetSAR 2.0. The ecotoxicity of compounds was predicted with the admetSAR 2.0 web tool. The bioactivity of the compounds was calculated using the computational software Molinspiration. In order to develop mathematical model, physicochemical properties (molecular weight, partition coefficient, refractivity) were used for correlation with biological activities (blood-brain barrier permeability, central nervous system permeability, lethal dose 50). Excel was used to perform mathematical calculations. To predict the molecular targets we used the Superpred database.

Results: Polycyclic aromatic hydrocarbons are small, lipophilic molecules (negative partition coefficient) with moderate solubility in water, according to solubility coefficient. All compounds comply with Lipinski and Veber druglikeness rules. No compound follows the Muegge rule. The compounds have high gastrointestinal absorption. They easily cross the blood-brain barrier and have a high permeability to the central nervous system (CNS), which demonstrates that they affect the CNS. Substances are rapidly metabolized in the body. The fact that they represent both substrates and inhibitors demonstrates that the concentration in which they are found in the body is important, at low concentrations they are substrates for cytochromes, and at high concentrations they can inhibit cytochromes. Most compounds have a low total clearance, which shows that they can be difficult to eliminate from the body. With regard to human health, polycyclic aromatic hydrocarbons cause adverse effects on the skin, eyes, mutagenicity, carcinogenicity and nephrotoxicity and immunotoxicity. It also affects various repellers and signaling pathways. According to the pkCSM and Protox II databases, they have no cytotoxic effects and do not cause hepatotoxicity. At the same time, it does not present reproductive, mitochondrial and respiratory toxicity according to the results of admetSAR 2.0. Naphthalene had the lowest bioactivity score for drug targets: G protein-coupled receptor, ion channel modulator, kinase inhibitor, nuclear receptor ligand, protease inhibitor, enzyme inhibitor. Ecotoxicity results showed that the chemicals analysed are toxic to phytoplankton, crustaceans and T. pyriformis, but not toxic to bees. The analysed compounds have low biodegradability. The best statistics of univariate correlation are shown by partition coefficient correlated with blood-brain barrier permeability. The most likely predicted target for the analyzed compounds is DNA-(apurinic or apyrimidinic site) lyase.

Conclusions: Computational methods offer perspectives for the design of new compounds that have fewer adverse effects, as well as the remediation of the effects of existing toxic compounds in a rapid and economic way, compared with *in vitro / in vivo* analysis.

- [1]. Patel AB, Shaikh S, Jain KR, Desai C, Madamwar D. Polycyclic Aromatic Hydrocarbons: Sources, Toxicity, and Remediation Approaches. Front Microbiol. 2020;11:562813.
- [2]. Mallah MA, Changxing L, Mallah MA, Noreen S, Liu Y, Saeed M, Xi H, Ahmed B, Feng F, Mirjat AA, Wang W, Jabar A, Naveed M, Li JH, Zhang Q. Polycyclic aromatic hydrocarbon and its effects on human health: An overeview. Chemosphere. 2022;296:133948.

QUALITY EVALUATION OF SOLID BIOFUEL FROM CO-FIRED AGRICULTURAL WASTES

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Keywords: co-firing; biomass; calorific values; pellets; combustion calorimetry

Introduction: Agricultural residues are defined as carbon –based materials generated into by-products through the harvesting and processing of agricultural crops, according to Directive EN 14588 of the European Committee, being ranked as a result of their origin in to four major classes: wastes from soil plantations, waste from food industry, breeding and slaughter wastes^{[1][2]}. The use of pure biomass firing in some industrial processes is unattractive due to its low bulk density, high moisture content and low calorific value. Co-combustion is the burning of more than one fuel to produce power. Co-firing biomass with coal reduces fuel costs, emission of NO_x, SO_x levels and fossil CO₂, reduce soil and water pollution. Burning biomass with fossil fuels, different additives and binding agents has a positive impact, both on the climate and the economics of power generation^{[3][4]}. The present work focuses on optimizing the characteristics in term of combustion for coarse ground grist of sorghum seeds, rape seeds, soyabean, sunflower seeds, grape pomace and corn cob by varying two different parameters: the type of co-firings apllied to the selected agricultural biomass pellets and the percentage used.

Materials and methods: In the present study, the agricultural by-products (coarse ground grist) of sorghum seeds, rape seeds, soyabean, sunflower seeds and their mixture with 20% coal; grape pomace, corn cob and their mixture with 10% waste rapeseed oil, sawdust and starch were used. The pellets were obtained by using a manual pellet press. The determination of calorific values of the investigated agricultural biomass pellets was performed in accordance with the ASTM D5865 Standard Test Method for Gross Calorific Value of Coal and Coke^[5] and standard operating procedure Parr 6200 Calorimeter^[6].

Results: Depending on the co-firing type used and the applied percentage, pellets with different calorific values were obtained. Among the studied samples, co-fired sunflower seeds grist presents the highest heating value, highest fixed carbon content and fuel value index, thus being a good alternative to fossil fuel in order to produce energy and reduce the domestic air pollution and the amount of wood needed. Waste rapeseed oil addition significantly increases the calorific powers in grape pomace and corn cob pellets. The highest calorific value was obtained for the grape pomace pellets containing 10% waste rapeseed oil, 22.14 MJ/kg, compared to grape pomace control pellets, of 21.35 MJ/kg. The calorific values of corn cob control pellets were also increased when adding 10% waste rapeseed oil, from 17.29 MJ/kg to 19.76 MJ/kg.

Conclusions: Pellets made from agricultural waste are some of the most popular biofuels. The biomass pellets from this study have a calorific value ranged between 16 to 22 MJ/kg.All the studied species are suitable due to the large quantities available and their calorific value being sufficiently high according to literature standards (EN14961-3) to justify the use of biomass, minimum value should be 15.5 MJ/Kg. The combustion heat of the studied pellets depends on the agricultural material they are made from. Significant differences were observed between the combustion heat of pellets from co-fired and non-cofired samples. Our studied samples, especially co-fired ones, offer an alternative material for energy use, which meets the requirements of minimizing CO_2 , NO_x and SO_x emissions. Biomass co-firing can be considered as a transition option towards a completely carbon-free power sector. The obtained results will complete the existing databases concerning the properties of solid biofuels from biomass containing the mentioned co-firings.

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- [1]. Europaisches Komitee fur Normung, 2010;EN14588-2010-10.
- [2]. Obi, F.O.; Uguruishiwu, B.O.; Nwakaire, J.N. Agricultural Waste Concept, Generation, Utilization and Management. Nig. J. Technol. 2016; 35: 957-964.
- [3]. Hughes, EE.; Tilmann, D.A. Biomass cofiring: status and prospects. Fuel Process Technol. 1998; 54: 127-42.
- [4]. Hamzah, N.; Zandi, M.; Tokimatsu, K.; Yoshikawa, K. Wood Biomass Pellet Characterization for Solid Fuel Production in Power Generation. Intl. J. Renew. Energ. Sources. 2018; 3: 32-40.
- [5]. ASTM D5865, Standard Test Method for Gross Calorific Value of Coal and Coke. 2013. www.astm.org
- [6]. Parr Instrument Company, 6200 Isoperibol Calorimeter, 2014. (http://www.parrinst.com/products/oxygenbombcalorimeters/6200isoperibolcalorimeter)

EXPLORING THE THERAPEUTIC POTENTIAL OF *ALOE VERA* AND HONEY FORMULATIONS FOR SKIN WOUND HEALING

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Keywords: Aloe vera; honey; antioxidant activity; collagen synthesis; wound healing

Introduction: *Aloe vera* and honey have been used in traditional medicine for thousands of years, including in Ancient Egyptian, Chinese, and Roman cultures. Nowadays, both natural sources of bioactive molecules continue to hold a significant place in modern medicine, exhibiting a wide array of beneficial properties, such as anti-bacterial, anti-oxidant, anti-inflammatory, and anti-tumor effects ^{[1][2]}. When used in biomedical applications, *A. vera* and honey have shown promising results in treating skin infections and burns, digestive disorders, and strengthening the immune system ^{[3][4]}. Given the health benefits provided by *A. vera* and honey, this study aims to investigate the effect of certain *A. vera*-honey extract mixtures on cell proliferation and collagen synthesis in human dermal fibroblasts (HDF) culture, cell protection against oxidative stress and cell migration capacity in biomimetic experimental models *in vitro*, in order to explore their potential use in novel formulations for skin wound healing promotion.

Materials and methods: The *A. vera* extract was obtained by 70% (v/v) ethanolic extraction of homogenized *A. vera* gel, which was then evaporated to dryness. Honey was dissolved in distilled water to reach 20% (w/v) solution. Total phenolic content was analyzed for each sample using the Folin-Ciocalteu method. For cell culture experiments, *A. vera* residue and honey solution were resuspended in cell growth medium and combined in 1:2, 1:1 and 2:1 (w/v) mixing ratios. HDF were seeded in 96-well culture plates and cultivated in standard conditions, in the presence of extract mixtures. After 48 h of cultivation, the number of viable cells was assessed using Neutral Red spectrophotometric assay. The Sircol soluble collagen test was conducted in harvested culture media to evaluate collagen synthesis by HDF cells. The anti-oxidant effect was assessed by simultaneously exposing HDF cells to hydrogen peroxide (H₂O₂) and extract mixtures, followed by cell viability assessment by means of the Neutral Red assay. Cell migration was examined in the presence of *A. vera* and honey extract mixtures using the scratch wound healing assay.

Results: The results showed that *A. vera* extract had higher phenolic content, compared to honey sample, which endows antioxidant properties. In cell culture, the formulations did not exhibit cytotoxicity and even stimulated HDF proliferation. Cells treated with each formulation exhibited increased collagen secretion, and *A. vera*-honey 1:2 had the highest stimulating effect. Additionally, all *A. vera* and honey formulations showed protective effect against H_2O_2 -induced oxidative stress in HDF cells. Also, they promoted cell migration in scratch assay and 15% higher rate of wound closure for *A. vera*-honey 1:2 formulation was registered, compared to untreated control.

Conclusions: In conclusion, the *Aloe vera* and honey extract formulations demonstrated complementary action to enhance cell proliferation and migration, collagen production, on one hand, and the anti-oxidant activity, on the other hand, in HDF culture. The highest stimulatory activity in main stages of wound healing process was found in case of *A. vera*-honey 1:2 formulation, acting as a promising agent in skin tissue regeneration.

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- [1]. Dorai AA.Wound care with traditional, complementary and alternative medicine. Indian J. Plast. Surg., 2019;45(2), 418-424.
- [2]. Yilmaz AC, Aygin D. Honey dressing in wound treatment: a systematic review. Complement. Ther. Med. 2020;51, 102388.
- [3]. Harinatha Reddy A, Sri Lakshmi B, Nageswari G, Shobha R, Venkatappa B. Phytochimical screening, TLC fingerprinting and antimicrobial activity of methanolic leaf extract of Aloe vera against clinical isolates of methicillin resistant Staphylococcus aureus. Mintage j. pharm. med. sci. 2015;5(1), 16-18.
- [4]. Krishnakumar GS, Mahendiran B, Gopalakrishnan S, Muthusamy S, Malarkodi Elangovan S. Honey based treatment strategies for infected wounds and burns: A systematic review of recent pre-clinical research. Wound Med. 2020;30, 100188.

UTILIZING MOVING BED BIOFILM REACTOR FOR CULTIVATING MICROALGAL-BASED CONSORTIA AND PLANT BIOSTIMULANT PRODUCTION

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Keywords: wastewater treatment, yeast, bacteria, high throughput screening, cucumber

Introduction: Aquaculture contributes to water nutrient enrichment by fish waste, particularly nitrogen and phosphorus, which can lead to eutrophication^[1]. Microalgae and their co-culture consortia help mitigate this by purifying wastewater^[2]. The aim of this research was to establish an integrated biotechnology for co-culturing microalgal consortia^[3], employing moving bed biofilm reactors (MBBRs)^[4], with the purpose of producing a plant biostimulant while treating wastewater.

Materials and methods: Microalgal-based consortia were chosen using high throughput screening (HTS), by assessing the compatibility of two microalgal strains (*Chlorella* sp. NIVA-CHL 137 and *Desmodesmus communis* NIVA-CHL 7) alongside several bacterial and yeast isolates. The chosen consortia were cultivated in synthetic wastewater similar to fish farm effluent, utilizing six types of MBBR, for 3 days. Growth parameters of microalgae such as optical density, turbidity, cell count, and water quality parameters such as COD, BOD, pH were monitored. The most desirable combination of MBBR and microalgal-based consortia was confirmed with Design Expert 11. The exces biomass was processed into a plant biostimulant and evaluated on cucumber plants (*Cucumis sativus*) in greenhouse settings, using concentrations of 4 mg/L and 8 mg/L.

Results: Based on HTS analysis, the bacterial strain P1T1 was chosen to co-culture with *D. communis*, and yeast strain TAzRr was selected for *Chlorella* sp. The *Chlorella*-yeast consortium, in combination with MBBR1, exhibited the highest microalgal growth, reaching an optical density of 0.5, and the lowest COD level in recycled water (22 mg O_2/L), Figure 1. The cucumber plants treated with the lower concentration (4 mg/L) of the biostimulant derived from the *Chlorella*-yeast consortium exhibited the highest chlorophyll fluorescence and photosynthetic rate. At the higher concentration (8 mg/L), there was a notable increase in stomatal conductance and respiration rate of the plants.



Figure 1. Interaction between Chlorella sp. consortium and D. Communis consortium in MBBR variant (SAB): a) OD; b) COD

Conclusions: Microalgal co-cultures on MBBR facilitated the reduction of organic matter by 76% and enhanced biomass production. The formulated plant biostimulant applied at 4 mg/L increased the photosynthetic rate in cucumber plants.

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- [1]. H. Milhazes-Cunha and A. Otero, "Valorisation of aquaculture effluents with microalgae: The Integrated Multi-Trophic Aquaculture concept," Algal Research, vol. 24, pp. 416-424, 2017/06/01/ 2017.
- [2]. L. Ferro, "Wastewater treatment and biomass generation by Nordic microalgae," U. UNIVERSITY, Ed., 2019.
- [3]. S. Zhu, L. Higa, A. Barela, C. Lee, Y. Chen, and Z.-Y. Du, "Microalgal Consortia for Waste Treatment and Valuable Bioproducts," (in en), Energies, Review vol. 16, no. 2, p. 884, 2023-01-12 2023.
- [4]. N. C. Boelee, H. Temmink, M. Janssen, C. J. N. Buisman, and R. H. Wijffels, "Balancing the organic load and light supply in symbiotic microalgal-bacterial biofilm reactors treating synthetic municipal wastewater," Ecological Engineering, vol. 64, pp. 213-221, 2014/03/01/ 2014.

UNDERSTANDING WATER IMPACT ON THE THERMAL BEHAVIOR OF DEEP EUTECTIC SOLVENTS: INSIGHTS FROM TGA ANALYSIS

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Keywords: reline, ethaline, decomposition, thermal stability, mass loss

Introduction: Deep eutectic solvents (DESs) are valued in green chemistry for their sustainability^[1]. This study explores how water influences the thermal behavior of ethaline (ChCl:EG 1:2 molar ratio) and reline (ChCl:U 1:2 molar ratio) as determined by TGA analysis^[2]. Understanding the role of water in the thermal properties of these DESs is crucial for tailoring the DES applications. By examining decomposition pathways and temperature profiles under varying water content, this research contributes to a broader comprehension of DESs and underscores the significance of water content in their design and usage.

Materials and methods: Analytical grade reagents were selected, i.e., choline chloride (>98% purity) as hydrogen bond acceptor (HBA), ethylene glycol, and urea (>99% purity) as hydrogen bond donor (HBD). The DESs (ethaline and reline) were prepared in a controlled environment, maintaining a 1:2 molar ratio of ChCl to HBD. The TGA analysis of the DES samples with varying water contents (0-60%) were conducted with a TA Instruments TGA Q5000IR. The samples were heated at 10°C per minute under N₂ flow, revealing decomposition, oxidation, or dehydration phase changes up to $450^{\circ}C^{[3]}$.

Results: The thermogram of ethaline (ChCl:EG 1:2) displays four distinct mass loss steps, influenced by the increase in water content (Fig. 1). The initial mass loss at 100°C is attributed to water removal, followed by intermediate acid formation (105-210°C) and choline chloride degradation. Low water concentrations (up to 20% in ethaline and 5-10% in reline – Fig. 2) initially stabilize DESs, increasing Tmax, then destabilize, decreasing Tmax, possibly due to disrupted hydrogen bonds. In ethaline, choline's (HBA) Tmax remains higher than in anhydrous DES.





Fig. 1. Thermogram of ChCl:EG 1:2 with different water concentrations

Fig. 2. Thermogram of ChCl:U 1:2 with different water concentrations

Conclusions: This study provides insight into the thermal properties of ethaline and reline DES and its aqueous solutions. The TGA analysis revealed distinct mass loss patterns with increasing water concentrations. The HBA and HBD in DES exhibited enhanced stability compared with individual components, probably due to the strong H-bonds formed.

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- Hansen, B.B.; Spittle, S.; Chen, B.; Poe, D.; Zhang, Y.; Klein, J.M.; Horton, A.; Adhikari, L.; Zelovich, T.; Doherty, B.W.;. Chem. Rev. 2021, 121:1232-1285.
- [2]. Delgado-Mellado, N.; Larriba, M.; Navarro, P.; Rigual, V; Ayuso, M.; García, J.; Rodríguez, F. J. Mol. Liq. 2018, 260:37-43
- [3]. E.-G. Brettfeld, T.D., C. A. Nicolae, D.; Constantinescu-Aruxandei, F.Oancea, BRChES, 2023, 10:59-66.

MODULATION OF RICE HUSK BIODEGRADATION BY *TRICHODERMA ATROVIRIDE* IRRADIATED WITH BLUE-LASER LIGHT: A SCALED-UP ATTEMPT

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Keywords: lignocellulose, blue-light, silicon, antioxidants, enzymes

Introduction: In fungi, light was discovered to trigger multiple signaling pathways crucial for metabolism, growth, and adaptation to stress caused by shifts in environmental conditions^[1]. The initial light effect documented for *Trichoderma* involved the stimulation of conidiation following brief exposure to blue or white light pulses^[2]. Light has the capability to regulate morphological and physiological processes in fungi^[3], as well as to influence the expression of certain enzymes, particularly those involved in lignocellulose degradation^{[4][5]}. This research delves into the impact of blue-light laser irradiation, a less conventional method of illumination, on the bioconversion of rice husk by *Trichoderma*, in an attempt to scale up the process.

Materials and methods: Mature spores of *Trichoderma atroviride* ATCC 74058 were transferred to ISM medium. To stimulate the production of biomass-degrading enzymes, the mycelium from ISM was cultured in water supplemented with rice husk in 2L flasks on a rotary shaker at 28°C for 15 days. The samples were exposed 3 times to blue-light laser for 60 sec. each at a specific intensity in different days. The supernatant underwent sterilization via filtration and was subsequently utilized to assess enzymatic activities, cellulases, α -amylases, proteases and LPMOs. The soluble silicon (Si), polyphenolic content, antioxidant activities, contact angle and interfacial tension were determined as well. Moreover, the microscopical features of mycelia were evaluated.

Results: Exposure of *T. atrovirid*e to blue-light laser was observed to impact the enzymatic activities. The highest protease and cellulase activities were observed after the 3^{rd} irradiation and were higher than the non-irradiated sample. The α -amylase and LMPO activities were not significantly affected by the blue light. The soluble Si content was significantly increased in the culture medium upon the three irradiations compared to the non-irradiated sample. The polyphenol content and the antioxidant activity had a heterogeneous behavior. The blue light decreased the surface tension and the contact angles of the samples. Exposing the samples to blue-light laser irradiation increased the production and the diameter of conidia in the irradiated ones.

Conclusions: Our findings suggest a rise in enzymatic activities of *T. atroviride* upon exposure to a moderate intensity of blue-light laser for 60 sec. The increase of the soluble Si content in the medium after irradiation indicates an enhancement of the breakdown process. The irradiation enhances the sporulation of *Trichoderma* and changes the cohesion and adhesion forces of the growth medium.

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- C. L. Baker, J. J. Loros, and J. C. Dunlap, "The circadian clock of Neurospora crassa," FEMS microbiology reviews, vol. 36, no. 1, pp. 95-110, 2012.
- [2]. J. Gressel and E. Galun, "Morphogenesis in Trichoderma: photoinduction and RNA," Developmental Biology, vol. 15, no. 6, pp. 575-598, 1967.
- [3]. Z. Yu and R. Fischer, "Light sensing and responses in fungi," Nature Reviews Microbiology, vol. 17, no. 1, pp. 25-36, 2019.
- [4]. H. Bazafkan, D. Tisch, and M. Schmoll, "Regulation of glycoside hydrolase expression in Trichoderma," Biotechnology and biology of Trichoderma, pp. 291-308, 2014.
- [5]. M. Schmoll, "Regulation of plant cell wall degradation by light in Trichoderma," *Fungal Biology and Biotechnology*, vol. 5, no. 1, p. 10, 2018.

SODIUM SELENITE TRIGGERS CALCIUM-DEPENDENT RESPONSES IN SACCHAROMYCES CEREVISIAE CELLS

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Keywords: S. cerevisiae mutants, chemogenomic screening, yeast cell growth, selenium nanoparticles, antioxidants

Introduction: Selenium is an essential micronutrient, exhibiting antioxidant activity and immunomodulatory effects. Selenium (Se) is described as 'both essential and toxic' due to the narrow interval between deficiency and toxicity ^[1]. Zero-valent Se is considered the least toxic form of selenium. Microorganisms, including yeasts, can reduce Se species, forming zero-valent selenium nanoparticles (SeNPs). The biogenic SeNPs have the advantage of lower toxicity and biological compatibility compared with inorganic Se forms. Yeasts can be designed as SeNPs *nano factories*, producing safer forms of Se with enhanced biological activities, such as antitumor, antimicrobial, and antioxidant ^[2]. Moreover, yeasts can be used as model microorganisms to provide a more comprehensive insight regarding the Se metabolism in eukaryotic cells ^[3]. The aim of this work was to assess the effect of Na₂SeO₃ on yeast cell growth and to highlight possible mechanisms involved in SeNPs biosynthesis.

Materials and methods: A partial chemogenomic screening was performed using a collection of *Saccharomyces cerevisiae* knock-out strains. Mid log growing cells (10⁷ cells/mL) of *S. cerevisiae* 'Wild-Type' (WT) BY4741 parental strain and knockout isogenic strains were serially diluted and stamped on Na₂SeO₃-enriched agar plates. Knock-out strains *cch1*Δ, *mid1*Δ, and *yvc1*Δ were exposed to different concentrations of Na₂SeO₃. The strains were cultured on Na₂SeO₃ enriched medium (Yeast Extract-Peptone-Dextrose) and observed after 4 days of incubation. The optic densities (OD_{600 nm}) of the yeast cell cultures exposed to Na₂SeO₃ were measured. The response to selenite exposure was investigated by observing the growth of *cch1*Δ, *mid1*Δ, *yvc1*Δ strains on media supplemented with different concentrations of Na₂SeO₃ and Ca²⁺ or calcium chelator EGTA. The effect of the antioxidants vitamin C, N-acetylcysteine (NAC) and dithiothreitol (DTT) on the growth of yeast cells exposed to Na₂SeO₃ was also assessed. The morphology of yeast cells was monitored with bright field optic and electronic microscopy.

Results: Concentrations over 1 mM Na₂SeO₃ significantly inhibited yeast cell growth. The screen indicated that the mutants defective in calcium transport behaved differently to selenite exposure. The *mid1* Δ strain (lacking Mid1 plasma membrane calcium channel) was the most sensitive to selenite-induced stress, whereas the *yvc1* Δ strain (lacking the vacuolar Yvc1 calcium channel) was the most resilient. An improved growth rate of Na₂SeO₃-exposed cells was observed on media supplemented with Ca²⁺, but not with the calcium chelator EGTA, especially in the case of *yvc1* Δ . Vitamin C and DTT exhibited protective effect on yeast cells exposed to selenite. NAC was the compound with the highest efficiency in combating selenite-induced stress in yeast cells. The yeast cells developed a red color during the incubation period, which confirmed, together with the microscopy analysis, that the microorganism reduced Se (IV) to Se⁰.

Conclusions: The behavior of *mid1* Δ , *cch1* Δ and *yvc1* Δ strains suggests that yeast cells adapt to Na₂SeO₃-induced stress by mobilizing external sources of Ca²⁺, especially through Mid1/CCh1 channel. The yeast cells exposed to non-toxic concentrations of selenite induced the formation of SeNPs.

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- [1]. Petrović, M. "Selenium: Widespread yet scarce, essential yet toxic." ChemTexts 7 (2021): 11. 10.1007/s40828-021-00137-y. https://doi.org/10.1007/s40828-021-00137-y.
- [2]. Asghari-Paskiabi, F., M. Razzaghi-Abyaneh and M. Imani. "Yeast as a cell factorybiological synthesis of selenium nanoparticles." In Mycosynthesis of nanomaterials. CRC Press, 27-49.
- [3]. Herrero, E. and R. E. Wellinger. "Yeast as a model system to study metabolic impact of selenium compounds." Microbial Cell 2 (2015): 139

STUDY ON PHOTOCATALYTIC DEGRADATION OF SOME REACTIVE DYES UNDER VISIBLE LIGHT USING HYBRID Fe₂O₃/TiO₂ SYSTEMS

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Keywords: titanium dioxide, photocatalytic degradation, organic pollutants, reactive dyes.

Introduction: The presence of toxic and persistent organic pollutants in wastewater causes serious environmental problems. The majority of the pollutants found in wastewater are organic dyes, which are waste products of the paint, textile, and tanneries industries. Reactive dyes are among the most commonly used organic dyes in textile industry. However, they are highly toxic and pose significant risks to both the environment and human health. This issue can be resolved by using advanced oxidation (AO) methods, which are a sustainable and effective way to remove non-biodegradable pollutants from aqueous effluents. Photocatalysis is one of the AO green method by producing reactive species during solar irradiation $^{[1][2]}$. This study presents an alternative method for decontamination using TiO₂ photocatalysts with Fe₂O₃ heterojunctions for application in the depollution of water effluents contaminated with reactive dyes $^{[3]}$.

Materials and methods: The photocatalytic nanoparticles were obtained through two methods: (i) synthesis of iron oxides using ferric chloride as precursor, in the presence of TiO₂ which finally lead to a hybrid photocatalyst and (ii) formation of a composite by directly wet milling of iron oxides with TiO₂. Synthesis of iron oxides was performed using a Discover 2.0 Microwave Flow Reactor, at the temperature of around 160°C, and at 300 W. The obtained samples underwent characterization using modern analytical methods to ensure that the photocatalysts possessed the desired properties. The photocatalysts with a styrene-acrylic film-forming material^[4]. These resulting materials were deposited onto glass plates and immersed in quartz vessels containing water contaminated with Drimaren yellow CL-2R (Reactive Yellow 176), Drimaren red K-4BL (Reactive Red 56) dyes (Clariant). The reaction vessels were illuminated using a Xenon arc lamp, and degradation of the chromophores was monitored using UV-Vis absorption spectroscopy.

Results: The synthesized photocatalysts were characterized using FTIR, SEM, BET and EDX. The results revealed several prominent absorption peaks corresponding to various oxygen functional groups. The impact of the doping ratio and the duration of UV-radiation were considered as the important two factors affecting TiO_2 -Fe₂O₃ synthesizing process. It seems that in the case of using solvents, a more compact mixture is obtained in which the components of the mixture are not highlighted. The structural type of the contaminant influences the decomposition mechanism and subsequently its decomposition speed.

Conclusions: New photocatalytic nanocomposites were prepared by a simple chemical process of iron oxides generation at the surface of TiO_2 nanoparticles by hydrolysis of iron chloride at microwaves and by wet milling of iron-oxides/TiO₂ mixtures. All the mixtures were evaluated for structural, morphologic, textural and optical properties. Performances of the composites were evaluated comparatively in photocatalytic decomposition of some reactive dyes from aqueous solutions, under arc-xenon light irradiation. The best result is obtained by wet grinding of P25 with Fe₂O₃, in which case nanometric particles of TiO₂ are deposited on the surface of micrometric particles of Fe₂O₃.

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- A. Kumar, "A Review on the Factors Affecting the Photocatalytic Degradation of Hazardous Materials", Mater. Sci. Eng. Int. J., vol. 1, nr. 3, pp. 106-114, 2017, doi: 10.15406/mseij.2017.01.00018.
- [2]. M. Crișan et al., Fe-doped TiO2 nanomaterials for water depollution. 2020.
- [3]. F. Giuffrida, L. Calcagno, G. Pezzotti Escobar, și M. Zimbone, "Photocatalytic Efficiency of TiO2/Fe2O3 and TiO2/WO3 Nanocomposites", Crystals, vol. 13, nr. 3, 2023, doi: 10.3390/cryst13030372.
- [4]. V. Raditoiu, A. Raditoiu, M. F. Raduly, V. Amariutei, I. C. Gifu, şi M. Anastasescu, "Photocatalytic behavior ofwater-based styrene-acrylic coatings containing TiO 2 sensitized with metal-phthalocyanine tetracarboxylic acids", Coatings, vol. 7, nr. 12, 2017, doi: 10.3390/coatings7120229.

VALORIZATION OF VITICULTURAL BY-PRODUCTS FOR THE DEVELOPMENT OF NANOMATERIALS WITH BIOACTIVE PROPERTIES

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Keywords: grapevine waste; natural extracts; phytochemicals; phytosynthesis; bioactive properties;

Introduction: Residual biomass accumulated as a result of the technological processes of grapes processing, as well as from the application of various techniques for the maintenance of grapevine crops, is not sufficiently exploited, thus presenting a low and limited economic value. The main goal of the works (Figure 1) was to reuse the viticultural waste through the development of new nanomaterials with bioactive properties in order to integrate them into the circular bioeconomy.

Materials and methods: The general objective of the study consisted in the valorization of viticulture and winemaking waste through the recovery of target phytoconstituents in order to phytosynthesize nanoparticles of noble metals, with potential bioactive properties. The first specific objective of the work included obtaining natural extracts from viticultural waste: application and optimization of classical (temperature classical extraction) and modern (microwave and ultrasound assisted extraction) extraction methods in order to obtain extracts rich in phytoconstituents. The extracts were characterized by determining the total phenolic content using the Folin Ciocâlteu spectrophotometric method. The secondary objective involved the phytosynthesis of nanomaterials and characterization of metallic nanoparticles using non-destructive techniques such as UV-Vis spectroscopy, X-ray diffraction, EDX and TEM. The final goal was to assess the effectiveness of the acquired nanostructures through the examination of their bioactive properties, including antioxidant activity (evaluated using the DPPH reagent assay), electrochemical properties (by cyclic voltammetry), and antimicrobial activity (determined through qualitative and quantitative tests on various bacterial strains).



Figure 1. Graphical concept of the proposed methodology.

Results: The study, covering a period of 12 months, led to the full achievement of the proposed outcomes; an innovative technology (protected by the patent application A0375/2023)^[1] was developed, proposing a methodology for valorification of viticulture and winery waste. In the same time, as the results obtained were disseminated through the publication of 3 articles in ISI rated journals ^{[2][3][4]}, 1 book chapter ^[5] and participation to 4 international scientific conferences.

Conclusions: The fulfillment of the study led to the development of advanced models focused on the most effective, fast and economic method for utilizing viticulture and winery waste by phytosynthesizing metallic nanomaterials with high bioactive properties with a various range of applications.

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- References:
 - Cosmetic formulation for sun protection and with antimicrobial effect based on silver nanoparticles and natural extract and method of obtaining it, Patent Application no. A0375/2023, authors: Baroi AM, Fierascu I, Brazdis (Matei) RI, Fistos T, Fierescu RC, Chican IE, Hosu IS, Raduly FM.
 - [2]. Fierascu IC, Fierascu I, Baroi AM, Ungureanu C, Spinu S, Avramescu SM, Somoghi R, Fierascu RC, Dinu-Parvu CE. Phytosynthesis of Silver Nanoparticles Using Leonurus cardiaca L. Extracts. Materials, 2023, 16(9):3472.
 - [3]. Baroi AM, Fierascu I, Ghizdareanu AI, Trica B, Fistos T, Matei (Brazdis) RI, Fierascu RC, Firinca C, Sardarescu ID, Avramescu SM. Green approach for synthesis of silver nano-particles with antimicrobial and antioxidant properties from grapevine waste extracts. IJMS, 2024 – under evaluation.
 - [4]. Lupuliasa AI, Baroi AM, Avramescu SM, Vasile BS, Prisada RM, Fierascu RC, Fierascu I, Toma DI, Ripszky Totan A, Voicu-Bălaşea B, Piţuru SM, Popa L, Ghica MV, Dinu-Pîrvu C. Application of common culinary herbs for the development of bioactive materials. Plants, 2024 – under evaluation.
- [5]. Baroi AM, Ungureanu C, Călinescu MF, Vizitiu D, Sărdărescu ID, Ortan A, Fierascu RC, Fierascu I. Role and application of nanosensors in crop protection for disease identification. In: Khan Z, Sutan NA, editors. Nanoformulations for Sustainable Agriculture and Environmental Risk Mitigation, 2023. pp. 118–141.

MICROAEROPHILIC FERMENTATION OF BEE POLLEN: IMPROVING THE FUNCTIONAL PROFILE OF A TRADITIONAL FERMENTED BEVERAGE

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Keywords: nutrition, antioxidant metabolites, borș, prebiotic, antimicrobial

Introduction: In a world oriented towards nutrition and dietary supplements, pollen has become increasingly attractive due to its high concentration of beneficial metabolites that can be released upon fermentation ^{[1][2]}. In Romanian gastronomy, *borş*, a traditional drink resulting from the natural fermentation of wheat and corn bran, has established itself as a symbol of authentic taste but also as an important source of natural antioxidants ^[3]. Our study focuses on improving the fermentation process of the mash by incorporating polyfloral pollen. This innovative approach aims to explore and harness the health benefits of pollen in a traditional beverage.

Materials and methods: The beverages were crafted using a traditional recipe, commencing with a *borş* starter that underwent a 24 h fermentation period at room temperature. Next, a portion of the already fermented bran was transferred to another container, into which fresh bran and varying concentrations of pollen were introduced, initiating a new fermentation process that extended for approximately 72 h. The total content of polyphenols, flavonoids, and hydroxycinnamic acids was determined, and the antioxidant activity was measured using the 2,2-diphenyl-1-picrylhydrazyl (DPPH), ferric and cupric reducing antioxidant power (FRAP, CUPRAC) methods. The soluble silicon and carbohydrate contents were analyzed as well. The prebiotic activity on *Limosilactobacillus reuteri* DSM 20016 was assessed, as well as the antibacterial activity against *Pseudomonas aeruginosa* ATCC 27853, *Enterococcus faecalis* ATCC 29212, *Staphylococcus aureus* ATCC 25923, and *Bacillus cereus* NCTC 10320. Furthermore, the cytocompatibility and *in vitro* antioxidant activity were investigated.

Results: After fermenting bran with bee pollen for 3-4 days, the resulting beverage demonstrates a remarkable increase in polyphenol, flavonoid, and hydroxycinnamic acid content, approximately 3- and for polyphenol content and 2-fold higher for flavonoid and hydroxycinnamic acids, respectively, compared to the unmodified drink. The antioxidant activity of the fermented drink enriched with bee pollen (BPol30) was considerably higher than that of traditional *borş* (B), exhibiting a 2-fold, 4-fold and 100-fold increase in the DPPH FRAP, and CUPRAC assay, respectively. The carbohydrate content and soluble silicon increased with the addition of pollen. After 24 h of incubation, a significant 50-80% increase in the beneficial lactic bacterium *L. reuteri* was observed with the B and BPol30 treatments compared to control. Both types of drinks, the traditional and pollen-modulated, exhibited antibacterial activity against the tested strains. Cell viability increased by approximately 10% compared to the control after 24 hours, with the highest potential for increasing the number of metabolically active viable cells observed at the concentration of 50 µg/mL BPol30, in contrast, B showed only a 3% increase.

Conclusions: By modulating the traditional beverage with pollen, a multibiotic product is obtained with a high content of polyphenols, carbohydrates, silicon, and antioxidant compounds. This beverage proved its effectiveness in stimulating the growth of the probiotic strain *L. reuteri*. In addition, a high potential for maintaining cellular viability was observed, with the number of viable metabolically active cells recorded in the beverage positively modulated by the addition of pollen.

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- N. Tritean et al., "Selenium-Fortified Kombucha–Pollen Beverage by In Situ Biosynthesized Selenium Nanoparticles with High Biocompatibility and Antioxidant Activity," Antioxidants, vol. 12, no. 9, p. 1711, 2023.
- [2]. J. S. Algethami et al., "Bee pollen: Clinical trials and patent applications," Nutrients, vol. 14, no. 14, p. 2858, 2022.
- [3]. A. Pasqualone, C. Summo, B. Laddomada, E. Mudura, and T. E. Coldea, "Effect of processing variables on the physicochemical characteristics and aroma of borş, a traditional beverage derived from wheat bran," Food chemistry, vol. 265, pp. 242-252, 2018.

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