Book of Abstracts

Exploratory Workshop

chemNEXT

"INNOVATIVE CROSS-SECTORAL TECHNOLOGIES"

VIIIth edition

May 25-26

2026

Organized by INCDCP – ICECHIM,
with the recognition of the European Chemical Society (EuChemS), under high patronage of the Technical Sciences Academy of Romania

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Book of Abstracts comprising scientific contributions presented at the

Exploratory Workshop *NeXT-Chem: Innovative Cross-Sectoral Technologies*

25-26 May 2026

National Institute for Research & Development
in Chemisty and Petrochemistry - ICECHIM Bucharest

ISSN: 2821 – 6784
ISSN-L: 2821 – 6784

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Foreword

The VIIIth edition of the **Exploratory Workshop** ***NeXT-Chem: Innovative Cross-Sectoral Technologies***, held on 25–26 May 2026 at the headquarters of the National Institute for Research and Development in Chemistry and Petrochemistry – ICECHIM Bucharest, marked another important step in the institute's continuous efforts to foster excellence in research and innovation.

Dedicated especially to master's and PhD students, as well as early-career researchers, NeXT-Chem VII offered a platform for young scientists to present their work, exchange ideas, and engage in cross-sectoral dialogue. By adopting a hybrid format, the workshop welcomed participants from across Romania and abroad, ensuring broader accessibility and encouraging international collaboration.

This year, 32 young researchers from cities including Bucharest and Iași – as well as from Kazakhstan and Pakistan – contributed presentations aligned with national priorities outlined in the National Plan for Research, Development and Innovation and the National Strategy for Research, Innovation and Smart Specialization (2022– 2027).

The workshop featured 39 submitted papers, enhanced by invited lectures delivered by established experts in chemical engineering, physical sciences, and agricultural research, offering participants valuable insights into current challenges and emerging directions in applied science.

We are confident that the knowledge shared and the connections made during this event will contribute to shaping the future of research, while inspiring the next generation of innovators.

Invited lectures

NANOSCALE BIODEGRADABLE POLYMERS FOR PACKAGING MICROSCALE FLUIDS

COARA PRINCIPLES – WHAT THEY ARE & HOW THEY APPLY FOR RESEARCH EVALUATION

ELECTRON MICROSCOPY: FROM SAMPLE PREP TO DATA INTERPRETATION

METHODOLOGICAL FRAMEWORKS FOR INTEGRATING BIODEGRADABLE MATERIALS INTO CONSUMER PRODUCT DESIGN

SIMPLE ACCESS TO COMPLEX INNOVATION

ALTERNATIVE APPROACH TO SCIENCE PRESENTATIONS

EUCHEMS & SCHR

NANOSCALE BIODEGRADABLE POLYMERS FOR PACKAGING MICROSCALE FLUIDS

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Introduction: Packaging microscale fluids requires thin, robust, and preferably biodegradable materials that can form directly at liquid interfaces without the use of organic solvents, complex equipment, or harsh processing conditions. In this talk, we present WRAPPINGS — Water-based, Room-temperature, Atmospheric Pressure Polymerization of INstant Glues controlled by Surfactants — as a simple interfacial route to nanoscale poly(cyanoacrylate) films[1,2].

WRAPPINGS uses cyanoacrylate vapor and cationic surfactant-laden water interfaces to facilitate surfactant-modulated anionic polymerization. This results in nanoscale, controllable thin polymer films with tunable, uniform thickness on a macroscopic scale and a growth rate of approximately 8 nm/min. The thickness of the film, color, shape, and mechanical properties can be adjusted by changing the polymerization time, wetting conditions, and patterned light exposure. This method enables in situ packaging of aqueous droplets, chemical and biological liquid cargos, and gases within solidified polymer shells. Because (poly)cyanoacrylates are biocompatible and biodegradable, WRAPPINGS provides a versatile platform for soft, programmable, and sustainable packaging of microscale fluids[1].

References:

[1]. Jampani, V. S. R. et al. Water-Templated Growth of Interfacial Superglue Polymers for Tunable Thin Films and In Situ Fluid Encapsulation. Advanced Materials 36, 2408243 (2024).

[2]. Jampani, V. S. R. & Anyfantakis, M. Packaging of Macroscopic Material Payloads: Needs, Challenges, Concepts, and Future Directions. Adv. Eng. Mater. 28, 9 (2026).

COARA PRINCIPLES – WHAT THEY ARE & HOW THEY APPLY FOR RESEARCH EVALUATION

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Introduction: The way research is assessed has a profound influence on scientific careers, funding decisions, institutional strategies, and the overall direction of research and innovation. In recent years, concerns have emerged regarding the excessive reliance on simplified quantitative indicators, such as publication counts, citation-based metrics, and journal impact factors, which may not adequately capture the quality, diversity, and societal value of research contributions. In response to these challenges, the international research community has initiated a broad reform movement aimed at promoting more responsible and holistic approaches to research assessment.

This presentation introduces the principles and objectives of the Coalition for Advancing Research Assessment (CoARA), placing them within the broader context of global initiatives such as the San Francisco Declaration on Research Assessment (DORA) and the Leiden Manifesto for Research Metrics. It explains the rationale behind the ongoing reform, the key principles promoted by CoARA, and the ways in which these principles are being implemented by research organizations, universities, and funding agencies across Europe.

Particular attention is given to the recognition of diverse research contributions, the responsible use of metrics, qualitative and context-sensitive assessment practices, and the growing role of Open Science in contemporary evaluation frameworks. At the same time, the presentation critically examines potential challenges associated with the reform process, including increased subjectivity, evaluator bias, difficulties in standardization, the resource demands of qualitative assessment, and tensions arising from misconceptions about Open Access publishing and research quality.

By exploring both the opportunities and limitations of the new assessment paradigm, the presentation aims to provide a balanced perspective on research assessment reform and to stimulate discussion on how institutions can achieve a more transparent, fair, and meaningful evaluation system that supports scientific excellence, innovation, and societal impact.

ELECTRON MICROSCOPY: FROM SAMPLE PREPARATION TO ADVANCED ANALYTICAL CHARACTERIZATION IN MATERIALS AND LIFE SCIENCES

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Introduction: Electron microscopy has become one of the most powerful and versatile characterization techniques in modern materials science, nanotechnology, engineering, and life sciences. The combination of high spatial resolution, analytical capabilities, and multimodal imaging enables the investigation of materials from the micrometer scale down to individual atomic columns. Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM) provide complementary information regarding morphology, structure, composition, crystallography, and functional properties that cannot be obtained using conventional optical microscopy.

A critical precondition for obtaining reliable and meaningful results is appropriate sample preparation. In SEM, proper mounting, dispersion, conductive coating, and charge mitigation are essential for achieving high-quality images and avoiding imaging artefacts such as charging, distortion, and loss of resolution. For TEM, specimen preparation is even more demanding because samples must be electron-transparent, typically below 100 nm in thickness. Techniques such as mechanical thinning, ion milling, focused ion beam (FIB) preparation, cross-sectional lamella fabrication, and cryogenic vitrification are employed to preserve the native structure of materials and biological specimens while minimizing preparation-induced damage. Poor preparation can introduce contamination, amorphization, aggregation, thickness variations, or structural artefacts that may lead to incorrect interpretation of results.

The importance of electron microscopy extends across both materials and life sciences. In materials research, SEM and TEM are indispensable for investigating grain structures, interfaces, thin films, coatings, nanomaterials, defects, dislocations, porosity, phase distributions, and failure mechanisms. In life sciences, these techniques enable visualization of cells, tissues, bacteria, viruses, biomaterials, and biological ultrastructures with nanometer and sub-nanometer resolution. Cryo-TEM has revolutionized structural biology by allowing biological specimens to be observed in a near-native hydrated state, while SEM provides detailed information on cell morphology, biofilms, tissue surfaces, and forensic evidence.

SEM primarily provides information regarding surface topography, morphology, particle size and shape, porosity, fracture mechanisms, and microstructural features through secondary electron (SE) and backscattered electron (BSE) imaging. When coupled with Energy Dispersive X-ray Spectroscopy (EDX/EDS), SEM additionally enables qualitative and semi-quantitative elemental analysis, elemental mapping, phase identification, contamination detection, and compositional distribution studies. These capabilities make SEM a valuable tool for quality control, failure analysis, forensic investigations, biomaterial characterization, and advanced materials development.

TEM offers substantially higher resolution and provides access to internal structural information. Conventional TEM imaging, high-resolution TEM (HRTEM), selected area electron diffraction (SAED) allows direct determination of crystal structure, lattice spacing, grain orientation, defects, interfaces, and atomic arrangements. Scanning Transmission Electron Microscopy (STEM), particularly High-Angle Annular Dark-Field (HAADF) and Annular Bright-Field (ABF) imaging, enables atomic-scale Z-contrast imaging and visualization of individual atomic columns. Advanced analytical TEM techniques further extend characterization capabilities. EDX mapping performed in STEM mode provides nanoscale elemental distribution, while Electron Energy Loss Spectroscopy (EELS) delivers information on light elements, oxidation states, bonding environments, electronic structure, optical properties, plasmonic behavior, and even single-atom spectroscopy. Combined TEM/STEM-EDX-EELS investigations allow simultaneous correlation of structure, chemistry, crystallography, and electronic properties from the same region of interest.

Modern electron microscopy therefore represents a comprehensive analytical platform capable of providing morphological, structural, crystallographic, compositional, chemical, electronic, optical, and three-dimensional information across an exceptionally broad range of materials and biological systems. The combination of advanced imaging modes with spectroscopic techniques such as EDX, EELS, STEM, tomography, electron holography, and in-situ experimentation continues to expand the scientific impact of electron microscopy, enabling researchers to directly correlate nanoscale structure with material performance and biological function.

METHODOLOGICAL FRAMEWORKS FOR INTEGRATING BIODEGRADABLE MATERIALS INTO CONSUMER PRODUCT DESIGN

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Keywords: biodesign; consumer product design; food waste; sensorial identity; practice-based design research; circular economy

Introduction: The catastrophic environmental impact of fossil-fuel-based plastics has triggered a radical paradigm shift in industrial and product design toward circular, bio-based methodologies. While the traditional plastics market continues to expand globally, Europe's market dynamics reveal a stagnation in recycling rates alongside a rapidly growing bioplastics sector driven by strict EU regulations. Concurrently, millions of tons of food waste are generated annually, offering an abundant, alternative source of second-generation raw materials rich in natural polymers.

This paper explores the integration of organic waste into everyday consumer products through advanced processing techniques, specifically highlighting extrusion, injection molding, and 3D printing. Rather than treating materials as passive substrates, modern biodesign synthesizes a Transdisciplinary Methodology that bridges scientific laboratory protocols with Practice-based Design Research and Material Tinkering. By analyzing the foundational frameworks of leading researchers, this study evaluates how "tinkering" acts as a cognitive tool where non-linear exploration and material dialogue take precedence.

Special emphasis is placed on the *Materials Experience* framework, examining how the unique Sensorial Identity of bio-composites—such as the natural olfactory aroma of spent coffee grounds, the iridescent visual textures of living bacteria, or the earthy tactile warmth of mycelium—serves as a crucial design tool. Altering raw biological parameters directly translates into evolutionary sensory qualities, fostering user empathy and emotional longevity, which in turn discourages premature product disposal. Finally, the paper addresses systemic barriers to commercialization, including unformalized supply chains and the current lack of scalable mass-production technologies, charting a course for the future transition from artisanal bio-artifacts to mass-manufactured, circular everyday objects.

ALTERNATIVE APPROACH TO SCIENCE PRESENTATIONS

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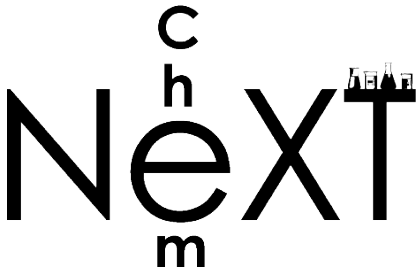
Introduction: Science and humor may seem like two different worlds, but together they create a powerful way to communicate knowledge. Humor makes complex scientific topics easier to understand, reduces stress, and captures the audience's attention. By combining accurate information with relatable jokes, science becomes more engaging, memorable, and human. In the end, laughter is not the opposite of seriousness, it is often the best way to connect people with science.

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



FINITE ELEMENT-BASED ASSESSMENT OF STRESS DISTRIBUTION IN DENTAL IMPLANTS UNDER DIFFERENT OSSEOINTEGRATION CONDITIONS

RAPID SCREENING METHOD FOR IMAZALIL AND THIABENDAZOLE IN CITRUS

ENGINEERING CALCIUM-BINDING POLYMERIC MEMBRANES VIA CROWN ETHER FUNCTIONALIZATION FOR IMPLANTOLOGY APPLICATIONS

BAGHDADITE AS A PROMISING CERAMIC FOR BONE TISSUE ENGINEERING: SYNTHESIS, BIOCOMPATIBILITY ASSESSMENT AND 3D PRINTING INTEGRATION

NITRONYL NITROXIDE DI- AND TRIRADICAL LIGANDS OBTAINED VIA SCHIFF CONDENSATION AND THEIR COMPLEXES

NEW INSIGHTS INTO ELECTROCHEMICAL SENSING OF LIPOPOLYSACCHARIDES BY BIOMIMETIC SENSORS MODIFIED WITH MOLECULARLY IMPRINTED POLYMERS

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PRELIMINARY ASSESSMENT OF FUNCTIONAL MONOMER-COCAINE INTERACTIONS WHEN PREPARING MOLECULARLY IMPRINTED POLYMERS

SYNTHESIS AND MAGNETIC PROPERTIES OF A FAMILY OF DINUCLEAR LANTHANIDE COMPLEXES DERIVED FROM 2(PHTHALIMIDOMETHYL)-NITRONYLNITROXIDE

MATERIALS CONTAINING CARBON DOTS FOR IMPROVED NAPROXEN RELEASE

NOVEL STRATEGIES FOR THE SYNTHESIS OF 4f AND 4f-4f' COMPLEXES DERIVED FROM SCHIFF BASE LIGANDS

PERSPECTIVES ON MICROPLASTICS FROM SPORTS ACTIVITIES

RATIONAL DESIGN OF POLY(2ISOPROPENYL-2-OXAZOLINE) HYDROGELS FOR CONTROLLED DRUG LOADING AND DELIVERY

MULTIFUNCTIONAL LUMINESCENT- THERMORESPONSIVE FILMS COMBINING EUROPIUM COMPLEXES AND CHOLESTERIC LIQUID CRYSTALS

PHYTO-DERIVED METAL AND METAL OXIDE NANOPARTICLES FOR BIOMEDICAL AND ENVIRONMENTAL APPLICATIONS

INFLUENCE OF Mg^{2+}, Sr^{2+}, AND Zn^{2+} DOPANT IONS ON CALCIUM PHOSPHATE COMPOSITE SCAFFOLDS FOR BIOMEDICAL APPLICATIONS

BIOLOGICAL DEGRADATION OF ARTIFACTS

CRYSTAL ENGINEERING OF 1,10 PHENANTHROLINE DERIVATIVES

INNOVATIVE ARTIFICIAL INTELLIGENCE TECHNOLOGIES FOR CHEMISTRY APPLICATIONS

DESIGN AND EVALUATION OF MOLECULAR WEIGHT-DEPENDENT CHITOSAN NANOPARTICLES FOR 5-FU DRUG DELIVERY

FINITE ELEMENT-BASED ASSESSMENT OF STRESS DISTRIBUTION IN DENTAL IMPLANTS UNDER DIFFERENT OSSEOINTEGRATION CONDITIONS

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Keywords: dental implants; osseointegration; finite element analysis; stress distribution; biomechanical modeling

Introduction: Dental implants represent one of the most effective solutions for oral rehabilitation, with long-term success strongly influenced by the degree of osseointegration between the implant surface and the surrounding bone tissue. Insufficient osseointegration may lead to stress concentration at the implant–bone interface, potentially affecting implant stability and long-term performance. Finite element analysis (FEA) is widely used in biomechanical studies for evaluating the mechanical behavior of implant systems and for predicting stress distribution under simulated loading conditions[1,2,3].

Materials and methods: A simplified three-dimensional finite element model was developed consisting of a titanium dental implant inserted into a bone structure composed of cortical and trabecular layers. Material properties were assigned according to literature data. Mechanical loading conditions simulating masticatory forces were applied both vertically and obliquely. Three osseointegration scenarios were considered by modifying the mechanical interaction between the implant and the surrounding bone tissue: low osseointegration, moderate osseointegration, and complete osseointegration. The resulting stress distribution was evaluated using the von Mises stress criterion.

Results: The numerical simulations indicate that the degree of osseointegration significantly influences the stress distribution in the implant–bone system. Reduced osseointegration leads to higher stress concentrations, particularly in the cervical region of the implant and in the adjacent cortical bone. Complete osseointegration results in a more uniform stress distribution and improved mechanical stability.

Conclusions: The results highlight the importance of adequate osseointegration for ensuring the mechanical stability and long-term performance of dental implants. Finite element modeling represents a useful predictive tool for investigating implant biomechanics and can support future experimental and clinical research.

References:

[1]. Geng JP, Tan KB, Liu GR. Application of finite element analysis in implant dentistry: a review of the literature. J Prosthet Dent. 2001 Jun;85(6):585-98. doi: 10.1067/mpr.2001.115251. PMID: 11404759.
[2]. Falcinelli C, Valente F, Vasta M, Traini T. Finite element analysis in implant dentistry: State of the art and future directions. Dent Mater. 2023 Jun;39(6):539-556. doi: 10.1016/j.dental.2023.04.002. Epub 2023 Apr 18. PMID: 37080880.
[3]. Nokar S, Jalali H, Nozari F, Arshad M. Finite Element Analysis of Stress in Bone and Abutment-Implant Interface under Static and Cyclic Loadings. Front Dent. 2020 Sep;17(21):1-8. doi: 10.18502/fid.v17i21.4315. Epub 2020 Sep 7. PMID: 33615298; PMCID: PMC7883651.

RAPID SCREENING METHOD FOR IMAZALIL AND THIABENDAZOLE IN CITRUS PATENT:RO-BOPI 11/2025, 138394 A_3 (51) G01N 30/02

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Keywords: citrus; imazalil and thiabendazole; HPLC

Introduction: The invention relates to the rapid screening method of imazalil and thiabendazole from citrus fruits with applicability in the field of food safety. The European Food Safety Authority (EFSA) in the technical report approved in March 2023, based on member countries' reports on official controls on pesticide residues in food products, stated among other things: citrus fruits, seed fruits, and fresh herbs are the product groups with the highest detection frequency of pesticide residues. More than 90% of the samples analyzed contained one or more residues.

Materials and methods: The method, according to the invention, consists of the following steps: (1) Preparation of standard stock solutions of imazalil and thiabendazole; (2) Preparation of working standard solutions; (3) Citrus sample extraction (i.e., grapefruit, oranges, lemons, limes and mandarines); (4) Chromatographic determination; (5) Instrumental determination; (6) Quantitative determination.

Results: Regarding the presence of the two fungicides in the analyzed samples, it is found that out of the 19 analyzed samples, 18 samples contain pesticide residues in variable quantities.

Conclusions: The proposed screening method is rapid (about 40 minutes), with a limit of detection (LOD) set at 0.003 mg/kg for imazalil and 0.00045 mg/kg for thiabendazole and a limit of quantification (LOQ) set at 0.01 mg/kg for imazalil and respectively 0.0015 mg/kg for thiabendazole, with high sensitivity regarding the simultaneous determination of the two pesticides from different categories of samples. By applying the invention, the following advantages are obtained: reduced working time (aprox. 40 minutes); reduced amounts of reagents; effective application of the screening method regardless of the studied citrus category; no equipment or consumables are needed in the sample preparation stage that require high costs, utilities or special training of the operator; working parameters are identical for citrus fruits (i.e., lemons, mandarines, grapefruits, oranges, limes), which allows the simultaneous determination of imazalil and thiabendazole from different categories of samples; low degree of toxicity of the resulting products (residues).

ENGINEERING CALCIUM-BINDING POLYMERIC MEMBRANES VIA CROWN ETHER FUNCTIONALIZATION FOR IMPLANTOLOGY APPLICATIONS

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Keywords: covalent functionalization; biomineralization; interface engineering; hybrid materials

Introduction: Surface engineering of polymeric membranes has emerged as an effective strategy for developing multifunctional materials with applications spanning water treatment and biomedicine[1]. Among these approaches, covalent functionalization enables the stable incorporation of active molecules while preventing their release into surrounding environments. In this context, macrocyclic compounds such as crown ethers offer unique selectivity toward specific ions, making them promising candidates for biomedical interface design[2].

Materials and methods: In this study, crown ethers were covalently immobilized onto polymeric membranes to obtain hybrid systems with enhanced ion-recognition capabilities. The developed materials were designed for biomedical applications, particularly as coatings for dental and orthopedic implants. The functionalization strategy aimed to promote calcium ion affinity, as elevated Ca^{2+} concentration at the material surface is known to stimulate biomineralization and improve osseointegration[3].

Results: Successful functionalization was confirmed through XPS and ATR-FTIR analyses, highlighting the incorporation of crown ether moieties within the membrane structure. The calcium retention capacity was quantified by ICP-MS measurements, demonstrating improved ion affinity compared to unmodified membranes. Biomineralization potential was further evaluated using a Taguchi experimental design, while morphological and structural changes were assessed by SEM, EDS, and XRD analyses. The results indicated enhanced calcium phosphate formation on functionalized membranes.

Conclusions: The developed crown ether–functionalized membranes exhibited significantly improved calcium ion retention and promoted *in vitro* biomineralization processes. These findings demonstrate the potential of such hybrid materials as advanced platforms for biomedical applications, particularly in implant surface modification and tissue integration.

References:

[1]. Oprea, M.; Voicu, S.I. Recent Advances in Composites Based on Cellulose Derivatives for Biomedical Applications. Carbohydr. Polym. 2020, 247, 116683.

[2]. Oprea, M.; Pandele, A.M.; Enachescu, C.I.; Antoniac, I.V.; Voicu, S.I.; Fratila, A.M. Crown Ether-Functionalized Polyethersulfone Membranes with Potential Applications in Hemodialysis. *Polymers* 2025, *17*, 2184.

[3]. Oprea, M.; Pandele, A.M.; Nicoara, A.I.; Nicolescu, A.; Deleanu, C.; Voicu, S.I. Crown-Ether Functionalized Cellulose Acetate Membranes with Potential Applications in Osseointegration. Int. J. Biol. Macromol. 2023, 230(1), 123162.

BAGHDADITE AS A PROMISING CERAMIC FOR BONE TISSUE ENGINEERING: SYNTHESIS, BIOCOMPATIBILITY ASSESSMENT AND 3D PRINTING INTEGRATION

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Keywords: baghdadite; sol-gel synthesis; biocompatibility; robocasting; rheological behavior.

Introduction: Baghdadite ($Ca_3ZrSi_2O_9$) is a promising ceramic biomaterial, known for its excellent role in bone regeneration by stimulating cell adhesion, proliferation, and osteogenic differentiation[1,2].The objective of this study was to evaluate the synthesis of baghdadite via the sol-gel method, assess its biocompatibility through in vitro cellular assays, and investigate its integration into 3D-printed scaffolds. To this end, the rheological behavior of baghdadite-based pastes was systematically characterized, and various combinations of additives and baghdadite powder were explored in order to optimize paste printability. The influence of formulation parameters on viscosity, extrudability, and shape retention was assessed, with the aim of identifying optimal ink compositions capable of producing structurally stable, porous scaffolds suitable for bone tissue engineering applications.

Materials and methods: $Ca_3ZrSi_2O_9$ (C_3ZS_2) powder was synthesized using the sol-gel method and its physicochemical properties were evaluated. Biocompatibility was evaluated in vitro according to ISO 10993-5[3], using human fetal osteoblasts (hFOB, 1×10^5 cells/mL) cultured for 6 days in direct contact with baghdadite pellets sintered under different thermal treatment conditions (1350°C, varying heating rates of 2–10°C/min and dwell times of 1.5–3h). Cell morphology was assessed by optical microscopy (Leica), while cell viability was quantified by confocal microscopy (Zeiss LSM 880) using the LIVE/DEAD assay. For 3D printing integration, baghdadite-based pastes were formulated by combining baghdadite powder with various organic additives, including HPMC (5%), Baymedix (polyurethane solution) and Pluronic F-127 (30%) and characterized rheologically via amplitude sweep tests (Anton Paar MCR 302e). Scaffolds were fabricated by robocasting using a 3D-BIOPLOTTER EnvisionTEC Starter. Thermal debinding and sintering profiles were established based on DSC-TG analysis.

Results: In vitro biocompatibility testing demonstrated that all sintered baghdadite samples supported hFOB adhesion, proliferation, and maintenance of osteoblastic morphology over 6 days, with high cell viability across all conditions as confirmed by the LIVE/DEAD assay. Rheological characterization of the optimal paste formulation (C_3ZS_2+ HPMC 5% + Baymedix) revealed a well-defined linear viscoelastic region with storage modulus G' ~10^5 Pa, a yield point at $\gamma \approx 0.1\%$ ($\tau \approx 900$ Pa), and a ductile yield behavior, all indicative of a paste suitable for robocasting. Among the tested formulations, this composition was the only one to produce stable, porous 3D-printed scaffolds (10×10×5 mm, 0°-45°-90°-135° layering pattern).

Conclusions: This study demonstrates the feasibility of fabricating porous baghdadite-based scaffolds via robocasting, integrating sol-gel synthesis, biocompatibility assessment, and rheological optimization into development of patient-specific, 3D-printed ceramic scaffolds for bone regeneration.

Acknowledgements: This work was supported by the Nucleu Program within the National Research Development and Innovation Plan 2022–2027, financed by Ministry of Research, Innovation and Digitization in the frame of contract no. 5N/2023 (Project: PN 23250201).

References:

[1]. Z.F. Lu, W.J. Zhang, Y.J. No, Y. Lu, S.M. Mirkhalaf Valashani, P. Rollet, L. Jiang, Y. Ramaswamy, C.R. Dunstan, X.Q. Jiang, H. Zreiqat, Baghdadite Ceramics Prevent Senescence in Human Osteoblasts and Promote Bone Regeneration in Aged Rats, ACS Biomater. Sci. Eng. 6 (2020) 6874–6885. https://doi.org/10.1021/acsbiomaterials.0c01120.

[2]. Z.F. Lu, G.C. Wang, I. Roohani-Esfahani, C.R. Dunstan, H. Zreiqat, Baghdadite ceramics modulate the cross talk between human adipose stem cells and osteoblasts for bone regeneration, Tissue Eng. Part A 20 (2014) 992–1002. https://doi.org/10.1089/ten.tea.2013.0470.

[3]. ISO 10993-5:2009(en), Biological evaluation of medical devices — Part 5: Tests for in vitro cytotoxicity, (n.d.). https://www.iso.org/obp/ui/en/#iso:std:iso:10993:-5:ed-3:v1:en (accessed February 18, 2026).

NITRONYL NITROXIDE DI- AND TRIRADICAL LIGANDS OBTAINED VIA SCHIFF CONDENSATION AND THEIR COMPLEXES

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Keywords: nitronyl nitroxide, radical, complex, EPR, magnetism

Introduction: The design of ligands incorporating nitronyl nitroxide (NN) unit(s) generally follows two principal synthetic strategies. In the first approach, aldehyde functionalities present in the molecular scaffold are converted into the corresponding NN radicals, thereby directly generating the target ligand[1]. In the second approach, a preformed NN radical is covalently attached to a substrate *via* suitable reactions such as cross-coupling[2], alkylation[3] or, as in the present case, Schiff condensation[4].

Results: The NN bearing free formyl unit, HL^1, has been used to form di- and triradical ligands with various amines: notably 4-amino-TEMPO (HL^2) andtris(2-aminoethyl)amine (H_3L^3) (Figure 1). The paramagnetic ligands have been reacted with hexafluoro acetyl acetonate ($hfac^-$) complexes ($[M(hfac)_2(H_2O)_2]$ and $[Ln(hfac)_3(H_2O)_2]$ where M = Co, Ni, Zn andLn = Gd, Tb, Dy) yielding mono-, di- and trinuclear complexes with various topologies. The structures have been analyzed using X-ray diffraction on single crystal both for the ligands and the complexes and the EPR spectra have been recorded for the ligands indicating exchange interactions between radical moieties.

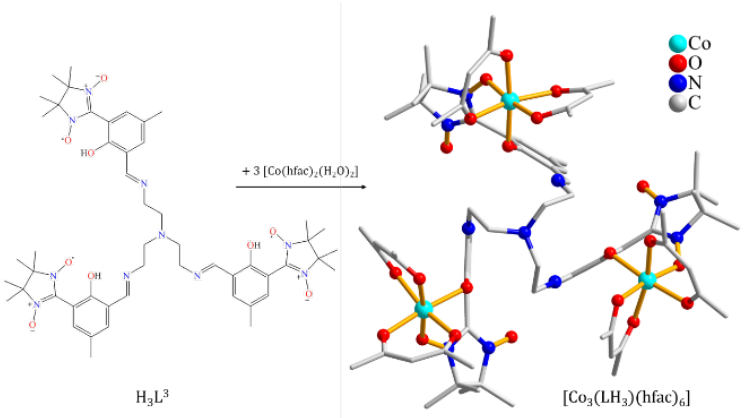

Figure 1. The crystalstructure of thetrinuclear complex $[Co_3(L^3H_3)(hfac)_6]$ obtainedfromtripodaltriradicalligand H_3L^3.

***Acknowledgements**: This work was supported by a grant of the Ministry of Education and Research, CCCDI - UEFISCDI, project number PN-IV-P6-6.1-CoEx-2024-0053, within PNCDI IV and from European Union through the Next Generation EU-PNRR−III-C9-2022-I8 program (contract no. 760230). The authors are grateful to Bing-Wu Wang, Anamaria Hanganu, and Victorița Tecuceanu for their assistance with the analyses.*

References:

[1]. Caneschi A, Gatteschi D, Rey P, Progress in Inorganic Chemistry, 1989;37:331-421.
[2]. Zayakin IA, Romanenko GV, Korlyukov AA, Tretyakov EV, Organometallics, 2025;*44*:892-8.
[3]. Dimitriu Ș, Răducă M, Tecuceanu V, Hanganu A, Andruh M, Revue Roumaine de Chimie, 2024;69:279-84.
[4]. Răducă M, Carrella LM, Ionita G, Toderașc AT, Rentschler E, Andruh M, Crystal Growth & Design, 2025;25:9475-86.
[5]. Pang, X., & Deng, B. (2008). *Investigation of changes in properties of water under the action of a magnetic field.* Science in China Series G: Physics, Mechanics & Astronomy, 51(11), 1621–1632. https://doi.org/10.1007/s11433- 008-0182-7.
[6]. Al-Khazan, M., & Al-Assaf, N. (2009). *Effect of magnetically treated water on tomato growth and yield*. World Applied Sciences Journal, 7(3), 399–404.

NEW INSIGHTS INTO ELECTROCHEMICAL SENSING OF LIPOPOLYSACCHARIDES BY BIOMIMETIC SENSORS MODIFIED WITH MOLECULARLY IMPRINTED POLYMERS

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Keywords: endotoxin detection; surfactants; molecularly imprinted silica particles; lipopolysaccharides

Introduction: The identification of bacterial endotoxins, also referred to as lipopolysaccharides (LPS), is essential for overcoming environmental and healthcare issues related to mutations and the worldwide spread of pathogenic microorganisms[1]. In addition to causing multiple diseases, including septic shock, LPS has lately been linked to the onset of Parkinson's disease. Conventional techniques used to detect LPS in clinical and research contexts, like the Limulus amebocyte lysate (LAL) assay and the enzyme-linked immunosorbent assay (ELISA), have serious limitations[2]. These conventional approaches frequently have poor sensitivity and require laborious, complex procedures. As a result, there is a growing need for the development of novel, economical, and effective techniques, such as electrochemical detection[3], particularly in the domains of environmental science and medicine. This work describes the design and embedment of amino functionalized MIPs silica particles for selective recognition of a specific targeted type of LPS (i.e., LPS from *P. aeruginosa*) into lab-made carbon paste formulation in order to obtain new and feasible biomimetic sensors for LPS detection.

Materials and methods: The amino-functionalized MIP silica particles were synthesized using the Stöber method in the presence of the target molecule LPS via polycondensation of the functional monomer 3-Aminopropyltriethoxysilane (APTES) and the structural monomer, tetraethyl orthosilicate (TEOS) in basic medium. Herein, two types of cationic surfactants namely cetyltrimethylammonium bromide (CTAB) and benzyl trimethyl ammonium chloride (BTAC) were utilized to stimulate and control the formation of silica nanoparticles. Further on, the MIP silica nanoparticles were embedded in a carbon paste containing ZnO electroactive nanoparticles, a polyether-based binder, and a compatible solvent. The obtained formulations were drop-casted on the working electrode of ceramic screen-printed carbon electrodes (SPCEs) and cured using thermal treatment.

Results: Computational docking has been assessed to anticipate the binding affinity of APTES towards LPS in order to assess the capacity of MIP nanoparticles to recognize LPS. The ^{1}H-NMR and XPS data supported the docking predictions. Other modern techniques, including structural and morphological analyses, were employed to characterize the obtained MIPs particles in both raw phase and after their embedment and deposition on the carbon electrode. The batch rebinding experiments on MIP particles alongside electrochemical analyses (Cyclic voltammetry, Differential pulse voltammetry and Electrochemical impedance spectroscopy) for the obtained biomimetic sensors were employed to determine the imprinting factor, LOD, LOQ, and electrochemical active surface area of the electrode. The assays were extended to other interferents, including LPS from other bacterial strains as *E. coli* and *S. enterica* and also bovine serum albumin (BSA) to examine their specificity and selectivity. Finally, the sensors were subjected to regeneration and reconditioning protocols for life-cycle assessment.

Conclusions: Overall, the obtained biomimetic sensors based on LPS-MIP silica nanoparticles proved to be effective for the detection of lipopolysaccharide from *P. aeruginosa*.

***Acknowledgements**: The authors gratefully acknowledge the financial support from the grant of the Ministry of Research, Innovation and Digitization, CNCS UEFISCDI, project number PN-IV-P2-2.1-TE-2023-1293, ctr. 40TE/2025, within PNCDI IV and the technical support through project AQUAMAT 2N/03.01.2023 (PN 23.06.01.01.)*

References:

[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 Disorders 2023,38, 1143–1155.
[3]. Neagu A-L et al. 3D inkjet printing of hybrid electroactive ink based on molecularly imprinted polymers for lipopolysaccharides detection, Electrochimica Acta, 506, 2024, 145044

VALORIZATION OF LACTIC ACID-MODIFIED NANOCELLULOSE IN THE PREPARATION OF BIONANOCOMPOSITES

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Keywords: cellulose nanofibers; (poly)lactic acid; (poly)3-hydroxybutyrate-co-3-hydroxyvalerate; bionanocomposites

Introduction: The rapid exhaustion of fossil resources and increasing awareness of the environmental problems arising from oil processing and use of oil-derived plastics, have sent the scientific world on a quest to develop biobased and biodegradable plastics to replace the traditional petroleum-based ones. (Poly)lactic acid (PLA) appears to be an attractive substitute for traditional plastics like polyethylene or polyethylene terephthalate, especially in the packaging industry, due to its origin from renewable resources, biodegradability in certain composting conditions, non-toxicity, good mechanical strength, and processability[1]. However, PLA presents rather poor gas barrier properties, high stiffness, and low crystallinity. Melt blending PLA with another well-known biopolymer, poly(3-hydroxybutyrate-*co*-3-hydroxyvalerate) (PHBV), can increase the crystallinity of PLA, improve its oxygen and water vapor barrier properties[2], and enhance its flexibility and biodegradability[1]. However, relative to PLA, PHBV possesses lower thermal stability, narrower processing window, with its melting temperature being close to its thermal degradation temperature, and is less commercially available and more expensive[1]. In addition, the miscibility of PLA and PHBV is rather poor and heavily dependent on their ratio in the blend, with various agents being added to the PLA/PHBV blends to improve the compatibility and miscibility between the two polymers[2]. In this work, we ventured towards the preparation of 50/50 w/w PLA-PHBV blends and the use of lactic acid-modified cellulose nanofibers (LACNF) to improve the compatibility between PLA and PHBV as well as the thermal and mechanical properties of the PLA-PHBV blends.

Materials and methods: LACNF were obtained by the esterification of microcrystalline cellulose with lactic acid followed by mechanical fibrillation. The PLA-PHBV blend and PLA-PHBV/LACNF nanocomposites with varying LACNF contents were obtained by melt-blending followed by compression molding. LACNF were characterized in terms of chemical structure, thermal stability, and morphology by Fourier-transform IR spectroscopy (FTIR), thermogravimetric analysis (TGA), and atomic force microscopy (AFM), respectively. The thermal characteristics of the resulting blend/composites were investigated by TGA and differential scanning calorimetry (DSC), their mechanical properties were evaluated by dynamic mechanical analysis, while their morphology and distribution of LACNF in the PLA/PHBV blends were studied by scanning electron microscopy (SEM) and AFM.

Results: At low amounts of LACNF in the PLA-PHBV blends of 0.5 and 1 wt%, respectively, LACNF facilitated crystallization and enhanced the thermal and mechanical performance of the blend. The SEM micrographs showed that NCLA acts as a capable compatibilizer that enhances the miscibility of PLA and PHBV.

Conclusions: LACNF shows potential as both compatibilizer and reinforcing agent in the PLA/PHBV system, while the resulting PLA-PHBV/LACNF bio-nanocomposites can be considered sustainable and easy-to-obtain alternatives for traditional petroleum-based plastics.

***Acknowledgements**: This work was supported by a grant of the Ministry of Education and Research, CNCS - UEFISCDI, project number PN-IV-P1-PCE-2023-1557, contract 37PCE/2025 (WASTE2COAT) within PNCDI IV and project PN23.06.01.01/2022 AQUAMAT, within PN23.06 Core Program-ChemNewDeal.*

References:

[1]. NaserA.Z., DeiabI., DarrasB.M.Poly(lactic acid) (PLA) and polyhydroxyalkanoates (PHAs), green alternatives to petroleum-based plastics: a review. RSC Adv.2021;11(28):17151–17196.

[2]. González-AusejoJ., Gámez-Pérez J., BalartR., LagarónJ.M., CabedoL., Effect of the addition of sepiolite on the morphology and properties of melt compounded PHBV/PLA blends,Polym. Compos. 2017;40(S1):E156-E168.

NITRONYL NITROXIDE STABLE RADICALS DERIVED FROM NITRO-*O*-VANILLIN AND BISPHENOL A AS LIGANDS TOWARDS 3D AND 4F METAL IONS

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Keywords: nitronyl nitroxide; radical ligands; heterospin complexes; qubit properties

Introduction: Heterospin compounds may be synthesized using stable radicals and metal ions.[1] The nitronyl nitroxide organic radical derived from nitro-*o*-vanillin with 3*d* (Mn, Co, Ni, Zn) and 4*f* (Gd, Tb, Dy) metal ions led to 2*p*-3*d*, 2*p*-4*f* and 2*p*-3*d*-4*f* heterospin complexes while the diradical derived from bisphenol A with 3*d* (Co, Ni) metal ions led to 2*p*-3*d* heterospin complexes.[2,3,4]

Materials and methods: The structures of the obtained compounds have been solved by single-crystal x-ray diffraction and investigated by X-ray powder diffraction, elemental analysis, mass spectrometry and spectroscopic techniques (IR, UV-Vis).

Results: The cryomagnetic studies have revealed a strong magnetic interaction within the molecules, results which are sustained by theoretical DFT calculations. The mononuclear nickel and zinc complexes containing the nitronyl nitroxide derived from nitro-*o*-vanillin were investigated through pulse EPR to determine the spin-lattice relaxation time, T_1, and phase memory time, T_m, probing the qubit properties.

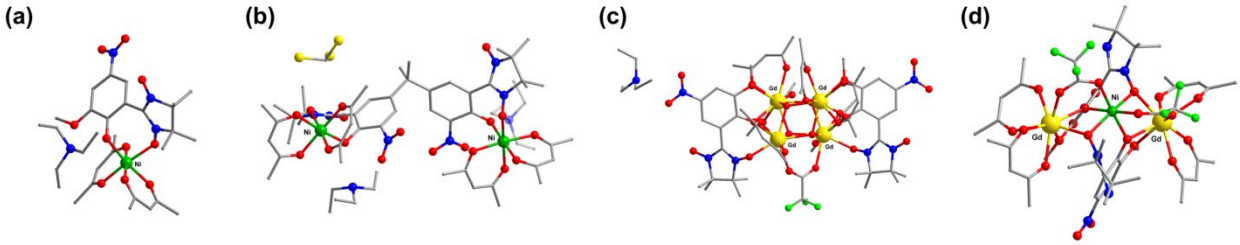

Figure 1. Crystal structure of (a), (b) 2*p*-3*d*, (c) 2*p*-4*f* and (d) 2*p*-3*d*-4*f* heterospin complexes.

***Acknowledgements**: This work was supported by a grant from Romanian Ministry of Education and Research, CCCDI - UEFISCDI, project number PN-IV-P6-6.1-CoEx-2024-0053, within PNCDI IV and from European Union through Next Generation EU-PNRR-III-C9-2022-I8 program (contract no. 760230).*

References:

[1]. Vaz MGF, Andruh M. Molecule-based magnetic materials constructed from paramagnetic organic ligands and two different metal ions. Coord Chem Rev. 2021;427: 213611.

[2]. Spinu CA, Pichon C, Ionita G, Mocanu T, Calancea S, Raduca M, Sutter JP, Hillebrand M, Andruh M. Synthesis, crystal structure, magnetic, spectroscopic, and theoretical investigations of two new nitronyl-nitroxide complexes. J Coord Chem. 2021;74:279–293.

[3]. Spinu CA, Martins DOTA, Mocanu T, Hillebrand M, Sutter JP, Tuna F, Andruh M. Two New 2p–3d Metal Complexes with a Nitronyl-Nitroxide Ligand Derived from o-Vanillin: Synthesis, Crystals Structures and Magnetic Properties. Magnetochemistry. 2024;10:86.

[4]. Spinu CA, Novitchi G, Hillebrand M, Mocanu T, Ionita G, Hanganu A, Tecuceanu V, Andruh M. Design of a new nitronyl-nitroxide biradical and its complexes: synthesis, crystal structures and magnetic properties. Cryst Eng Comm. 2025;27:6462–6472.

PRELIMINARY ASSESSMENT OF FUNCTIONAL MONOMER-COCAINE INTERACTIONS WHEN PREPARING MOLECULARLY IMPRINTED POLYMERS

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Keywords: functional monomers; cocaine; selective binding; molecularly imprinted polymers

Introduction: The rising use of illicit drugs has become an important concern for public health, environmental protection, and forensic analysis. Among these substances, cocaine remains one of the most commonly abused psychoactive stimulants[1]. Because of its pronounced activity on the central nervous system and its frequent recreational use, the development of reliable, sensitive, and selective methods for cocaine recognition is still highly relevant[2]. In this context, molecularly imprinted polymers (MIPs) offer an attractive approach for this purpose, as they can provide selective recognition sites together with good chemical stability and relatively low production costs[3]. Their recognition efficiency largely depends on the interactions established between the template and the functional monomer before polymerization. For this reason, evaluating the strength and nature of cocaine–monomer interactions is a key step in the rational design of selective imprinted materials[4]. In this work, both experimental and computational methods were used for an initial investigation of the interactions between cocaine and selected functional monomers. The aim was to identify suitable and cost-effective binding systems that could support the development of cocaine-MIPs with enhanced recognition performance.
Materials and methods: Cocaine–monomer pre-polymerization mixtures were examined by ^{1}H-NMR spectroscopy to identify intermolecular interactions through chemical shift variations. Molecular docking simulations were conducted to estimate preferential binding sites and relative binding affinities, while calculated logP (clogP) values were used to assess hydrophobicity, ionization behavior, and system compatibility. Preliminary adsorption experiments were also carried out to evaluate the binding behavior of the synthesized polymers, and the imprinting factor was calculated by comparing the performance of the MIPs with that of the corresponding non-imprinted polymers (NIPs).
Results: ^{1}H-NMR analysis indicated evidence of interactions between cocaine and the investigated functional monomers, reflected by modifications in proton chemical shifts within the pre-polymerization mixtures. These findings were further supported by molecular docking simulations, which predicted favorable binding regions and provided estimates of the relative affinities between the template and monomers. By combining computational screening with ^{1}H-NMR evaluation, an improved imprinting approach was developed, which required smaller amounts of cocaine than those typically reported in the literature. Despite the reduced template concentration, the preliminary adsorption studies revealed encouraging binding properties and a measurable imprinting factor, demonstrating that efficient molecular imprinting can be achieved while using lower template concentrations.
Conclusions: The results indicate that the proposed strategy could offer a cost-effective route for preparing molecularly imprinted polymers by reducing template consumption while preserving good recognition performance. The integration of experimental evaluation with computational pre-screening strategy demonstrates significant potential for optimizing cocaine-imprinted polymers designed for selective recognition applications.

***Acknowledgements**: The authors gratefully acknowledge the financial support from the grant of the Ministry of Research, Innovation and Digitization, CNCS UEFISCDI, project number PN-IV-P2-2.1-TE-2023-1293, ctr. 40TE/2025 Drug-Scan, within PNCDI IVand the technical support through project AQUAMAT 2N/03.01.2023 (PN 23.06.01.01.)*

References:

[1]. UNODC, World Drug Report 2025 (United Nations publication), 2025, https://www.unodc.org/unodc/data-and-analysis/world-drug-report-2025.html.
[2]. NestlerE.J., *The Neurobiology of Cocaine Addiction*, Sci. Pract. Perspect., 2005:3(1), 4.
[3]. Gavrila A.M., Diacon A., Iordache T.V., Rotariu T., Ionita M., Toader G., *Hazardous Materials from Threats to Safety: Molecularly Imprinted Polymers as Versatile Safeguarding Platforms*, Polymers 2024:16, 2699.
[4]. Fu X., Yang Q., Zhou Q., Lin Q., Wang C., *Template-Monomer Interaction in Molecular Imprinting: Is the Strongest the Best?,*Open J. Org. Polym. Mater., 2015:5(2).

SYNTHESIS AND MAGNETIC PROPERTIES OF A FAMILY OF DINUCLEAR LANTHANIDE COMPLEXES DERIVED FROM 2-(PHTHALIMIDOMETHYL)-NITRONYL-NITROXIDE

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Keywords: nitronyl-nitroxide; heterodispin complexes; magnetic properties; crystal structure; alkylation reaction

Introduction: Nitronyl-nitroxides have a rich coordination chemistry, allowing the synthesis of complexes with various spin topologies that show intriguing magnetic properties. While most radicals reported in the literature are obtained starting from the corresponding aldehydes,[1] methods of grafting the nitronyl-nitroxide moiety onto a substrate through coupling or alkylation[2] reactions have also been described, benefiting from simpler procedures and higher yields.

Results: This work focuses on the previously scarcely explored potential of alkylation reactions with 2-(chloromethyl)-nitronyl-nitroxide[1] in building new paramagnetic ligands. N-, O-, C-, and S-alkylation reactions have been studied in this regard, with substrates including amines, phenols, and acetylacetones employed. Particularly interesting results were obtained in the case of alkylated phthalimide, which afforded two structural families of complexes (Figure 1): mononuclear transition metal (Ni^{II}, Co^{II}) complexes with two radical molecules bound to the metal ion, and dinuclear lanthanide (Pr^{III}, Nd^{III}, Eu^{III}, Gd^{III}) complexes with the radical moiety acting as a bridge. The magnetic properties of the second family have been investigated, revealing, in the case of the gadolinium complex, a ferromagnetic interaction (J_1 = 6.8 and J_2 = 0.2 cm^{-1}, $-J_{12}S_1S_2$ convention).

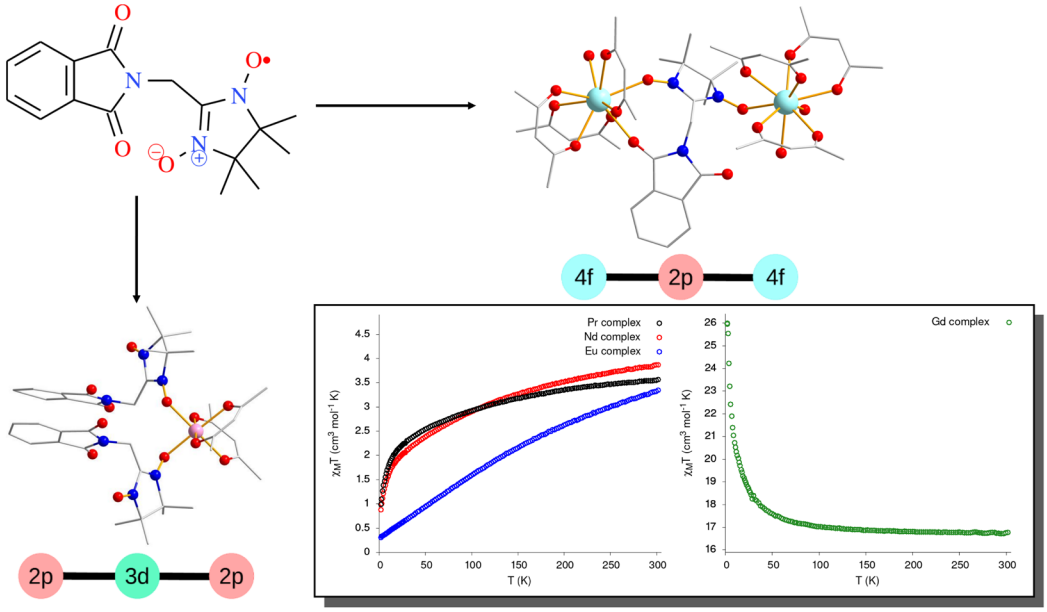

Figure 1. The structure of 2-(phthalimidomethyl)-nitronyl-nitroxide, its complexes with transition metals and lanthanide ions, and the $\chi_M T$ versus T plots recorded for the lanthanide complexes

***Acknowledgements**: This work was supported by a grant of the Ministry of Education and Research, CCCDI - UEFISCDI, project number PN-IV-P6-6.1-CoEx-2024-0053, within PNCDI IV.*

References:

[1]. Ullman EF, Osiecki JH, Boocock DGB, Darcy RJ. Studies of Stable Free Radicals. X. Nitronyl Nitroxide Monoradicals and Biradicals as Possible Small Molecule Spin Labels. J Am Chem Soc. 1972;94:7049.

[2]. Osada S, Igarashi K, Nogami T, Ishida T. Amino Acid Spin Labels. An Application of Chelation Ability to a Nickel(II) Ion. Chem Lett. 2010;39:576.

MATERIALS CONTAINING CARBON DOTS FOR IMPROVED NAPROXEN RELEASE

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Keywords: carbon dot, collagen, cyclodextrin, naproxen release

Introduction: Carbon dots (CDOTs), with fluorescence properties and low toxicity, have been used as promising multifunctional nanocarriers for biomedical applications[1]. In this study, we report the development of a novel drug delivery platform based on collagen-coated β-cyclodextrin (β-CD) inclusion complexes co-loaded with naproxen (Np) and bamboo-derived CDOT, aiming to achieve controlled drug release.

Materials and methods: CDOT were synthesized *via* one-step hydrothermal method using bamboo powder, nitric acid, and thiourea. Inclusion complexes were prepared by co-encapsulating Np and CDOT into β-CD, followed by coating with collagen to form the materials. Those were characterized using Scanning Transmission Electron Microscopy (STEM), fluorescence spectroscopy or circular dichroism. *In vitro* drug release was investigated at pH 6.8 and 7.4 and analyzed using different kinetic models (Higuchi, Korsmeyer–Peppas, Gompertz, and Weibull).

Results: The synthesized CDOTs exhibited quasi-spherical morphology with an average size of 6.44 nm and strong excitation-dependent fluorescence (Figure 1).

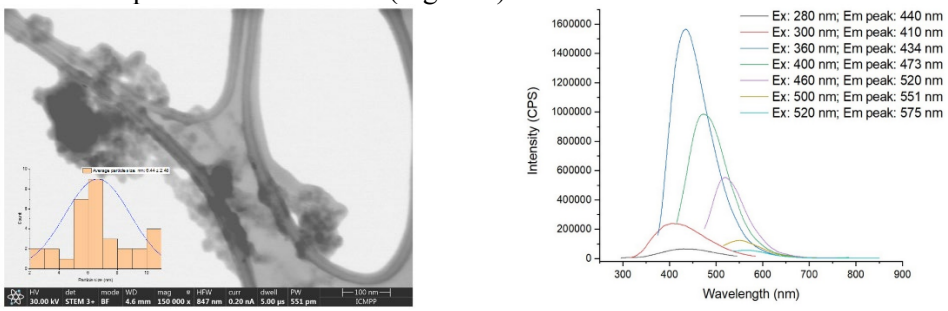

Figure 1. STEM image and fluorescence spectra of CDOT

After coating the inclusion complexes with collagen, circular dichroism spectroscopy (Figure 2) confirmed their formation, evidencing structural rearrangements and β-sheet supramolecular organization[2]. All the materials, demonstrated antioxidant activity, significantly enhanced in CDOT-containing samples.

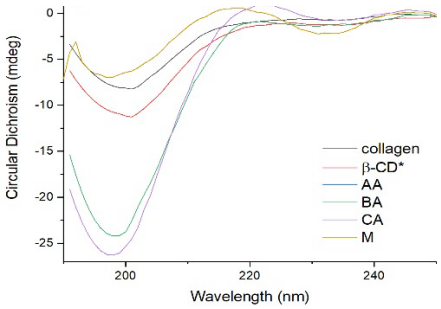

Figure 2. Circular dichroism spectra of collagen covered materials (AA-β-CD-Np; BA-β-CD-CDOT; CA-β-CD-CDOT-Np; M- Np)

Drug release studies revealed that naproxen release follows the Weibull kinetic model (R^2=0.9973-0.9987), indicating complex diffusion and matrix-controlled mechanisms. The release behavior was strongly influenced by formulation composition and environmental pH. Generally, the presence of CDOT slowed drug release due to noncovalent binding domains (π–π and hydrogen bonding) or tighter interfacial packing with collagen.

Conclusions: The systems presented in this study represent a promising platform for advanced controlled Np delivery. CDOT play a dual role by influencing release kinetics and providing imaging capability, highlighting their potential in biomedical applications.

***Acknowledgements**: This work was financially supported by a grant from the National Research Authority, project no. PNRR-III-C9-2022-I8-291, IntelDots, contract no. 760081/23.05.2023, within the National Recovery and Resilience Plan.*

References:

[1]. GhosalK., Ghosal A.Carbon dots: The next generation platform for biomedical applications. Mater. Sci. Eng. 2019; 96:887–903
[2]. Mandal T.N., Mal S., Das D., Cho S., Jana A. Cyclodextrin-mediated circularly polarized luminescence in achiral two-dimensional blue perovskites. Mater. Today Phys. 2025; 59:101885.

NOVEL STRATEGIES FOR THE SYNTHESIS OF 4*f* AND 4*f*-4*f*' COMPLEXES DERIVED FROM SCHIFF BASE LIGANDS

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Keywords: lanthanides, schiff base ligands, coordination compounds

Introduction: Numerous lanthanide-based coordination compounds, which are known for their remarkable magnetic and luminescent properties, have been obtained employing Schiff base ligands[1,2]. This is primarily due to the fact that these ligands can be easily designed by selecting suitable precursors, which allow control over the number and type of donor atoms[2]. Thus, these ligands must fulfill two important conditions: they should posess oxygen donor atoms as lanthanide ions are known for their oxophilic nature, and they should present a significant number of donor atoms to generate higher coordination numbers, which are preferred by lanthanide ions. Moreover, multi compartmental ligands of varying sizes can be generated, which are able to acommodate different lanthanide ions, in a selective way, based on their ionic radii.

Materials and methods: The Schiff base ligands used in this study are formed by the 2:1 condensation of various aldehydes, such as 3-bromo-5-chlorosalicylaldehyde (H_2**L**^{1}), o-vanillin (H_2**L**^{2}), 2,3-dihydroxybenzaldehyde (H_4**L**^{3}) or 2-hydroxy-3-hydroxymethyl-5-methylbenzaldehyde (H_4**L**^{4}) with 1,8-diamino-3,6-dioxaoctane.The lanthanide complexes derived from these Schiff base ligands are characterized by single crystal and powder X-ray diffraction, as well as UV-Vis and IR spectroscopies.

Results: In this work, we report the synthesis and characterization of novel 4*f* and 4*f*-4*f*' complexes starting from a variety of side-off bicompartmental type Shiff base ligands. By varying the reaction ratios between these ligands and different lanthanide precursors, either mononuclear or polynuclear lanthanide-based complexes are generated. Luminescence or magnetic properties of some complexes have been investigated.

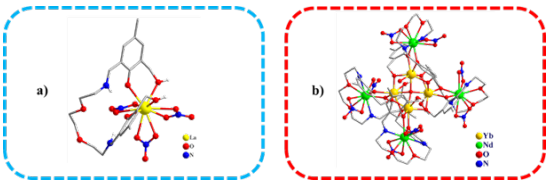

Figure 1. Molecular structure of a) 4*f* and b) 4*f*–4*f*' complexes derived from H_4**L**^{4}

Conclusions: Various synthetic strategies have been employed to develop new 4*f* and 4*f*–4*f*' polynuclear complexes. These compounds have been characterized both structurally and spectrally, and for certain examples, their luminescent or magnetic properties have been studied.

Acknowledgements: *The financial support from the grant of the Ministry of Education and Research, CCDI - UEFISCDI, project number PN-IV-P6-6.1-CoEx-2024-0053 (Contract no. 5CoEx/2026) within PNCDI IV and from European Union through Next Generation EU, programme-PNRR-III-C9-2023-I8 (contract no.760230) is gratefully acknowledged.*

References:

[1]. Marin R., Brunet G., Murugesu M. Shining New Light on Multifunctional Lanthanide Single-Molecule Magnets. *Angew. Chem. Int. Ed.* 2021;60:1728-46

[2]. Andruh M. The exceptionally rich coordination chemistry generated by Schiff-base ligands derived from o-vanillin. *Dalton Trans.* 2015;44:16633-53.

PERSPECTIVES ON MICROPLASTICS FROM SPORTS ACTIVITIES

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Keywords: microplastics; sportswear; wastewater; circular economy

Introduction: In Zero Pollution Action Plan (2021)[1], the European Commission has set a target of reducing microplastics (MPs) released into the environment by 30% by 2030. To support this objective, the Commission is integrating this target into the broader framework of strategies on plastics, circular economy, and chemicals (including the new Circular Economy Action Plan)[2]. Therefore, the prevention of the formation of MPs from the degradation of macroplastics is also addressed, for example by reducing plastic waste in the sea and improving plastic production design. The aim of this paper is to identify the perspectives of the main sportswear's companies such as NIKE Inc., Adidas AG, and Macron S.p.A. on MPs released from sports activities into Municipal Wastewater Treatment Plants (WWTPs). WWTPs are considered important point sources of MPs in the environment. The literature data showed that such textiles represent a significant source of MPs which end up in wastewater[3]. These particles accumulate in sewage sludge and its processed by-products as biosolids[4]. Also, some strategies of sportswear companies have been highlighted.

Materials and methods: The most important types of textile materials used by NIKE Inc., Adidas AG., Macron S.p.A. sportswear companies have been identified. Modern approaches for detecting and characterizing MPs in sportswear use attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR), chromatographic methods, μ-Raman spectroscopy, optical microscope, and FT-IR analysis.

Results: Water analysis from WWTPs indicated the presence of MPs, including their final effluents[5]. Filaments with sizes between 1 mm and 125 μm were the most prevalent[6]. Sustainable sportswear is mainly composed of virgin polyester (PET), recycled polyester (rPET), elastane (EL), polypropylene (PP), polyamide (PA), (PA/EL), and cotton (CO) (Fig. 1).

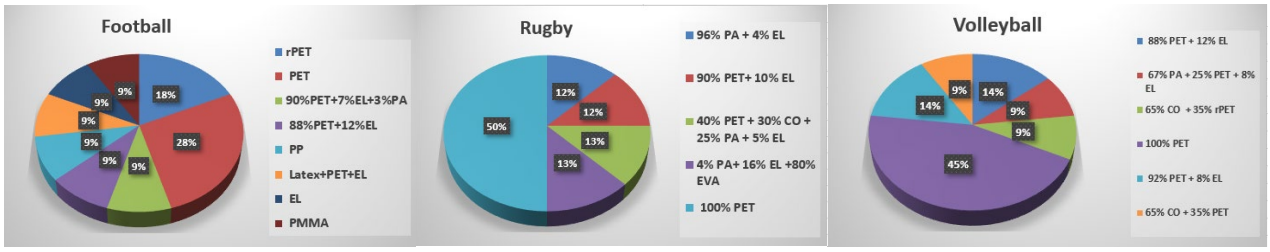

Figure 1. Identification of materials used in sports articles, classified by sports branches

These investigated companies have started a campaign to reduce MPs, as follows: NIKE Inc. is rethinking its fundamental processes from the perspective of sustainability and the circular economy. The company is focusing its efforts on reducing its carbon footprint, managing waste, using water efficiently and optimizing chemicals. Adidas AG. is prioritising decarbonisation, circular economy, conserving biodiversity, and sustainable water management. Macron S.p.A. is monitoring and assessing the use of resources, their impact, and the risks/opportunities associated with the circular economy, through sustainable policies, using certified materials, andoptimizing material flows[7].

Conclusions: The main significant sources of microplastics from sports, are textile materials. These MPs end up in wastewater through their deterioration. The main leaders on the sportswear market, NIKE Inc., Adidas AG., Macron S.p.A. have implemented sustainable strategies to reduce the environmental pollution associated with the release of MPs. Their current efforts prioritize **textile-to-textile recycling** and **advanced wastewater filtration**. Standardizing methodologies and implementing EU and national regulations on the detection and monitoring of MPs are essential to reducing pollution and protecting

human health.

References:

[1]. Zero Pollution Action Plan, https://environment.ec.europa.eu/strategy/zero-pollution-action-plan_en.Accessed in 25 Dec 2025.
[2]. Circular Economy, https://environment.ec.europa.eu/strategy/circular-economy_en.Accessed in 25 Dec 2025.
[3]. S. A. Carr, J. Liu, and A. G. Tesoro, "Transport and fate of microplastic particles in wastewater treatment plants," Water Research, vol. 91, pp. 174-182, Mar 2016, doi: 10.1016/j.watres.2016.01.002.
[4]. J. P. da Costa, P. S. M. Santos, A. C. Duarte, and T. Rocha-Santos, "(Nano)plastics in the environment - Sources, fates and effects," Science of the Total Environment, vol. 566, pp. 15-26, Oct 2016, doi: 10.1016/j.scitotenv.2016.05.041.
[5]. Stancu, A.; Râpă, M.; Popa, C.; Dontu, S.; Matei, E.; Covaliu-Mirela, C. Degradation of Emerging Plastic Pollutants from Aquatic Environments Using TiO2 and Their Composites in Visible Light Photocatalysis. MOLECULES 2025, 30, doi:10.3390/molecules30153186.
[6]. Alexandra Gabriela Stancu; Maria Rapa; Ecaterina Matei; Andra Mihaela Predescu; Cristian Predescu; Recovery of Microplastics from a Synthetic Water. Scientific Bulletin UPB, Submission ID 15209. 2024
[7]. Sustainability Report, https://about.macron.com/en/sustainability/sustainability-report-2024/#bilancio-di-sostenibilita-2024. Accessed in 08 Feb 2026

RATIONAL DESIGN OF POLY(2-ISOPROPENYL-2-OXAZOLINE) HYDROGELS FOR CONTROLLED DRUG LOADING AND DELIVERY

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Keywords: hydrogels; drug delivery; controlled release; RNA

Introduction: Poly(2-isopropenyl-2-oxazoline) (PiPOx) has gained significant attention as a versatile polymer for designing hydrogel materials in biomedical applications. Its favorable characteristics, including biocompatibility, improved hydrophilicity, thermal stability, and immunomodulatory properties, make it an excellent candidate for a wide range of medical applications.[1] Exploiting the reactive 2-oxazoline groups, PiPOx can be cross-linked with dicarboxylic acids to form hydrogel networks.[2,3]

Materials and methods: Poly(2-isopropenyl-2-oxazoline) hydrogels were prepared through a one-pot aqueous cross-linking reaction carried out at 60 °C, using bio-based and non-toxic amino- or hydroxy-substituted dicarboxylic acids as cross-linking agents. The physicochemical and mechanical properties of the hydrogels, including water uptake and cross-linking density, were tailored by varying the type of cross-linker. Their potential as drug delivery systems was evaluated *in vitro* using propranolol hydrochloride, 5-fluorouracil, sodium diclofenac, and nafcillin sodium as model drugs. The degradation behavior and drug-release profiles were investigated under simulated physiological conditions. In addition, enzymatic degradation studies were performed in the presence of lipase and esterase to further assess the biodegradability of the hydrogels.

Results: The PiPOx-based hydrogels showed tunable water absorption, cross-linking density, and mechanical stability depending on the cross-linker type and composition. The cross-linker influenced the degradation rate and drug-release behavior in all investigated physiologic media. The exceptional versatility of PiPOx hydrogels as drug delivery systems arises from their ability to establish various non-covalent interactions with drug molecules, including ionic, cation-π, ion-dipole, hydrophobic, and hydrogen-bonding interactions, through both the 2-oxazoline rings and the network's junction points. Furthermore, the weakly basic nature of the 2-oxazoline groups allows their protonation under acidic conditions, enabling pH-responsive regulation of drug loading and release. The chemical structure of the cross-linkers can additionally influence release behavior through secondary physical interactions with the incorporated drugs, contributing to sustained and controlled drug release profiles.

Conclusions: PiPOx-based hydrogels demonstrated significant promise as biodegradable, biocompatible materials for controlled drug delivery and tissue engineering applications. The cross-linker had a pivotal role in tuning the release behavior of PiPOx hydrogels, as hydroxy/aminoacid-based cross-linkers promote sustained drug release through stable electrostatic, ion-dipole, and hydrogen-bonding interactions. These structure-property relationships also enabled the rational use of PiPOx hydrogels for RNA loading and delivery by taking advantage of the interactions between polyanionic RNA and the cationic 2-oxazolinium groups.[4]

***Acknowledgements**: The authors acknowledge the Romanian Ministry of Research, Innovation and Digitalization, CNCS/CCCDI – UEFISCDI, project number PN-IV-P6-6.1-CoEx-2024-0088 within PNCDI III, for the financial support.*

References:

[1]. Kroneková, Z., Mikulec, M., Petrenčíková, N., Paulovičová, E., Paulovičová, L., Jančinová, V., Nosál', R., Reddy, P.S., Shimoga, G.D., Chorvát, D., Jr., Kronek, J., Ex Vivo and In Vitro Studies on the Cytotoxicity and Immunomodulative Properties of Poly(2-isopropenyl-2-oxazoline) as a New Type of Biomedical Polymer. Macromolecular Bioscience, 2016. 16(8): p. 1200-1211.

[2]. Jerca, F. A.; Anghelache, A. M.; Ghibu, E.; Cecoltan, S.; Stancu, I.-C.; Trusca, R.; Vasile, E.; Teodorescu, M.; Vuluga, D. M.; Hoogenboom, R.; Jerca, V. V, Poly(2-isopropenyl-2-oxazoline) Hydrogels for Biomedical Applications. Chemistry of Materials, 2018.

[3]. Ghibu E.,Vasile V., Caras I.,Giol E.D., Banu N.D., Vuluga D.M.,Stan R., Jerca V.V., Jerca F.A., Poly(2-isopropenyl-2-oxazoline) hydrogels with biodegradable junction points for drug-delivery applications, *Chemistry of Materials, 2024,* 36(15), 7459-7475.

[4]. Ghibu, E.,Vuluga D.M., Stan R., Jerca F.A., Jerca V.V., Poly(2-isopropenyl-2-oxazoline) hydrogels as multipurpose drug delivery systems: Tailoring molecular interactions for controlled loading and release. European Polymer Journal, 2026. 242: p. 114407.

MULTIFUNCTIONAL LUMINESCENT- THERMO-RESPONSIVE FILMS COMBINING EUROPIUM COMPLEXES AND CHOLESTERIC LIQUID CRYSTALS

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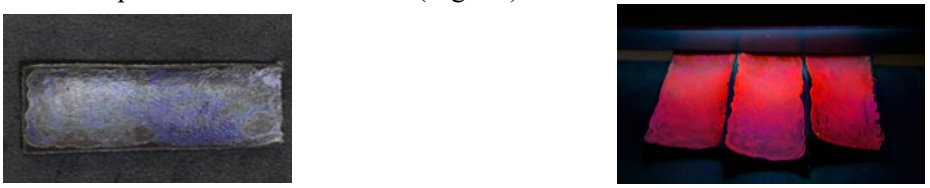
Keywords: hybrid film; cholesteric liquid crystal*; *thermoresponsive; luminescent

Introduction: In this presentation, we describe the development, the design and the fabrication of thermo-responsive luminescent composite films based on a europium (III) polyoxometalate integrated with a cholesteric liquid crystal into a PMMA matrix. The europium polyoxometalate anion shows intense red emission upon excitation at 254 nm, offering high luminescent efficiency in the visible region. By blending this complex with thermo-responsive cholesteric liquid crystals (CLC) and a PMMA matrix, we have engineered films that couple strong red luminescence with temperature-dependent structural changes of the cholesteric phase.[1] The cholesteric part, characterized by its helical pitch sensitive to temperature fluctuations, induces modulation of the optical response, enabling a reversible variation in selective reflection and photoluminescence with thermal stimuli. The composite films keep robust red emission under UV irradiation while showing clear thermally induced changes in their optical features.[2] These changes arise from modifications in the molecular organization and intermolecular interactions within the liquid crystalline environment as temperature varies[3] (t= 37-40 °C).

Materials and methods: The CLC mixtures were prepared by the mixing of cholesteryl pelargonate with oleyl cholesteryl carbonate. The Eu(III) hybrid material was obtained in two steps. In the first one the 1-Methylimidazole was mixed with 1-Bromotetradecane in acetonitrile at 85°C to yield the imidazolium bromide salt. The obtained product was coupled with the sodium salt of the decatungstoeuropate(9-) anion. Both components, CLC and the europium-containing polyoxometalate hybrid material, were mixed by magnetic stirring with PMMA in dichloromethane. The new film forming polymer was dried and analyzed by POM. This mixture was used for leather and cardboards coating in view of thermochromism and luminescent effects generation.

Results: The natural bovine leather was coated with the product and both thermochromic effect (Fig.1a) and luminescent upon excitation at 254 nm (Fig. 1b) were observed.



a) b)

Fig. 1. CLCs mixed with europium component deposited on leather surface a); exposed to UV light b)

Conclusions: The preparation of those hybrid films shows potential as stimuli-responsive optical materials for temperature sensing, smart coatings, and security applications where tunable luminescence and structural responsiveness are advantageous. The work highlights a promising strategy for developing multifunctional luminescent materials by merging lanthanide photophysics with thermally adaptive liquid crystal platforms.

Acknowledgements: This research was funded by the National Research Authority under Core Program 6N, PN 23 26 03 02-BIO-LEATHER project and was performed in the framework of Contract 18211_C_1/2020.

References:

[1]. Xu, L.; Et Al. Circularly Polarized Luminescence Of Cholesteric Liquid Crystal Polymer Networks With A Europium (Iii) Complex As An Emitter. Acs Applied Materials & Interfaces, 2024, Acs Applied Materials & Interfaces.
[2]. Knyazev, A. A.; Et Al. Thermosensitive Luminescent Film Sensors Based on A Europium (III) Liquid Crystalline Complex. Liquid Crystals, 2026, Liquid Crystals (Taylor & Francis).
[3]. Choudhury P. K., Ibrahim A.-B. M.A, Introductory Chapter: Liquid Crystals and Applications, 2022.

PHYTO-DERIVED METAL AND METAL OXIDE NANOPARTICLES FOR BIOMEDICAL AND ENVIRONMENTAL APPLICATIONS

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Keywords: silver nanoparticles; biohybrids; antioxidant; antimicrobial

Introduction: This study presents eco-strategies for the valorization of various vegetal wastes to develop phyto-derived metal (MNPs) and metal oxide (MONPs) nanoparticles with great potential in biomedical and environmental applications. These phyto-nanostructures possess antioxidant, antimicrobial and urease inhibitory activities[1,2], and, consequently, they can constitute building blocks for the further development of multifunctional biohybrids.

Materials and methods: "Green" bottom-up approaches were used to develop bioactive materials based on phytosynthesized MNPs and MONPs. The aqueous vegetal extracts were obtained by various plants and vegetal waste, and were characterized by biochemical (Folin-Ciocalteu assay), spectral (UV-Vis absorption) and chromatographic (HPLC) methods. The phytosynthesis of nanoparticles was confirmed by spectral methods (UV-Vis, DLS). The antioxidant properties were tested by DPPH assay, and the antibacterial activities were investigated by agar disc diffusion. Urease inhibitory activity was evaluated by electrical conductivity measurements.

Results: The chromatographic and bio-physico-chemical characterization of vegetal extracts revealed the presence of bioactive phyto-compounds which played a key role in the synthesis of phyto-MNPs and phyto-MONPs. The spectral fingerprints of phyto-derived metal (MNPs) and metal oxide (MONPs) were identified on the UV-Vis absorption spectra. DLS measurements revealed the nanoscale dimension of these particles. The obtained NPs showed antioxidant and antibacterial properties.

Conclusions: The phyto-derived nano-structures proved to be good antioxidant agents and good biocides, and therefore they can be used in biomedical and environmental fields. Our future research will focus on the integration of these NPs in various biocomposites, for development of novel materials with improved bioactivities.

***Acknowledgements**: This work was supported by a grant of the Ministry of Education and Research, CCCDI -UEFISCDI, project number PN-IV-P7-7.1-PED-2024-0690, within PNCDI IV [31PED/2025, Eco-innovative novel phyto-derived 3D hybrid bioarchitectures for a better life (ECOPHYTO)].This work was also supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS/CCCDI—UEFISCDI, project number COFUND-WATER4ALL-WATER Green Treat-1, No. 59/2024, within PNCDI IV. This work was supported by the Culture Collection of Microorganisms of Industrial Importance (CMII-ICCF-WFCC 232, MIRRI-RO).*

References:

[1]. Barbinta-Patrascu, M.-E.,Nichita, C., Enculescu, M., Maraloiu, V.-A.,Bacalum, M., Ungureanu, C.,Negrila, C.C.,Zgura, I. Bioactive Hybrids Containing Artificial Cell Membranes and Phyto-Gold–Silver Chloride Bio-Nanoparticles. Int. J. Mol. Sci. 2024, 25: 11929. https://doi.org/10.3390/ijms252211929.

[2]. Barbinta-Patrascu, M.-E.,Nichita, C.,Bita, B.,Antohe, S. Biocomposite Materials Derived from *Andropogonhalepensis* – Eco-design and Biophysical Evaluation, Materials 2024, 17(5): 1225. https://doi.org/10.3390/ma17051225

INFLUENCE OF Mg^{2+}, Sr^{2+}, AND Zn^{2+} DOPANT IONS ON CALCIUM PHOSPHATE COMPOSITE SCAFFOLDS FOR BIOMEDICAL APPLICATIONS

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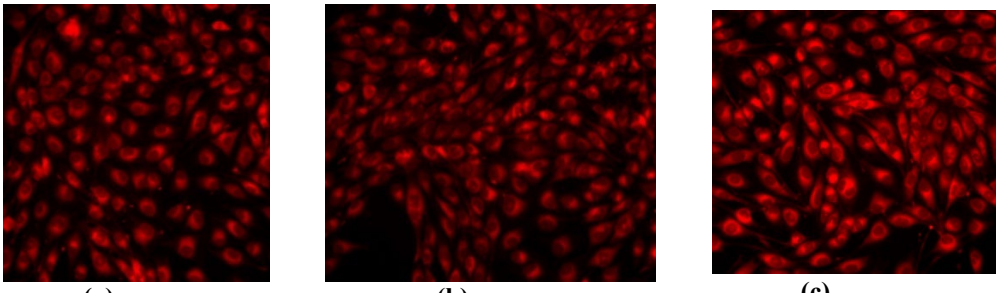
Keywords: dopant ions; calcium phosphate; scaffolds; biomedical applications

Introduction: Biomedical applications involve materials and complementary technologies designed to support effective and personalized treatments. In hard tissue engineering, research focuses on reproducing the natural bone structure, including its surface characteristics, porous three-dimensional architecture, cellular matrix, and chemical composition. Bone tissue consists of inorganic and organic phases, where the inorganic phase is mainly based on hydroxyapatite and metallic ions, while the organic phase contains collagen fibers and specialized cells[1,2,3]. Together, these components form the complex structure of bone tissue. Scaffold-based composite materials have emerged as a promising strategy for mimicking this architecture and supporting bone regeneration. These materials promote cell attachment, proliferation, osteoconductivity, and osteoinductivity[2]. Furthermore, the incorporation of metallic ions improves the similarity to natural bone, enhancing the biocompatibility and overall physicochemical and biological properties of the composites[3].

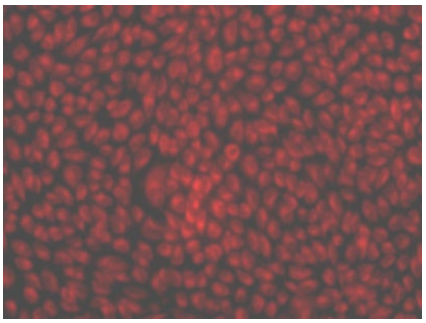
Materials and methods: The current study was divided into two main directions: the synthesis of calcium phosphate doped with metallic ions (Mg^{2+}/Sr^{2+}/Zn^{2+}) at specific concentrations using the co-precipitation method, and the mimicry of bone structure through the fabrication of scaffolds based on doped calcium phosphate, polyvinyl alcohol, and glycerin using the replication method. The ceramic powders and composite materials were characterized to evaluate the effect of dopant ions on improving the biocompatibility and physicochemical properties of the materials for future biomedical applications.

Results: XRD and FT-IR analyses confirmed the presence of a single β-tricalcium phosphate ceramic phase together with the incorporated metallic ions. SEM observations revealed a honeycomb-like porous structure of the scaffold materials, influenced by the ceramic suspension and the composition of the proposed materials. The most significant results were related to the interaction between the composite scaffolds and the THP-1 cell line (human monocyte cell line), highlighting the effect of metallic ions on the biological behavior of the composite structures.

Conclusions: The proposed composite scaffold materials demonstrated good interaction with the cell line, promoting enhanced cell proliferation and strong adhesion on the material surface. Structural characterization confirmed the presence of a single β-tricalcium phosphate ceramic phase together with the incorporated dopant ions. The addition of metallic ions significantly improved the overall properties of the materials, particularly their mechanical resistance.



(a) **(b)** **(c)**



(d)

Figure 1. Cell proliferation and fluorescence microscopy of composite materials in contact with THP-1 cell culture: (a) calcium phosate dopped with 5%Mg^{2+}, (b) calcium phosphate dopped with 5%Sr^{2+} (c) calcium phosphate with 5%Zn^{2+} and (d) calcium phosphate.

References:

[1]. Zahra M., Håvard J.H., Dagnija L., Filippo R., Giuseppe P., Amirhossein M., Qianli M. Review on the strategies to improve the mechanical strength of highly porous bone bioceramic scaffolds. J. Eur. Ceram. Soc. 2024, 4(1): 23-42.
[2]. Sheikh Md M.H., Md Abdul K., Min-Su L., Jin-Kyu K., Do-Kyun K., Hwan-Hee L. and Young-Yul K., Biomimetic Strategies for Bone Regeneration: Smart Scaffolds and Multiscale Cues. Biomimetics. 2026, 11(1), 12.
[3]. Xuan W., Shan H. and Qian P. Metal Ion-Doped Hydroxyapatite-Based Materials for Bone Defect Restoration. Bioengineering. 2023, 10(12), 1367

BIOLOGICAL DEGRADATION OF ARTIFACTS

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Keywords: microbiology; bacteria; degradation; hydrogels; artifacts,archaeology

Introduction: The relevance of the project lies in the technological backwardness of current museums[1] and the importance of preserving historical artifacts. The main problem is formulated as the lack of safe and manageable methods of suppressing biological activity in museum and laboratory conditions[2]. Three types of materials were used for the study: ceramics, iron and bone. Biological gels from bacteria block oxygen to bacteria and chemically neutralize their poisons right at the moment of their release, flowing into the pores in the form of water, and then transformed inside into an elastic mesh. As an example, for ceramics, the composition is based on ethyl cellulose and thymol. When mist gets on the surface, micro drops penetrate into the capillaries of the baked clay. After evaporation of alcohol, the polymer forms an ultrathin mesh, which envelops mineral grains, strengthening them and preventing Arthrobacter bacteria and Streptomyces gain a foothold in the pores. Mist application ensures that the inhibitor gets into all cavities and under the edges of the rust flakes. To confirm this, an experiment was conducted with the breeding of bacteria on the surface of high-quality artifacts. The materials were placed in an incubator.

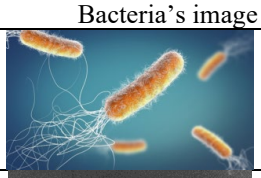
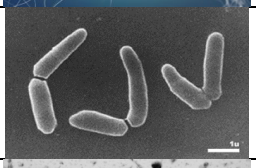
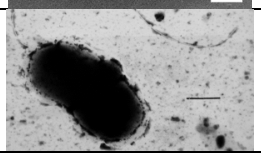
Materials	Bacteria's name	Bacteria's image
Bone	Pseudomonas,Clostridium	
Ceramics	Arthrobacter, Bacillus, Streptomyces	
Iron	Desulfovibrio,Thiobacillus	

Table 1. Studied bacterias[4]

Image 1. The prototype

The operation of the developed mechanism is a controlled and step-by-step process of chemical treatment of archaeological and museum objects in a closed laboratory chamber. The design is based on a sealed working container made of chemically inert materials and equipped with transparent walls, which allows the restorer to continuously monitor the condition of the object during the entire procedure. The artifact is

placed on a slowly rotating platform, which ensures uniform surface treatment without the need for manual turning of the object and without direct mechanical contact with the operator.

Materials and methods: (1) Collecting information about the properties of bacteria; (2) Practical part, experiments, verification of results; (3) Calculating the mass before and after artifacts, documenting changes in the biological environment of artifacts.

Results: Experimental data confirm that the developed composition based on acrylic polymers and thymol forms a stable crystalline phase of the antiseptic directly in the zone of potential bio-contamination. Absence of vegetative forms. The microflora (mycelium) on the prints after 24 hours of incubation proves the high efficiency of the chosen direction in comparison with previously used organic substrates.

Conclusions: This method of processing artifacts is safe and effective against biological degradation, which solves an important problem relevant to archaeologists. Also, the development of the technological part in archeology contributes to the assistance of museum staff and laboratory technicians, which will increase the demand for this field. The problem of biodegradation, developed abroad[3], should also develop in Kazakhstan for the sake of preserving culture and heritage.

***Acknowledgements**: We are grateful to our school and our teachers for providing us such an opportunity to develop our ideas and showcase them on events as NEXT Chem and EuroChem conferences.*

References:

[1]. Scientific article by V. V. Chaga and A. A. Brazhnikov "Conservation and restoration of archaeologicalobjects".
[2]. "Fundamentals of restoration and conservation", S. M. Gromovoy and B. V. Pomaskin.
[3]. "Desk processing of archaeological finds: laboratory restoration and conservationof archaeological objects" by L.I. Maslikhova.
[4]. Article “The Control of Cultural Heritage Microbial Determination". Microbial Colonization Researchof Cultural Heritage Objects.

CRYSTAL ENGINEERING OF 1,10 PHENANTHROLINE DERIVATIVES

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Keywords: 1,10 phenanthroline; crystal engineering; molecular tectons; supramolecular assembly; coordination chemistry

Introduction: 1,10-Phenanthroline derivatives are versatile building blocks for crystal engineering due to their rigid aromatic structure, chelating ability, and propensity for supramolecular interactions. Functionalization with carbonyl, oxime, or imine fragments enables the tuning of interaction sites and crystal-packing preferences.

Materials and methods: 1,10-Phenanthroline was used as starting material to obtain 1,10-phenanthroline-5,6-dione, which served as a key intermediate for the synthesis of 1,10-phenanthroline-5,6-dioxime and dihydropyrazine-functionalized derivatives.

Results There were obtained and characterized 1,10-Phenanthroline-5,6-dione, 1,10-phenanthroline-5,6-dioxime and dihydropyrazine-functionalized derivatives as potential tectons for crystal engineering.

Conclusions: Owing to their rigidity, coordinating ability, and capacity to engage in hydrogen bonding, metal coordination, and π–π interactions, these compounds represent promising molecular building units for supramolecular assembly and the design of crystalline materials.

Acknowledgements *The financial support from European Union through NextGeneration EU-PNRR–III-C9–2022-I8 programm (High performance chiral materials for circularly polarized luminescence (CPL) and chirality induced spin selectivity (CISS) (CRUNCHINESS), contract no 760230) is grateful acknowledged.*

References:

[1]. Akhmedov, T. N.; Kumar, A.; Starkenburg, D. J.; Chesney, K. J.; Abboud, K. A.; Akhmedov, N. G.; Xue, J.; Castellano, R. K. Beilstein J. Org. Chem. 2024, 20, 1037–1052.

INNOVATIVE ARTIFICIAL INTELLIGENCE TECHNOLOGIES FOR CHEMISTRY APPLICATIONS

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Keywords: artificial intelligence; chemistry studies; therapeutic design; deep learning; machine learning

Introduction: Artificial intelligence (AI) technologies are increasingly significant methods to enhance speed and reduce costs in the development of important fields, such as healthcare, chemistry, biology and biotechnology, chemical engineering, and industrial processes[1]. In terms of drug discovery, many researchers proved that the cost of production is quite expensive, so AI tries to address this problem by combining the progress in computation and constructive virtual screening (VS) methodologies. Most common approaches are machine learning (ML) and deep learning. Multiple researchers used both algorithms to conduct studies that are beneficial for society's health and resources[2].
Materials and methods: Machine learning (ML) is a popular computer vision approach, which implies automatic learning of computer systems through given datasets on which the systems are trained. Then, the computer should make a decision based on the identified patterns and predictions established with statistics. It is important to note that ML learns from its own experience, becoming smarter and smarter without human interventions. In other words, the machine learns the patters in the input and generates the output based on its learning[3]. Comparing to ML, which can involve smaller datasets, deep learning needs several layers in between the input and the output of a neural network. This complex process leads to deep learning paying more attention to details. Thus, deep learning becomes suitable for questions that require very detailed analysis and that have high risks if not managed with a proper accuracy. ML and deep learning are very useful in generative chemistry, therapeutic design, protein structure prediction and many other applications[4].
Results: Traditionally, with the structure of the target protein available, structure-based approaches including molecular docking studies and molecular dynamic simulations can be applied to explore the potential receptor-ligand interactions and to virtually screen a large compound set for finding the plausible lead. Then, with the identified active molecules for the given target, ligand-based approaches such as pharmacophore modeling can be conducted for modifying known leads and for finding future compounds[5]. In a study, disseases were classified by using medical imaging performed by experts in medicine and by artificial intelligence. The findings showed that deep learning diagnostic performance was equivalent to the one of healthcare professionals, with a pooled sensitivity of 87% for deep learning and 86.4% for healthcare professionals, respectively, a pooled specificity of 92.5% for AI models and 90.5% for healthcare experts[6].
Conclusions: This study was focused on how artificial intelligence tackles pressing challenges, using machine learning and deep learning for optimizing modern world medical tasks in therapeutical design, chemical and biological discoveries, followed by numerous relevant innovations.

***Acknowledgements**: The authors would like to thank the International Computer High School of Bucharest for collaboration with National Institute for Research & Development in Chemistry and Petrochemistry—ICECHIM on Project Science for future researchers: experiments and knowledge PN-IV-P10-SS-SC-2024-0045(2SSSC/2025).*

References:

[1]. Nedungadi P.etal.Big Data and AI Algorithms for Sustainable Development Goals: A Topic Modeling Analysis. IEEE Access. 2024;12:188519 – 188541.
[2]. Akshaya Karthikeyan & U Deva Priyakumar Artificial intelligence: machine learning for chemical sciences J. Chem. Sci. 2022;134:2
[3]. Pandey D. Machine Learning Algorithms: A Review IRJET 2019;06: 916-922.
[4]. Sharma N. et.al. Machine Learning and Deep Learning Applications-A Vision Global Transitions Proceedings 2021;2:24-28.
[5]. Yuemin Bian & Xiang-Qun Xie Generative chemistry: drug discovery with deep learning generative models, J.of Molec.Model. 2021;27:71.
[6]. Xiaoxuan Liu et.al. A comparison of deep learning performance against health-care professionals in detecting diseases from medical imaging: a systematic review and meta-analysis 2019;1-27.

DESIGN AND EVALUATION OF MOLECULAR WEIGHT-DEPENDENT CHITOSAN NANOPARTICLES FOR 5-FU DRUG DELIVERY

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Keywords: chitosan; 5-Flourouracil; nanoparticles

Introduction: Research on chitosan nanoparticles has been widely focused on their use as drug delivery carriers, largely due to their biodegradable nature and compatibility with biological systems[1]. Despite notable advancements in this field, there remains a need for further investigation to refine and improve the production methods for drug-loaded nanoparticles. The final structure and morphology of chitosan nanoparticles are affected by several key factors, including their concentration, pH conditions, average molecular weight, and degree of deacetylation[2].

Materials and methods: The objective of this work is to develop and compare two formulations of chitosan nanoparticles (CNPs) with low and medium molecular weights, loaded with the therapeutic agent, 5-Fluorouracil (5-FU) at concentrations of 1.25 and 2.5 mg/ml. The nanoparticles were synthesized through ionic gelation, using tripolyphosphate (TPP) as a crosslinking compound. The resulting systems were characterized in terms of their hydrodynamic and structural properties using dynamic light scattering (DLS) and FTIR spectroscopy. In addition, encapsulation efficiency (EE%) was determined, along with the in vitro release behavior drug from the nanoparticle systems.

Results: The formulated chitosan nanoparticles (CNPs) exhibited an average hydrodynamic diameter ranging from 166 to 216 nm, with low polydispersity indices (PdI < 0.194 for low molecular weight samples and PdI < 0.231 for medium molecular weight samples). Loading with 5-Fluorouracil (5-FU) resulted in a reduction of the average particle size, consistent with typical colloidal behavior.

FTIR analysis of the 5-FU-loaded CNPs revealed characteristic absorption bands, including a C=O stretching vibration at 1662 cm^{-1} and an amide-related band at 1247 cm^{-1}, confirming the presence of the drug within the polymer matrix. Encapsulation efficiency showed a clear decrease as the concentration of 5-FU increased. For low molecular weight CNPs, EE% values were 72.84% and 18.40% for 1.25 mg/ml and 2.5 mg/ml, respectively. In medium molecular weight CNPs, the corresponding EE% values were 65.74% and 17.6%.

In vitro release experiments demonstrated a typical biphasic profile for 5-FU, consisting of an initial burst release phase (26–36%), followed by a more sustained and controlled release phase (40–45%), independent of the type of chitosan nanoparticles used.

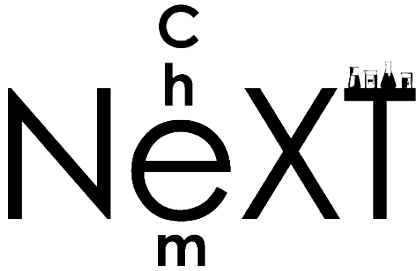
Conclusions: In this study, successful synthesis of nanoparticles intended for biomedical use was achieved using both low and medium molecular weight chitosan at a fixed concentration of 0.125%. Dynamic light scattering (DLS) and FTIR results confirmed that the drugs were effectively entrapped within the chitosan nanoparticle matrix. In addition, encapsulation efficiency was found to be slightly higher for nanoparticles based on low molecular weight chitosan compared to those with medium molecular weight.

***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).*

References:

[1]. K. V. Jardim, J. L. N. Siqueira, S. N. Báo, A. L. Parize, *In vitro* cytotoxic and antioxidant evaluation of quercetin loaded in ionic cross-linked chitosan nanoparticles, Journal of Drug Delivery Science and Technology, 74 (2022), 103561.
[2]. D. Zhao, S. Yu, B. Sun, S. Gao, S. Guo, K. Zhao, Biomedical applications of chitosan and its derivative nanoparticles, Polymers, 10 (2018), No. 4.

Section 2 - Bioresources, biotechnologies and biorefining



DERMACOSMETIC CREAM BASED ON LIPOSOMES WITH GRAPE POMACE EXTRACTS FROM RED GRAPES

STIRRED-TANK BIOREACTOR SCREENING FOR β -CAROTENE BIOSYNTHESIS BY RHODOTORULA RUBRA ICCF 220

FROM GLYCEROL TO BIOFUEL ADDITIVES / VALUE-ADDED PRODUCTS: A CATALYTIC APPROACH

BIMETALLIC NITROGEN-DOPED CARBON NANOFRAMEWORKS AS EFFICIENT CATALYSTS FOR FURFURAL HYDROGENATION

CONTROLLED CELL LINES STOCK – AN IMPORTANT STEP FOR VACCINES DEVELOPMENT

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BIOACTIVE MUCOADHESIVE DEXTRAN FROM WATER KEFIR ENRICHED WITH AGRO-INDUSTRIAL BY-PRODUCTS

EFFECTS OF ENCAPSULATED THYME ESSENTIAL OIL ON SEED GERMINATION AND EARLY GROWTH OF VIGNA RADIATA SEEDLINGS

DERMACOSMETIC CREAM BASED ON LIPOSOMES WITH GRAPE POMACE EXTRACTS FROM RED GRAPES

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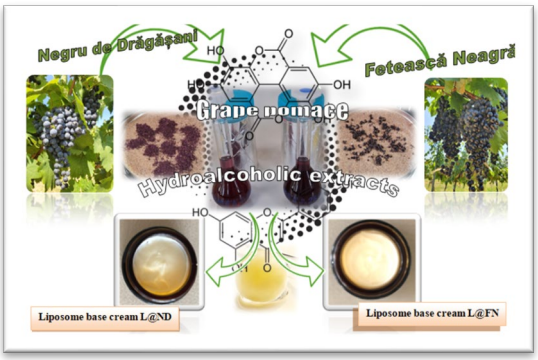
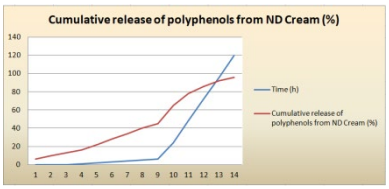
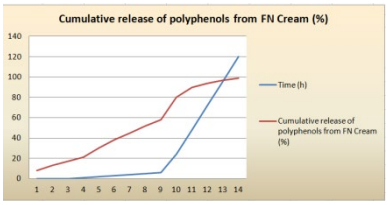
Keywords: grape pomace; hydroalcoholic extract; polyphenols; green cosmetics



Introduction: The use of grape pomace to produce dermatocosmetic creams is one of the most promising directions for winemaking by-products. This is due to its extremely high content of polyphenols, vitamins, lipids, and minerals, which can have direct beneficial effects on the skin. [1]. In addition to polyphenols, grape pomace contains residual oils rich in unsaturated fatty acids (linoleic, oleic) and phytosterols, compounds with emollient, regenerative, and skin barrier-restoring properties.[2] The liposome-based dermatocosmetic cream containing grape pomace extracts from red grapes can be used in the dermatocosmetic field to moisturize and improve skin elasticity, with anti-aging, antimicrobial effects, and protection against UVA and UVB radiation. The cream has the following composition: xanthan gum 0.5%, propylene glycol 8%, Calendula officinalis oil 5%, Argania Spinosa oil 5%, Helianthus annuus oil 5%, liposomes with hydroalcoholic extract of red grape pomace (Fetească Neagră and Negru de Drăgășani) 2%, vitamin E 0.5%, cetearyl alcohol 3%, olive oil-based emulsifier 6%, and purified water up to 100%. Natural ingredients promote the current concept of 'green cosmetics', giving the dermatocosmetic product moisturizing, anti-aging, antimicrobial, and anti-inflammatory properties, and protection against UVA and UVB radiation, while the use of liposomes as carriers for delivering the bioactive substances from hydroalcoholic extracts leads to a gradual release of the actives in the skin.

Materials and methods: Creams enriched with liposomes containing extracts from red grape pomace were prepared using the components mentioned above. In a laboratory vessel, the components of the oil phase were mixed and heated in a water bath at 70°C for 15 minutes. In another laboratory vessel, xanthan gum was dispersed in water and left to fully swell for 30 minutes, after which propylene glycol was added. The components of the aqueous phase were mixed and heated to 70°C for 15 minutes to form the aqueous phase. After heating, the oil phase was gradually added to the aqueous phase, continuously stirring, until a uniform and smooth paste was obtained. The liposomes with extracts were added after the mixture had cooled to 40°C. The resulting cream was then packaged in amber glass containers and stored in the refrigerator at 4-8°C until further use.





Results: The analyses demonstrated that all the evaluated dermatocosmetic creams exhibit strong antioxidant activity, with a slight superiority of the ND and FN samples. These results confirm the potential of the products to help protect the skin against oxidative damage and support their use in formulations aimed at maintaining the health and youthful appearance of the skin. After 120 hours, the cumulative release was >95% for all samples. Overall data suggest that liposomal encapsulation in cream matrices can provide controlled and prolonged release of bioactive polyphenols.

Conclusions: Overall, the results demonstrate that the use of grape pomace in dermatocosmetic products is feasible, sustainable, and

effective, offering a concrete example of transforming an agro-industrial waste into a high-value-added ingredient. These formulations have real potential for application in the cosmetics industry, simultaneously contributing to reducing environmental impact and developing natural products with proven biological efficacy.

***Acknowledgements**: List funding sources in compliance to funder's requirements.*

References:

[1]. Ferreira, S. M., & Santos, L. (2022). Unveiling the Utilization of Grape and Winery By-Products in Cosmetics with Health Promoting Properties. Applied Sciences, 15(3), 1007.

[2]. Teixeira, A., Baenas, N., Dominguez-Perles, R., Barros, A., Rosa, E., & Ferreira, I. C. (2014). Natural bioactive compounds from grape by-products and their possible health benefits. Food Chemistry, 160, 585–592.

STIRRED-TANK BIOREACTOR SCREENING FOR β -CAROTENE BIOSYNTHESIS BY *RHODOTORULA RUBRA* ICCF 220

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Keywords: Rhodotorula rubra; β-carotene; carotenoids; culture medium; bioprocess parameters.

Introduction: Carotenoid-producing yeasts represent an attractive microbial route for obtaining natural pigments with antioxidant potential. Among these, β-carotene is of particular interest due to its applications in food, feed, and biotechnology. The present work reports a preliminary screening study aimed at identifying culture-medium components and cultivation conditions that promote β-carotene biosynthesis by *Rhodotorula rubra* ICCF 220, while maintaining adequate biomass formation. The outcome is intended to define a practical operating window to support subsequent optimization and scale-up[1-3].

Materials and methods: Submerged cultivations were carried out at laboratory scale using *R. rubra* ICCF 220. Key factors were screened by varying: initial pH (tested range 3–8, with emphasis on the 6–7 interval), inoculum concentration (0.5–5%), carbon source and concentration (glucose in the 1–6% range; additional carbon sources such as maltose, sucrose, fructose, lactose, molasses, and glycerol), and nitrogen source (ammonium-based salts, with NH_4NO_3 used as reference). The effect of nutritional supplements was also evaluated, including yeast extract (0.15%) and selected additives (e.g., alanine 0.1%, threonine 0.2%, and oleic acid 0.2–0.5%), as well as other amino acids tested at different concentrations. Biomass formation was monitored during cultivation, and β-carotene was extracted from harvested biomass using solvent-based protocols and quantified by UV–Vis spectrophotometry.

Results: The screening highlighted a clear dependence of pigment accumulation on cultivation conditions. Overall, mildly acidic to near-neutral pH and moderate substrate levels favored β-carotene formation, whereas deviations from these ranges tended to shift the balance toward lower pigmentation and/or altered growth. Carbon and nitrogen sources affected both biomass and pigment profiles, indicating that nutrient balance is a primary driver of carotenogenesis in *R. rubra* ICCF 220. Supplementation with yeast extract and selected additives (notably lipid-related supplementation) showed a positive tendency toward improved pigmentation, supporting the role of nutrient availability and membrane-associated metabolism in β-carotene accumulation.

Conclusions: This preliminary screening defines an initial set of medium compositions and cultivation conditions that support enhanced β-carotene biosynthesis by *Rhodotorula rubra* ICCF 220. The findings provide a solid foundation for structured optimization (e.g., design of experiments) and for future process intensification and scale-up toward a controllable microbial bioprocess for natural β-carotene production.

References:

[1]. Šovljanski O, Beronja M, Saveljić A, Travičić V, Tomić A. Microorganisms as biotechnological source of carotenoids. In: Ramawat KG, Mérillon J-M, editors. Natural Products. Berlin, Heidelberg: Springer; 2025.

[2]. Adamantidi T, Lafara M-P, Venetikidou M, Likartsi E, Toganidou I, Tsoupras A. Utilization and bio-efficacy of carotenoids, vitamin A and its vitaminoids in nutricosmetics, cosmeceuticals and cosmetics' applications with skin-health promoting properties. Appl Sci. 2025;15(3).

[3]. Di Salvo E, Lo Vecchio G, De Pasquale R, De Maria L, Tardugno R, Vadalà R, Cicero N. Natural pigments production and their application in food, health and other industries. Nutrients. 2023;15.

FROM GLYCEROL TO BIOFUEL ADDITIVES / VALUE-ADDED PRODUCTS: A CATALYTIC APPROACH

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Keywords: zeolites; hierarchical; glycerol; acetalization; biofuels

Introduction: Hierarchical zeolites were obtained by applying post-synthetic modifications (PSM) to zeolites with different Si/Al ratios. Structural analyses have confirmed the creation of hierarchical porosity while maintaining the crystalline framework and acidity, thereby enhancing molecular diffusion and accessibility [1]. The novelty of this study lies in the combination of conventional and advanced methods, including pore-directing agent (PDAs) and microwave-assisted (MW) treatments. The catalytic evaluation showed high efficiency in the acetalization of glycerol (Gly) with various carbonylic compounds. The most stable catalyst retained its activity over at least three recycling cycles.

Materials and methods: A series of different zeolitic structures (beta-Hβ, mordenite-HMOR, L-KLTL, and ultra-stable Y-HUSY) were subjected to demetallation, namely desilication and dealumination, based on their Si/Al ratio. Desilication was performed using conventional means (Des-C) and ethylenediamine (Des-EDA) as the PDA. Dealumination was carried out conventionally (Deal-C) and via microwave irradiation (Deal-MW). Samples subjected to both desilication and dealumination are denoted as Desal-C and Desal-MW, respectively.

Results: XRD patterns (Fig. 1A) of both pristine and modified Hβ-12.5 zeolites highlights the pronounced and intense reflections characteristic of β zeolite, which indicate that the crystalline structure remained well-developed after PSM, with the exception of Hβ-12.5-Des-C, where a partial collapse was observed. These catalysts were further used in glycerol acetalization, which is highly important as five and six-ring ketals are produced as fuel additives that boost octane, cold flow, and reduce emissions[2,3]. Under the optimized reaction conditions, hierarchical zeolites showed high efficiency in converting all carbonylic compounds (Fig. 1B).

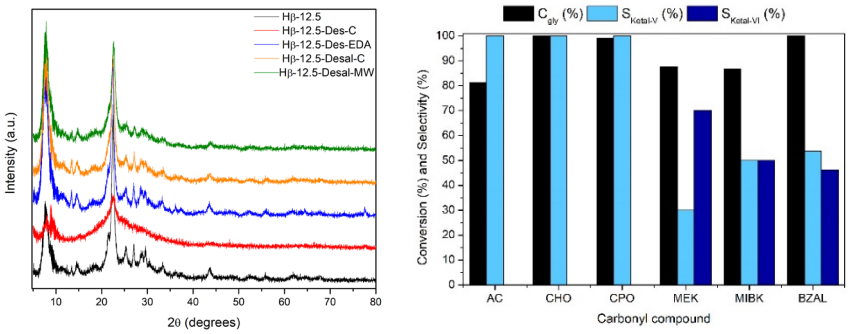

Figure 1. XRD patterns for Hβ-12.5 and modified catalysts (A) and catalytic results for Hβ-12.5-Desal-MW (B).(acetone - AC, cyclohexanone - CHO, cyclopentanone - CPO, methyl ethyl ketone - MEK, methyl isobutyl ketone - MIBK and benzaldehyde – BZAL)

Conclusions: Hierarchical zeolite-based catalysts were prepared using various PSMs to introduce additional porosity. Desilication with PDAs and MW-assisted dealumination showed improvement over conventional method while, preserving the zeolitic framework. The prepared catalysts were further employed in the acetalization of glycerol to produce value-added products. The influence of the textural, acid/base, density, distribution of active sites, and type of PSM properties on the efficiency of the catalysts in the afore mentioned processes is discussed.

***Acknowledgements**: Oana-Adriana Petcuta kindly acknowledges the Council of Doctoral Studies (C.S.U.D), University of Bucharest, Romania for supporting this work.*

References:

[1]. Wang D, Sun H, Liu W, Shen Z, Yang W. Hierarchical ZSM-5 zeolite with radial mesopores: Preparation, formation mechanism and application for benzene alkylation. Front Chem Sci Eng. 2020;14:248-57.

[2]. Bornes C, Santos-Vieira ICMS., Vieira R, Mafra L, Simões MMQ, Rocha J. Challenges and opportunities for zeolites in biomass upgrading: Impediments and future directions. Catal Today. 2023;419:114159.

[3]. Trifoi AR., Agachi PȘ., Pap T. Glycerol acetals and ketals as possible diesel additives. A review of their synthesis protocols. Renew Sustain Energy Rev. 2016;62:804-14.

BIMETALLIC NITROGEN-DOPED CARBON NANOFRAMEWORKS AS EFFICIENT CATALYSTS FOR FURFURAL HYDROGENATION

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Keywords: carbon; bimetallic; furfural; hydrogenation; biomass

Introduction: Furfuryl alcohol (FOL) is an important biomass-derived alcohol, obtained by hydrogenation of furfural (FAL), used in the production of resins, lubricants, synthetic fibers, lysine, and vitamin C[1]. The selective production of FOL requires efficient catalysts that can operate under solvothermal conditions. The current study emphasizes the use of bimetallic nitrogen-doped carbon nanoframeworks (NCFs), prepared from zeolitic-imidazolate frameworks (ZIFs) using emerging silica-assisted strategies[2], as highly selective catalysts for FOL production under mild reaction conditions.

Materials and methods: A series of bimetallic $M_{0.1}Co_{0.9}$-ZIFs (M = Fe, Ni, Cu, Zn) were obtained under solvothermal conditions. Subsequent annealing at high temperatures under inert atmosphere, using a silica-protection shell, yielded to corresponding $M_{0.1}Co_{0.9}$-NCFs catalysts.

Results: The carbonization of bimetallic $M_{0.1}Co_{0.9}$-ZIFs resulted in nitrogen-rich graphitic carbon matrix, characterized by a broad reflection around 26°, containing well-dispersed small metal nanoparticles with reflections mainly attributed to Co^0 (Figure 1A). Catalytic hydrogenation tests revealed the high activity of $M_{0.1}Co_{0.9}$-NCFs in FOL production under mild reaction conditions (100ºC, 15 bar H_2, 3h) using ethanol as solvent (Figure 1B). For the bimetallic samples, Fe- and Ni-doped catalysts were the most efficient, affording a 95-99% FAL conversion and 97-99% FOL selectivity, outperforming other dopants (i.e. Cu and Zn) as well as unmodified Co-NCF samples.

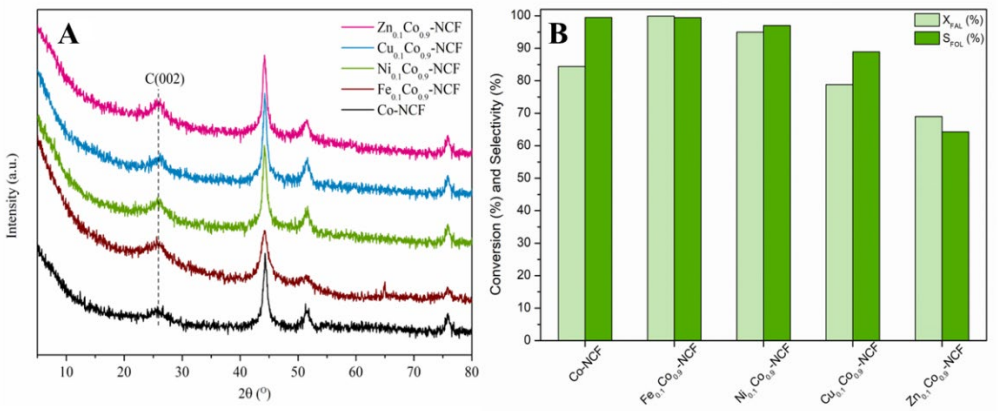

Figure 1. XRD patterns of $M_{0.1}Co_{0.9}$-NCF (A) and catalytic hydrogenation of FAL on $M_{0.1}Co_{0.9}$-NCF (B)

Conclusions: Bimetallic NCF catalysts were prepared *via* a silica-assisted carbonization of $M_{0.1}Co_{0.9}$-ZIF precursors. The NCF catalysts were found highly efficient in FOL production, with Fe- and Ni-modified samples achieving outstanding results. Their catalytic efficiency was attributed to the exposure of a high concentration of active sites and a synergistic effect of Co and the metal dopants in the hydrogen dissociative chemisorption.

***Acknowledgements**: We kindly acknowledge the Romanian Ministry Research and Digitalization, grant PNRR-III-C9-2022-I5-18, ResPonSE - Project, No. 760010/2022for the financial support.*

References:

[1]. Yang Z, Cong X-S, Teng D-G, Wei X-Y, Li Z-X, Xie H-S. Facile selective hydrogenation of bio-based furfural to furfuryl alcohol via a ZIF-67-derived Co-based catalyst. Fuel Process. Technol.;239:107507.

[2]. Bordeiasu M, Goscianska J, Panek R, Nicolaev A, Jurca B, Parvulescu VI, Coman SM. Magnetic Fe,Co-Nanocarbon Frameworks Derived fromFe-Doped Zeolitic Imidazolate Framework-67 as Highly Active Catalysts for 5-Hydroxymethylfurfural Oxidation. ChemSusChem;18:e202500678.

CONTROLLED CELL LINES STOCK – AN IMPORTANT STEP FOR VACCINES DEVELOPMENT

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Keywords: Cell-based vaccine; influenza; cell line; cell lines stock; MDCK; Vero

Introduction: Influenza viruses are a constant health threat, having a high potential to cause epidemics or even pandemics[1]. Vaccination is still the most effective protective measure against ongoing forms of influenza virus infections. Cell-based influenza vaccines are effective alternatives to the conventional embryonated chicken eggs platforms, as they reduce the overall production time, and can be made readily available, provided a stock of well characterized and well-maintained cell lines is created. MDCK (Madin-Darby Canine Kidney) cell line is a well-established substrate for influenza viral multiplication/viral vaccines studies; the viral propagation is comparative to that obtained using embryonated chicken eggs and offers high titers. Genetically engineered cell lines, like MDCK STAT 1 KO[2] and MDCK SIAT1[3] have been selected for influenza production yield and titration assays. Vero (African green monkey kidney) cells[4] have likewise gained widespread use in virus propagation studies. Both Vero and MDCK cells are adherent, however for large-scale production processes they require adaptation to suspension growth or cultivation on microcarriers in serum free media. In this study, we aimed to establish a well characterized in-house working stock of three cell lines- two MDCK variants and one VERO variant sub-cultured, monitored to evaluate the growth rates and morphological characteristics across serial passages, until the optimal cell density for cryopreservation was reached.

Materials and methods: Thawing and initial passage were conducted based on the producer's recommendations. For MDCK STAT 1 KO and Vero E6, the medium used was DMEM Low Glucose and for MDCK SIAT1 DMEM High Glucose. All cell lines were cultured in T-flasks, starting from 25 cm^2 surface area and gradually expanded by cultivation at 37°C, with 5% CO_2. The cells were passaged upon reaching 80-90% surface coverage, maintaining a cellular density of 1-3 x 10^4 cell/ cm^2 in the subsequent passages. After reaching the desired density to establish sufficient aliquots for the cell bank stocks, the cells were cryopreserved and the supernatants were tested for *Mycoplasma* contamination using both an enzymatic assay and PCR quantification.

Results: The cell lines were successfully cryopreserved, at the density of 4 x 10^6 cells/ml, in case of MDCK, Vero E6 at 2.9 x 10^6 cells/ml, and both MDCK STAT1 KO and MDCK SIAT1 cell lines were cryopreserved at 2.5 x 10^6 cells/ml. The *Mycoplasma* control performed showed no contamination, for both test methods used.

Conclusions: The cell lines stock obtained is essential for ensuring experimental reproducibility and it provides immediate access to a well characterized and controlled starting material for future studies.

Acknowledgements: This work was funded through the project ***Dezvoltarea cercetării translaționale pentru vaccinuri, seruri și alte medicamente biologice* - CANTAVAC 2.0, cod SMIS: 326920.**

References:

[1]. H. Kim, R. G. Webster, and R. J. Webby, "Influenza Virus: Dealing with a Drifting and Shifting Pathogen," *Viral Immunol.*, vol. 31, no. 2, pp. 174–183, Mar. 2018, doi: 10.1089/vim.2017.0141.

[2]. Q. Wang *et al.*, "Deficiency of IFNAR1 Increases the Production of Influenza Vaccine Viruses in MDCK Cells," *Viruses*, vol. 17, no. 8, Aug. 2025, doi: 10.3390/v17081097.

[3]. A. Abdoli *et al.*, "Comparison between MDCK and MDCK-SIAT1 cell lines as preferred host for cell culture-based influenza vaccine production," *Biotechnol. Lett.*, vol. 38, no. 6, pp. 941–948, Jun. 2016, doi: 10.1007/s10529-016-2069-4.

[4]. Y. Genzel, C. Dietzsch, E. Rapp, J. Schwarzer, and U. Reichl, "MDCK and Vero cells for influenza virus vaccine production: A one-to-one comparison up to lab-scale bioreactor cultivation," *Appl. Microbiol. Biotechnol.*, vol. 88, no. 2, pp. 461–475, Sep. 2010, doi: 10.1007/s00253-010-2742-9.

INTEGRATED BIO-HYBRID SYSTEMS OF ALGAE-BACTERIA-HYDROGELS FOR ANTIBIOTICS DEGRADATION, RETENTION AND MONITORING IN AQUATIC RESOURCES

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Keywords: bacteria; microalgae; bioremediation; antibiotics; biosensing; hydrogels

Introduction: Tetracycline is a broad-spectrum antibiotic used as treatment of various bacterial infections for both human and zoonotic diseases, having a high use rate among treatment facilities leading to widespread water contamination. Conventional methods of eliminating antibiotics from the environment are proven to be effective, but disadvantages of costs, use of aggressive reactants, secondary pollution and low yields make alternative biodegradation methods increasingly interesting, as bacterial resistance to antibiotics presents a high medical risk[1]. Through our study, we aimed to create a complex, semi-autonomous system that combines hydrogels for capturing antibiotics (e.g. tetracycline-TC) from contaminated waters, their biodegradation through a hybrid alga–microorganism consortium, and dynamic monitoring of the process efficiency using tetracycline-specific aptasensor.

Materials and methods: The bio-remediation process was monitored in a synthetic water matrix containing 5% TC and 1% inoculum. Tests were conducted on combinations of *Chlorella vulgaris* (AICB 329) with *Pseudomonas aeruginosa* (ATCC 27853) and *Bacillus subtilis* (ATCC 6051), in order to determine the most effective consortium towards TC degradation. Thus, for a period of 10 days, both TC concentration and cell density were monitored spectrophotometrically at the appropriate wavelengths. Optimization of glucose concentration (100-1000 mg/L), pH (6-9) and incubation temperature (25°C-35°C) was performed for enhanced TC bioremediation. Scanning electron microscopy (SEM) and FTIR studies were used to observe the morphological differences generated after TC biodegradation[2]. Different hydrogel matrices based on polyvinyl alcohol (PVA) combined with chitosan and laponite were used to determine the optimal retention capacity of TC. Monitoring the decrease in tetracycline concentration in the water samples was performed by electrochemical detection using the specific tetracycline aptasensor developed by immobilizing the specific aptamer on screen-printed carbon paste electrodes modified with in-situ synthesized diazonium salts.

Results: During the test period, a considerable decrease in TC concentration was achieved using *C. vulgaris* individually, as well as in consortium with *B. subtilis*. Thus, a significant decrease in TC concentration was observed during the first 48 hours, due to adsorption by the *C. vulgaris* and *B. subtilis* consortium, followed by a steady reduction through biodegradation, resulting in up to 70% removal of TC by the end of the experimental period. Microscopic analysis did not show any notable morphological changes in *P. aeruginosa* and *C. vulgaris*, whereas *B. subtilis* cells showed elongation upon exposure to TC. Adsorption was confirmed by changes in the functional groups present in the cell wall. The efficiency of TC adsorption by hydrogels was observed to increase with the biopolymer concentration and the presence of laponite inorganic filler, associated with the decrease in pore size dimensions. The aptasensor was used for the detection of tetracycline in electrochemical impedance spectroscopy (EIS), being incubated for 45 minutes with water samples containing inoculum and different concentrations of TC, being observed a decrease in charge transfer resistance (Rct) with increasing of tetracycline concentration.

Conclusions: Microalgae and bacterial consortia prove to be a viable option for bioremediation of TC-contaminated waters. Also, the use of the biopolymer-based hydrogels increases the adsorption rate of these contaminants from the tested medium. Further studies will continue to identify the degradation limits, efficiency against different classes of antibiotics and adaptability to different environmental conditions while maintaining their degradation function.

***Acknowledgements**: This work was supported through the PN 23.06 Core Program - ChemNewDeal, project no. PN 23.06.01.01-AQUAMAT and within PN-IV-P7-7.1-PED-2024-1277-SafeBioChain.*

References:

[1]. Alrefaey K. A., et al., 2025. https://doi.org/10.1039/d5ew00346f.
[2]. Zhou, Y., et al., 2023. https://doi.org/10.1016/j.chemosphere.2023.138240.

DESIGN OF OPTICALLY ACTIVE COORDINATION COMPOUNDS USING ENANTIOPURE COMPARTIMENTAL SCHIFF-BASE LIGANDS: SYNTHESIS, CHARACTERIZATION AND OPTICAL PROPERTIES

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Keywords: coordination compounds; compartimental ligands; circularly polarized luminescence

Introduction: The chiroptical properties of Ln(III) coordination compounds originate from parity-forbidden 4f–4f electronic transitions, which exhibit significant magnetic dipole character. The magnitude of the optical anisotropy parameter (g_{lum}) is determined by the ratio of magnetic to electric dipole transition moments. The inherent structural modularity of coordination chemistry allows efficient transmission of chiral information within the coordination sphere of the lanthanide ion. Along with the narrow emission bands of lanthanide ions, these characteristics render such complexes promising for optoelectronic applications.

Materials and methods: Our activity focuses on the synthesis of optically active 3d–4f coordination compounds incorporating enantiopure ligands to control the interplay of point, axial, and helical chirality. The inclusion of diamagnetic Zn(II) centers preserves 4f-centered luminescence and promotes the chirality transfer from the ligand to the metal ion, facilitating circularly polarized luminescence (CPL).

Results: Preliminary investigations include a Zn(II)–Sm(III) enantiomeric pair, in which the Sm(III) center exhibits CPL activity (Figure 1).

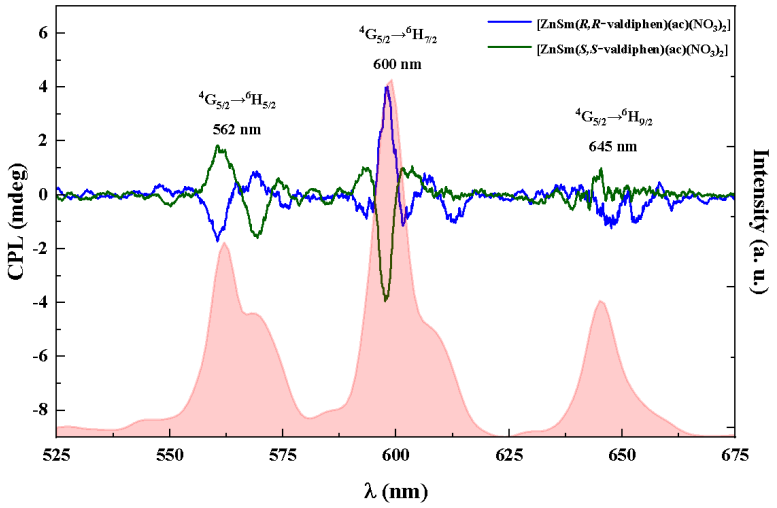

Figure 1. The CPL spectra of the enantiomeric pair (R,R) and (S,S) [ZnSm(valdiphen)(ac)$(NO_3)_2$].

Conclusions: By employing enantiopure ligands and diamagnetic Zn(II) centers, we achieve controlled chirality transfer to Ln(III) ions, enabling circularly polarized luminescence, as demonstrated in a Zn(II)–Sm(III) enantiomeric pair.

*1) **Acknowledgements**: High performance chiral materials for circularly polarized luminescence (CPL) and chirality induced spin selectivity (CISS) (CRUNCHINESS); PNRR-III-C9-2023-I8, CF 6/23.07.2023 (Contract nr. 760230/28.12.2023).*

References:

[1]. Lu, H., Di Bari, L.; Favereau, L. Nat. Photon. 2025;19;1041;
[2]. Tubau, A.; Zinna, F.; Di Bari, L.; Font-Bardia, M.; Vicente, R. Dalton. Trans. 2024;53;13566.

INFLUENCE OF ETHANOLIC SOLVENT CONCENTRATION ON BIOACTIVE COMPOUNDS EXTRACTION FROM *ALOE ARBORESCENS* LYOPHILIZED POWDER

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Keywords: Aloe arborescens; extraction; phytochemical properties; FTIR; UV-VIS; HPLC-DAD; GC-MS

Introduction: *Aloe arborescens* is extensively used due to its pharmacological properties and decorative applications. The phytochemical profile can be assigned to various bioactive compounds such as polysaccharides, proteins, water and fat-soluble vitamins, fatty acids, phenolic compounds, organic acids and minerals[1]. These compounds are widely used in the cosmetic and pharmaceutical industries. The composition of *Aloe arborescens* lyophilized powder and its ethanolic extracts was analyzed and described in the present study.

Materials and methods: *Aloe Arborescens* lyophilized powder was characterized by FTIR spectroscopy, elemental analysis (C, H, N, O). The aloe powder was extracted using 50%, 60%, 70% (v/v) ethanolic solvents by the ultrasound-assisted extraction (UAE) method and Ultra-Turrax extraction method at room temperature. The UV-VIS technique was applied to determine the total polyphenols content, total flavonoids content, photosynthetic compounds content[2] and antioxidant activity[3] of the obtained extracts. Based on the results, the extract with the highest bioactive compounds content was selected for further quantitative analyses. The GC-MS method and FTIR spectroscopy were used for further identification of bioactive compounds. The selected extract was analyzed by HPLC for phenolic acids determination and by ICP-OES for metal content evaluation.

Results: The obtained results highlighted the influence of both extraction method and ethanol concentration on the phytochemical profile of the *Aloe arborescens* extracts. The spectrophotometric analyses revealed the presence of photosynthetic pigments and antioxidant compounds in all extracts. FTIR spectroscopy and GC-MS analysis allowed the identification of several classes of bioactive compounds characteristic of Aloe species, also reported in other studies[4]. Furthermore, HPLC-DAD analysis enabled the quantification of phenolic acids present in the selected extract, while ICP-OES analysis revealed the presence of essential and trace elements.

Conclusions: These findings highlight the importance of optimizing extraction parameters in order to selectively recover specific classes of bioactive compounds from Aloe-based materials for potential pharmaceutical, nutraceutical, and cosmetic applications.

***Acknowledgements**: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CCCDI - UEFISCDI, project number PN-IV-P7-7.1-PTE-2024-0749, within PNCDI IV and by Nucleu Program, project 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.*

References:

[1]. Rodriguez DJ, Angulo-Sánchez Jl, Teixeira da Silva JA, Aguilar-Gonzale CN. Review of Aloe Species Medicinal Properties and Bioactive Compounds. Floriculture Ornamental and Plant Biotechnology: Advances and Topical Issues. 1st ed. Global Science Books, UK; 2006.

[2]. Bista R, Ghimire A, Subedi S. Phytochemicals and Antioxidant Activities of Aloe vera (Aloe barbadensis). Journal of Nutritional Science and Healthy Diet. 2020;1(1):25–36.

[3]. Kim DO, Lee KW, Lee HJ, Lee CY. Vitamin C Equivalent Antioxidant Capacity (VCEAC) of Phenolic Phytochemicals. Journal of Agricultural and Food Chemistry. 2002;50(13):3713–3717.

[4]. Olennikov DN, Rokhin AV, Zilfikarov IN. Method for determining content of phenolic compounds in Aloe arborescens. Chem Nat Compd., 2008; 44, 715–718.

BIOACTIVE MUCOADHESIVE DEXTRAN FROM WATER KEFIR ENRICHED WITH AGRO-INDUSTRIAL BY-PRODUCTS

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Keywords: biophysical properties; prebiotic; cytocompatibility; antioxidant; mucin binding efficiency

Introduction: Throughout the fermentation of water kefir, the microbial consortium synthesizes exopolysaccharides (EPS), which are essential for the organization and structural stability of kefir grains. The primary EPS is dextran (DEX), an α-glucan produced from sucrose through the action of the enzyme dextransucrase. Its structure, dominated by α-(1→6) bonds and secondary branches, confers flexibility and strength to the polysaccharide matrix[1]. Due to its increased biocompatibility and biodegradability, dextran is of major interest for food and pharmaceutical applications[2]. The aim of this study was to investigate the biophysical characteristics, bioactivity and mucoadhesive properties of dextran following the supplementation of water kefir with agro-industrial by-products, in order to support the cellular homeostasis for biomedical applications.

Materials and methods: Dextrans from fermented kefir grains (DEX120) and fermented kefir grains enriched with agro-industrial by-products (DEXGP120) were characterized by Transmission- and Scanning Electron Microscopy (TEM, SEM), X-Ray Diffraction (XRD), rheology, Dynamic Light Scattering (DLS), Zeta potential. The mucin binding efficiency was assessed using the periodic acid-Schiff (PAS) method. The antioxidant activity was determined by FRAP and PFRAP assays. The total carbohydrate content (TCC) was determined by phenol-sulfuric acid method. Cell viability and proliferation were assessed on HGF-1 cells (ATCC CRL-2014) by LIVE/DEAD and Cell Counting Kit-8 (CCK-8) assays. The cytoskeleton was highlighted by labelling actin filaments with Alexa Fluor 488-conjugated phalloidin. The nuclei were marked with DAPI. The *in vitro* antioxidant activity was determined by labeling and quantifying total intracellular ROS with 2',7'-dichloro-dihydro-fluorescein diacetate (H_2DCFDA). The prebiotic activity was investigated on *Limosilactobacillus reuteri* (DSM 20016).

Results: Based on TEM analysis, DEX120 exhibited a relatively compact structure, whereas DEXGP120 displayed a granular structure. SEM analysis indicated that DEX120 had a relatively homogenous and compact structure with large pores, and DEXGP120 exhibited a homogeneous network-like morphology with small pores. XRD analysis showed that DEXGP120 had higher crystallinity compared to DEX120. The Zeta potential of DEX120 was −11.27 ± 1.18 mV, and DEXGP120 exhibited a Zeta potential of −5.01 ± 0.97 mV. The SBL model in DLS indicated that the average hydrodynamic diameter was 67.51 nm for DEX120 and 57.81 nm for DEXGP120, based on molecule number. DEXGP120 had a TCC nearly two times higher than that of DEX120. DEXGP120 exhibited an antioxidant activity about 3.5 times higher than DEX120 by using the FRAP method and about 9 times higher according to the PFRAP assay. The mucin binding efficiency of DEXGP120 was significantly higher compared to DEX120, according to the PAS assay and the rheological measurements. DEX120 and DEXGP120 showed a high degree of cytocompatibility and *in vitro* antioxidant activity, with no changes in cell morphology compared to the cytotoxicity negative control. At 48h post-treatment, DEXGP120 stimulated *L. reuteri* growth by 170.66 ± 6.63% compared to the positive control, whereas DEX120 induced a stimulation of 159.91 ± 3.95% at a concentration of 2.5 mg/mL.

Conclusions: By modulating the fermentation of water kefir through enrichment with agro-industrial by-products, a higher-bioactive dextran is obtained, with significant potential for supporting the cell homeostasis.

***Acknowledgements**: This work was supported by the Romanian Ministry of Agriculture and Rural Development, project "Research regarding development of sustainable technologies for obtaining and valorizing innovative ingredients and foods, for nutritional equilibration of modern consumer's diet" - ADER 17.1.2.*

References:

[1]. Martínez-Torres A, Gutiérrez-Ambrocio S, Heredia-del-Orbe P, Villa-Tanaca L, Hernández-Rodríguez C. Inferring the role of microorganisms in water kefir fermentations .Int J Food Sci Technol. 2017;52:559-571.
[2]. Daba GM, Elnahas MO, Elkhateeb WA.Contributions of exopolysaccharides from lactic acid bacteria as biotechnological tools in food, pharmaceutical, and medical applications. Int J Biol Macromol. 2021;173:79-89.

EFFECTS OF ENCAPSULATED THYME ESSENTIAL OIL ON SEED GERMINATION AND EARLY GROWTH OF *VIGNA RADIATA* SEEDLINGS

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Keywords: volatiles; nanoemulsion; seed treatment; mung bean; saline stress

Introduction: Thyme essential oil (TEO), rich in phenolic bioactive compounds such as thymol and carvacrol, was found to improve seed germination and seedling development under stress conditions, acting as a plant biostimulant[1]. Among the shortcomings of using essential oils is the fact that they are highly unstable due to their volatile nature and they were also shown to have a hormetic response, higher, antimicrobial doses being considered phytotoxic. To overcome this, one solution could be encapsulating them in nanostructured delivery systems, ensuring a slower, controlled release of the bioactive compound. The aim of this study was to investigate the effects of encapsulated and non-encapsulated TEO on mung bean seed germination and seedling growth parameters, as well as on seed tolerance to saline stress, under various conditions.

Materials and methods: For the encapsulation of TEO in a nanostructured delivery system a phase inversion emulsification process was used[2]. In order to address the biostimulant activity of encapsulated and non-encapsulated TEO, two approaches were used. For the first approach (indirect contact) sterilized dry mung bean seeds were either pretreated for 72 h before germination or germinated in the presence of the volatile components from TEO or emulsion. For the second approach (direct contact of the seeds with the products) freshly sterilized seeds were pretreated for 5 h with different doses of encapsulated and non-encapsulated TEO. For the direct contact approach, two controls were used: untreated seeds and seeds treated with 2.5% (v/v) dimethylsulfoxide, and for the indirect contact approach, the water control was used.The final experiments were performed both in the presence and in the absence of saline stress. All the tests were set in a growth chamber with controlled temperature, light and humidity[3]. The experiments were stopped after 5 days, seedlings photographed and the following parameters were investigated: mean germination time (MGT), germination rate (GR), germination percentage (GP), germination energy (GE), root length, shoot length, seedling length and vigour index (VI), root weight, shoot, cotyledon, leaf weight, and seedling weight.

Results: In the case of the indirect contact approach, the 72h pre-treatment on dry seeds did not have any significant effect. The TEO volatiles released during seed germination had significant inhibitory effects on seedlings, whereas encapsulated TEO (eTEO) significantly stimulated seedling development, in the absence of salt stress. At 50 mM NaCl, TEO and eTEO increased GP from 85% to 100% and eTEO slightly stimulated seedling development, but not statistically significant. In the case of the direct contact approach, the effects ranged from slightly stimulatory to significant inhibitory in the absence of salt, depending on the dose. Both TEO and eTEO increased the salt tolerance of seedlings under high saline stress (100 mM NaCl), but had no significant effect under moderate saline stress (50 mM NaCl).

Conclusions: In the absence of salt, significant positive effects on seedlings were obtained by volatile release from eTEO, but negative effects by volatile release from TEO, at the dose tested. Under high saline stress, both TEO and eTEO applied directly on seeds protected the seedlings, at the doses tested. Under moderate saline stress, the effects were less significant. The nanoemulsion eTEO has the potential as a better biostimulant than TEO under certain conditions, due to the controlled release of active ingredients.

***Acknowledgements**: This research was funded by project PN 23.06.02.01 InteGral, Nucleu Programme, funded by Ministry of Education and Research.*

References:

[1]. Ben-Jabeur M, Vicente R, López-Cristoffanini C, Alesami N, Djébali N, Gracia-Romero A, Serret MD, López-Carbonell M, Araus JL, Hamada W. A novel aspect of essential oils: coating seeds with thyme essential oil induces drought resistance in wheat. Plants 2019; 8 (10), 371-88.

[2]. Ostertag F, Weiss J, McClements DJ. Low-energy formation of edible nanoemulsions: factors influencing droplet size produced by emulsion phase inversion. J Colloid Interface Sci. 2012; 388 (1),95-102.

[3]. Tritean N, Trică B, Dima ȘO, Capră L, Gabor RA, Cimpean A, Oancea F, Constantinescu-Aruxandei D. Mechanistic insights into the plant biostimulant activity of a novel formulation based on rice husk nanobiosilica embedded in a seed coating alginate film. Front. Plant Sci. 2024; 15, 1349573-601.

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