POLISH - PORTUGUESE SYMPOSIUM ON BIOMATERIALS

PROGRAM AND BOOK OF ABSTRACTS

AGH UNIVERSITY OF KRAKOW

8TH OCTOBER 2025

To exchange ideas, research results, and perspectives within the field of biomaterials science and engineering. To meet, discuss, seek collaboration, and enhance partnership between Polish and Portuguese biomaterials scientists.

Organizers

Prof. Elżbieta Pamuła
Dr. Patrycja Domalik-Pyzik
Dr. Konrad Kwiecień

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Faculty of Materials Science and Ceramics,
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ENGINEERING OF BIOMATERIALS
THE OFFICIAL JOURNAL OF THE POLISH SOCIETY FOR BIOMATERIALS AND THE FACULTY OF MATERIALS SCIENCE AND CERAMICS / AGH UNIVERSITY OF KRAKOW

ENGINEERING OF BIOMATERIALS

THE OFFICIAL JOURNAL OF THE POLISH SOCIETY FOR BIOMATERIALS AND THE FACULTY OF MATERIALS SCIENCE AND CERAMICS / AGH UNIVERSITY OF KRAKOW

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The Journal Engineering of Biomaterials publishes refereed original articles and review papers on biomedical aspects of engineering. It deals with application of materials engineering principles and methods to problems associated with human health. This includes the design and manufacturing of biocompatible materials, implants, artificial organs, controlled drug delivery systems and various medical devices. The journal encourages to present the research results focused on the areas of biomaterials technology and analysis of interaction between implant surfaces and the biological environment/living tissue to improve the biocompatibility and the biofunctionality of biomaterials.

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Program

10:00 - 10:15	Opening remarks
	Experts' Panel
10:15 – 10:40	**Cristina Barrias** *Modular Bottom-up Strategies for Microvascular Network Assembly*
10:40 – 11:05	**Aneta Zima** *New Trends in Bioceramics Materials for Bone Regeneration*
11:05 – 11:30	**Judite Barbosa** *Immunomodulatory Biomaterials as a Bridge Between Inflammation and Tissue Regeneration*
11:30 – 12:00	**Coffee break (onsite)/Networking**
	Next Gen Biomaterials: Stories from the Lab
12:00 – 12:15	**Konrad Kwiecień** *Inhalable Dry Powders from Polyanhydride Microparticles as a Weapon Against Pulmonary Infections*

Short oral presentations by PhD and MSc students to see the most up-to-date research results

1. **Paulina Armatys**, Elżbieta Długoń, Alina Dudinskaya, Ewa Stodolak-Zych
   Sol–Gel Derived Zirconia and Zirconia–Siloxane Coatings for Antibacterial Protection of Tracheostomy Implants
2. **Wiktoria Bulanda**, Anna Ścisłowska-Czarnecka, Ewa Stodolak-Zych
   Electrospun Membranes Functionalized with Exosomes for Enhanced Skin Regeneration
3. **Zuzanna Burkiewicz**, Paulina Armatys, Ewa Stodolak-Zych
   Metal Ion-Modified Nanostructured Titanium Surfaces for Infection-Resistant Implants
4. **Julia Godzwon**, Joanna Czechowska, Kinga Kowalska, Piotr Pańtak, Aneta Zima
   Ceramic Scaffolds for Dental Applications: β-TCP and Hydroxyapatite with Controlled Drug Delivery
5. **Szymon Jaśniewski**, Andrzej Kotarba, Gabriela Jajko-Liberka
   Decoration of Polymeric Biomaterials with Heparin Nanoparticles via Sonochemistry
6. **Agnieszka Kłapcia**, Dorota Lachowicz, Szczepan Zapotoczny
   Cyclodextrin-Based Carriers for Curcumin: Improved Solubility and Lipid Membrane Integration
7. **Hubert Knap**, Weronika Jaśko, Izabella Ślęzak-Prochazka, Alicja Kazek-Kęsik
   Preliminary Analysis of Antibacterial Coatings Formed on Ti Alloys
8. **Kinga J. Kowalska**, Joanna P. Czechowska, Magdalena Szumera, El Sayed Yousef, Aneta Zima
   From Bioactivity to Multifunctionality: Gold-Doped Phosphate Bioactive Glasses and Glass-Ceramics for Bone Regeneration

9. **Anna Kusibab**, Ana Beatriz Sousa, Judite Novais Barbosa, Justyna Drukała, Elżbieta Pamuła
   Effects of Combining Quercetin and Curcumin on Viability, Morphology and Migration of L929 Fibroblasts and Macrophages Viability
10. **Aleksandra Lisowska**, Antonette Jessica Arunkumar
    Effect of Engineered Surface Features on Flow Dynamics and Endothelial Cell Response in a Biomimetic Vessel Model
11. **Maciej Łach**, Magdalena Bańkosz, Bożena Tyliszczak
    3D/4D-Printed Functional Hydrogels as Transdermal Platforms for Targeted Skin Cancer Therapy
12. **Teresa Matlak**, Roman Jędrzejczyk, Agnieszka Kyzioł, Karol Kyzioł
    Sustainable Synthesis of Silver Nanoparticles with Antioxidant Activity for Potential Biomedical Applications
13. **Justyna Matysek**, Anna Górska-Ratusznik, Jonasz Czajkowski, Barbara Pucelik, Patrycja Domalik-Pyzik
    Drug-Loaded κ-Carrageenan and HP-β-Cyclodextrin Hydrogel Films: A Potential Approach for Diabetic Foot Treatment
14. **Jakub Nowak**, Andrzej Kotarba, Gabriela Jajko-Liberka
    Surface Functionalization of Polymers with Ibuprofen Nanoparticles
15. **Katarzyna Sala**, Magdalena Bańkosz, Bożena Tyliszczak
    Janus Nanoparticles – Research into Active Substance Carriers in Targeted Skin Cancer Therapy
16. **Issam Thamer**, Magdalena Mazurek-Budzyńska, Vignesh Kumaravel
    Sustainable Extraction Techniques for Functional Biopolymers with Improved Antibacterial Features
17. **Kamila Walczak**, Katarzyna Reczyńska-Kolman, Elżbieta Pamuła
    Effect of Processing Conditions on The Degree of Hyaluronic Acid Oxidation and Biological Tests on Hyaluronic-Acid Based Hydrogels
18. **Weronika Wałczyk**, Małgorzata Noworyta, Magdalena Jankowska, Andrzej Świeży, Filip Petko, Klaudia Trembecka-Wójciga, Joanna Ortyl
    Novel Photocurable Resin with High-Density Packing of Bimodal Zirconia Particles for 3D Printing of Bone-Mimetic Scaffolds
19. **Dominika Wanat**, Magdalena Bańkosz, Bożena Tyliszczak
    New Generation of Drug Carriers: Transfersomes in Dermato-Oncology Therapy
20. **Krzysztof Stafin**, Paweł Śliwa, Marek Piątkowski
    Chitosan-Templated Biomimetic Mineralization of Calcium Phosphate: Theoretical vs. Experimental Studies

Experts Panel

Prof. Dr. Cristina Barrias

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Cristina Barrias is a Principal Investigator and Leader of the Bioengineered 3D Microenvironments (BEMIC) group at i3S – Instituto de Investigação e Inovação em Saúde, University of Porto (www.i3s.up.pt), and an Invited Associate Professor at Instituto de Ciências Biomédicas Abel Salazar (ICBAS), University of Porto. She also serves as Vice-President of Instituto de Engenharia Biomédica (INEB), Vice-President and Journal Liaison Officer of the European Society for Biomaterials (ESB), and is Managing Editor of Materials Today Bio. Her research focuses on engineering bioinspired 3D microenvironments to direct cell–matrix assembly and function. Her group employs molecularly designed biomaterials, microtissues and organoids as building blocks to recreate key aspects of human tissue development, regeneration, and disease progression. A major focus is the bottom-up engineering of perfusable microvascular networks, essential for sustaining tissue function, mediating repair, and modeling pathological conditions. These efforts support the development of advanced regenerative strategies and physiologically relevant in vitro models for fundamental research and therapeutic screening. She is the author of more than 120 scientific articles (h index 41, citations 5250).

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Modular Bottom-up Strategies for Microvascular Network Assembly

Bottom-up tissue engineering (TE) approaches using microscale living materials as building blocks offer an exciting avenue for generating complex 3D constructs akin to native tissues. These microtissue units typically present high cell densities and a rich extracellular matrix (ECM) composition. Their biological relevance can be improved by the rational integration of different cell types, promoting the establishment of pivotal cell-cell and cell-ECM interactions. This allows the recreation of biomimetic micro-niches and the recapitulation of complex morphogenetic processes. Significantly, microtissues with stable capillary beds can be generated by the co-assembly of blood vessel-forming endothelial cells with supporting stromal cells. These vascular units (VUs) can be further combined with other types of microtissues, organoids and/or biomaterials to build large-scale vascularized tissues from the bottom up through a modular TE approach. Structurally complex and perfusable constructs can be obtained by combining VUs with other technologies, such as 3D bioprinting and microfluidics. This talk will feature some examples of scaffold-based and scaffold-free VUs developed by our group[1-6] and their application in regenerative medicine and organ/disease modelling.

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Aneta Zima is an Associate Professor at AGH University of Krakow, where she leads the Bioceramics Group in the Department of Ceramics and Refractories. Her research focuses on biomaterials, composites, and hybrid materials, with particular emphasis on calcium phosphate-based biomaterials for bone tissue engineering and regenerative medicine. She is a member of the Polish Society for Biomaterials, the Polish Ceramic Society, and the Biomedical Engineering Discipline Council at AGH. Professor Zima has served as an expert, reviewer, and panelist for the Foundation for Polish Science and the National Science Centre, and she has contributed to the Organizing Committees of numerous international conferences, including Ceramics in Europe 2022. In 2023, she completed a research internship at Anna University in Chennai, India. Professor Zima has supervised three doctoral dissertations, over 20 master's theses, and more than 30 engineering theses. She is the author of over 90 peer-reviewed publications (h-index: 19; 1,087 citations, Scopus) and the inventor/co-inventor of 11 patents and patent applications. She has also led and participated in numerous research projects.

Aneta Zima

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New Trends in Bioceramic Materials for Bone Regeneration

Bioceramics have emerged as a vital class of materials in modern medicine, valued for their exceptional mechanical strength, biocompatibility, and their ability to interact with biological systems. Among them, calcium phosphate bioceramics, particularly hydroxyapatite (HAp) and tricalcium phosphate (TCP or whitlockite), are widely used across various medical fields, including orthopaedics, maxillofacial surgery, restorative dentistry, tissue engineering, regenerative medicine, and targeted drug therapy.

Particularly promising are intelligent materials, known as smart biomaterials, which are designed to interact with their environment and respond to external stimuli such as temperature, pH, magnetic fields, or the presence of enzymes. Smart bone substitute materials can dynamically adapt to physiological conditions and integrate with the host tissue, making them highly desirable for medical applications. This intelligent approach has the potential to revolutionize biomaterial engineering and transform the treatment of severe bone tissue damage by offering solutions that are significantly more effective than conventional implants.

The latest advancements in bone substitute materials focus on the development of hybrid biomaterials. These hybrid bone substitutes integrate organic and inorganic components, effectively supporting bone regeneration. Thanks to the synergy between both types of constituents, these materials offer enhanced tissue integration, mechanical strength and controlled biodegradation.

Another rapidly developing approach is the design of bioceramics and composites with intrinsic antibacterial properties. Drugs and biologically active agents incorporated into advanced bioceramic or hybrid implants are released locally at the implantation site, reducing systemic exposure and minimizing the risk of side effects. Given the growing resistance of bacteria to antibiotics, the creation of materials with built-in antimicrobial functionality is becoming increasingly essential.

In addition to material innovation, advanced manufacturing technologies are playing a transformative role in medicine. At the forefront of these technologies is 3D printing, which allows for fine-tuned control over scaffold pore geometry and internal architecture. This method enables the fabrication of customized, patient-specific implants that precisely replicate the unique anatomy of bone defects. Such customization greatly improves implant integration, vascularization, and the overall regenerative potential of the scaffold, pushing the boundaries of current bone tissue engineering.

Combining 3D printing techniques with smart biomaterials that promote tissue regeneration, alongside hybrid composites with antibacterial activity, opens new perspectives for the effective treatment of complex bone defects

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The Use of Specialized Pro-Resolving Mediators for the Development of Immunomodulatory Biomaterials

The implantation of a biomaterial will lead to the immediate onset of an acute inflammatory response, which is of key importance in shaping the quality of the repair process. However, the return to homeostasis is critical to prevent a chronic inflammatory response that may impair the healing process (1). The resolution of the inflammatory response is now recognized as an active and highly regulated process, being described as specialized immunoresolvents that have a fundamental role in the termination of the acute inflammatory response. These mediators collectively coined as specialized pro-resolving mediators (SPMs) are a family of endogenous molecules that include lipoxins (Lx), resolvins (Rv), protectins (PD), maresins (Mar), Cysteinyl-SPMs (Cys-SPMs) and n-3 docosapentaenoic acid-derived SPMs (n-3 DPA-derived SPMs). SPMs have important anti-inflammatory and pro-resolutive actions such as decreasing the recruitment of polymorphonuclear leukocytes (PMNs), inducing the recruitment of anti-inflammatory macrophages, and increasing macrophage clearance of apoptotic cells through a process known as efferocytosis (2).
The advent of tissue engineering and regenerative medicine led to the development of new biomaterials with the capability of enhancing tissue repair and regeneration. The recognition of the key importance of the immune system in tissue healing moved researchers to the development of a new class of biomaterials that present the ability to modulate inflammatory responses—the immunomodulatory biomaterials (3). During this talk examples of the use of specialized pro-resolving mediators in biomaterial-based immunomodulation will be explored (4-7).

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Next-Gen Biomaterials: Stories from the Lab

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Inhalable Dry Powders from Polyanhydride Microparticles as a Weapon Against Pulmonary Infections

Chronic lung diseases such as COPD are often associated with chronic bacterial colonization, leading to recurrent exacerbations. Systemic antibiotics are limited by poor biodistribution to the lungs, and therefore, high doses required, side effects, and bacterial resistance. Inhalable dry powder formulations (DPIs) offer a promising alternative, but few antibacterial DPIs are clinically available.

This work investigated polyanhydrides as carriers for antibacterial drugs in DPIs. Five polymers were synthesized from sebacic acid with ether comonomers (either PEG250 or PEG600, namely PSAEG250 or PSAEG600, respectively) and characterized by NMR, FTIR, DSC, and surface properties. Microparticles in the range of diameters 1–5 µm, i.e. a proper size distribution for inhalation, were successfully produced using oil-in-water emulsification. However, exhibited agglomeration, leading to a much higher size distribution of the generated aerosol. On the other hand, the low density of polymeric powder improved its aerodynamic properties, leading to an aerodynamic size distribution much better than the physical one, i.e. fraction below 5 µm was around 21% and 66% for the same formulation regarding physical and aerodynamic diameters, respectively.

Hydrophobic drugs, particularly azithromycin (AZM), showed high encapsulation efficiency (up to 100%) due to conjugation with the polymeric matrix during manufacturing. Thanks to this, they were efficient against various strains of *Staphylococcus aureus*, either methicillin-sensitive or -resistant, in non-toxic concentrations, as shown by *in vitro* studies with human lung epithelial cells and *ex vivo* with precision-cut lung tissue slices from rats.

The results indicated that PSAEG250 microparticles loaded with azithromycin are a promising inhalable formulation for treating lung infections, particularly in patients with chronic lung diseases.

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Short oral presentations

Paulina Armatys

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Sol–Gel Derived Zirconia and Zirconia–Siloxane Coatings for Antibacterial Protection of Tracheostomy Implants

Tracheostomy tubes are essential in long-term mechanical ventilation, yet their continuous exposure to both internal and external environments promote bacterial colonization and biofilm formation, leading to ventilator-associated pneumonia (VAP). VAP is one of the most severe complications of mechanical ventilation, associated with increased mortality, prolonged hospitalization, and significant healthcare costs. Currently, no effective and durable antibacterial solutions are clinically available for such devices, making the development of innovative protective coatings an urgent and strategic research challenge. [1-2].

A major challenge in long-term tracheostomy care is the prevention of bacterial colonization and biofilm formation on implant surfaces. A promising strategy to address this issue is the application of zirconia- and zirconia–siloxane-based sol–gel coatings applied by dip-coating. In this study, functional layers were obtained using siloxane sols [dimethyldiethoxysilane (DEDMS) and methyltriethoxysilane (TEOS)], zirconia sol [zirconium (IV) tetrapropoxide], and mixed zirconia–siloxane sols.

The implants were coated with a single sol-derived layer and thermally cured (70 °C, 7 days). Successful deposition was confirmed by SEM and EDS analyses. Contact angle and surface free energy measurements indicated changes in surface physicochemistry, with increased hydrophobicity (from ≈84° to >100°) and reduced surface free energy in zirconia-containing coatings (from ~35 mJ/m² to ~25 mJ/m²). Microbiological evaluation following JIS L 1902:2002 standards demonstrated strong antibacterial activity of zirconia-based coatings, with bacterial reduction of ≈70% for zirconia–siloxane sols and ≈99% for zirconia sols. In contrast, siloxane coatings alone showed no antibacterial effect.

The dip-coating process proved effective for modifying implants with complex geometries, such as tracheostomy tubes. Importantly, zirconia-based layers remained stable after plasma sterilization and autoclaving, confirming their robustness and translational potential as clinically relevant antibacterial coatings.

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Electrospun Membranes Functionalized with Exosomes for Enhanced Skin Regeneration

Chronic wounds and impaired skin regeneration remain a major challenge due to persistent inflammation and insufficient cellular activity. Electrospun fibrous scaffolds have emerged as attractive candidates for regenerative medicine, since their morphology closely resembles the extracellular matrix (ECM). Among various polymers, polylactic acid (PLA) stands out for its biodegradability and mechanical stability, but its limited bioactivity restricts wider therapeutic applications [1]. One strategy to address these drawbacks is aminolysis, which introduces reactive amine groups and allows immobilization of bioactive agents such as exosomes, nanoscale vesicles that modulate immune responses and support tissue repair [2].

In this work, PLA membranes were electrospun into uniform nanofibers and subsequently surface-activated by aminolysis carried out for 5, 10, and 15 minutes. To enhance bioactivity, commercial exosomes were immobilized. Surface chemistry was verified by ninhydrin assay and the XPS method, while morphology and porosity were assessed by SEM and the capillary flow porometry. Physicochemical characterization included FTIR, DSC, TG, and wettability analysis. For biological studies, RAW 264.7 macrophages and HaCaT keratinocytes were used to evaluate cytocompatibility, viability, and cytokine secretion.

SEM analysis confirmed, that the electrospun PLA membranes exhibited a uniform fibrous architecture without beads formation. After the aminolysis, the fibers preserved structural integrity with slight roughening, while XPS and the ninhydrin confirmed time-dependent amine formation, with 5-min treatment proving to be the most effective for further functionalization. The thermal and FTIR analyses indicated a thermal stability and polymer structure with no significant degradation. The exosomes immobilization markedly decreased water contact angle and increased surface free energy, improving hydrophilicity and creating a more cell-friendly interface. *In vitro* studies used, RAW 264.7 macrophages showed the highest viability on unmodified and 5-min aminolyzed PLA membranes, whereas the HaCaT keratinocytes proliferated most on the membranes functionalized with animal-derived exosomes.

The combination of the aminolyzed PLA nanofibers with the exosome-based bioactivation represents a promising strategy for skin regeneration. This approach enhances scaffold-cell interactions and opens the way to personalized wound-healing therapies, yet further studies are needed to optimize functionalization and fully understand cell–material interactions.

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Metal Ion-Modified Nanostructured Titanium Surfaces for Infection-Resistant Implants

Implant-related infections are a major clinical challenge, enhanced by the rising antibiotic resistance of bacteria. Titanium endoprostheses are particularly susceptible to biofilm formation, with infection rates reaching up to 30% depending on the surgical site. Developing implant surface modifications that combine antibacterial efficacy with biocompatibility is therefore a critical need.

In this study, titanium substrates were oxidized with 30% H_2O_2 and chemically modified with metal salts: biocidal agents ($AgNO_3$, $Zn(NO_3)_2 \cdot 6H_2O$) and a bioactive agent ($Mg(NO_3)_2 \cdot 6H_2O$). Nanostructuring increased surface area and oxygen content, forming a nanostructured titanium oxide layer. The surfaces were characterized by the contact angle analysis, SEM, ICP measurements, bacterial reduction assays, and cellular studies.

Results demonstrated that silver and zinc significantly inhibited bacterial growth: silver reduced *E. coli* by 99.99% and *S. aureus* by 83.7%, while zinc reduced *E. coli* by 10.1% and *S. aureus* by 46.1%. Magnesium exhibited no antibacterial activity but enhanced cell viability. All modifications increased surface free energy without altering nanostructure, and ion release was confirmed after 7 and 14 days.

These findings highlight the potential of tailored metal-salt surface modifications to achieve both antimicrobial activity and biocompatibility. Such dual-functional coatings represent a promising strategy for next-generation titanium implants, balancing infection prevention with support of cellular integration and offering a translational pathway toward improved clinical outcomes.

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Ceramic Scaffolds for Dental Applications: β-TCP and Hydroxyapatite with Controlled Drug Delivery

Calcium phosphate ceramics, such as hydroxyapatite (HAp) and β-tricalcium phosphate (β-TCP), are well-known as promising biomaterials in regenerative medicine [1]. Their bioactivity, chemical similarity to natural bone, and ability to support new tissue formation make them attractive for a broad range of applications in orthopedics and implantology, including alveolar ridge reconstruction. Beyond their structural role, these scaffolds have the potential to serve as local drug delivery systems, providing a dual therapeutic effect: mechanical stability combined with controlled release of therapeutic molecules [2].

In this study, preliminary research was aimed at the characterization of calcium phosphate powders intended for scaffold fabrication. The analysis included determination of the specific surface area (BET) and particle size distribution (DLS), which are critical parameters influencing sintering behavior, porosity, and drug incorporation efficiency. These measurements provide insight into the suitability of the powders for further processing into porous scaffolds enriched with anti-inflammatory drugs.

The obtained data confirmed that both HAp and β-TCP powders exhibit physicochemical properties favourable for scaffold fabrication. Notably, the BET surface area of HAp (22.523 m^2/g) exceeded that of β-TCP (6.638 m^2/g), indicating a higher potential for drug adsorption and controlled release. In contrast, the wider particle size distribution of HAp facilitated more efficient sintering, whereas the higher porosity preserved in β-TCP compacts is advantageous for scaffold applications, as interconnected pores enhance both tissue ingrowth and drug delivery.

The initial characterization of calcium phosphate powders forms the foundation for the development of porous ceramic scaffolds capable of controlled release of anti-inflammatory agents. Such systems hold potential to accelerate healing, reduce inflammation, and minimize the risk of complications following dental surgery. Future work will focus on scaffold fabrication, structural evaluation, and drug release profiling, to validate their clinical applicability.

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Decoration of Polymeric Biomaterials with Heparin Nanoparticles via Sonochemistry

The implantation of various medical devices carries a real risk of thrombosis, which is particularly relevant for polymeric implants in long-term blood contact (PICC lines, vascular grafts). Immobilization of sodium heparin onto polymeric surfaces is an effective strategy to improve hemocompatibility.

We developed nanoscale heparin particles with anticoagulant activity using a sonochemical synthesis approach and anchored them onto polymer-based materials. The use of ultrasonic irradiation led to the formation of stable nanoparticles, suitable for surface attachment. Polyurethane and parylene C films were modified with cold oxygen plasma to introduce polar functional groups, which significantly improved particle immobilization compared to untreated surfaces. Surface analysis techniques, including AFM, XPS, and ATR-IR, verified the chemical changes and showed that the nanoparticles were evenly distributed. In addition, molecular dynamics simulations helped us understand how the drug interacts with the modified surfaces on a molecular level.

Our findings show that this combination of sonochemistry and plasma treatment is a practical way to add anticoagulant properties to polymeric materials. This method could be useful in designing drug-releasing coatings and implants with controlled performance.

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Cyclodextrin-Based Carriers for Curcumin: Improved Solubility and Lipid Membrane Integration

Curcumin, a natural polyphenol with well-documented anticancer and anti-inflammatory effects, suffers from limited bioavailability due to its low aqueous solubility and hydrophobic character. To overcome these limitations, inclusion complexes were developed using cyclodextrins—compounds with a characteristic structure capable of hosting guest molecules within their hydrophobic cavity. The host–guest interaction leading to the formation of inclusion complexes between cyclodextrin (host) and curcumin (guest) is illustrated in Figure 1.

Three types of cyclodextrins — β-cyclodextrin, its polymeric derivative (β-CDpoly), and 2-hydroxypropyl-β-cyclodextrin (HP-β-CD) — were used to encapsulate curcumin. Binding constants determined by spectrophotometric titration confirmed the successful formation of the inclusion complexes. The influence of these complexes on model lipid membranes was evaluated using Langmuir monolayers composed of DPPC. The isotherm analysis revealed improved compatibility of the cyclodextrin complexes with the lipid monolayer compared to free curcumin. Physicochemical characterization using DLS, FT-IR, and TG-DTA confirmed the formation of host–guest inclusion complexes, their stability in aqueous solutions, and improved thermal resistance, respectively. Additionally, UV-VIS spectrophotometric analysis demonstrated a significant increase in the aqueous solubility of curcumin after its release from previously dissolved lyophilized inclusion complexes.

These results highlight the potential of cyclodextrins as carriers for hydrophobic anticancer drugs, with curcumin serving as a model compound.

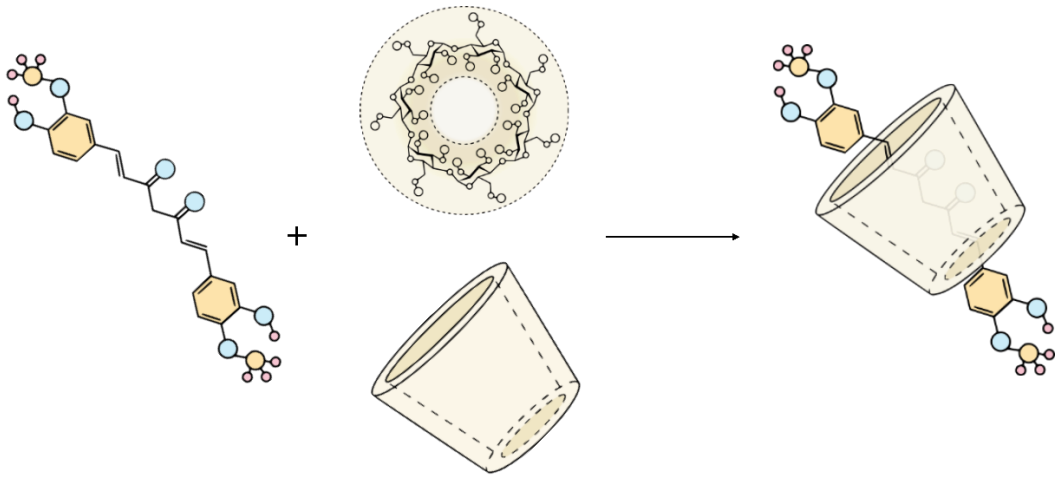

Fig. 1 Scheme of complexation reaction between curcumin molecule and β-CDs.

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Preliminary Analysis of Antibacterial Coatings Formed on Ti Alloys

Surface modification of titanium and its alloys is still growing field of biomaterial engineering. Today's trends put an emphasis on regenerative properties of implanted implants and developing of antibacterial properties of the obtained surfaces. Currently, there is research being carried out into modifying surface of titanium implants using electrochemical methods as well as conducting post–treatment to put active substances on the surface of modified implant. For example, there was research published [1] which investigated the combination of clindamycin as an active substance and PLGA as polymer which was used as carrier for the drug. This kind of the coating could inhibit *S. aureus* ATCC 25923 growing whereas the number of living mouse fibroblast cells L929 was 95% after 3 days of cells culture with the extracts collected from the dental implant. Only a singular bacteria were attached to the implant surface but with the visible changes in their morphology (scanning electron microscopy) [1]. Additionally, research was undertaken to examine the possibility of using benzydamine chloride as drug for creating bacteriostatic layer, as well as using MXenes nanoparticles for this purpose. For example, the MXenes could be deposited on previously anodized surface using ultrasonic coating machine (Sono-Tek, NY, USA) [2].

Now, the biggest challenge for researchers working in the field of biomaterials is using and researching new active substances or nanoparticles which would allow us to develop new bacteriostatic layers, that could combat bacterial infections even against drug-resistant strains of bacteria. Some of the researched substances might have the ability to biodegrade, which would minimize harmful effects of waste and releasing of them into the environment. Additionally, to this effort, more throughout investigation into the biological mechanism of infections and implant integration with the tissues should be carried out to deepen the knowledge of these processes and help us in using the right dose of active substances to achieve goal of antibacterial layer.

In conclusion, new challenges in the field of biomedical engineering are focusing on new active substances to be used for development of bacteriostatic layers. Integration of electrochemical methods into this goal could help us achieve highly biocompatible layers with additional bacteriostatic properties.

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From Bioactivity to Multifunctionality: Gold-Doped Phosphate Bioactive Glasses and Glass-Ceramics for Bone Regeneration

Bioactive glasses and glass-ceramics have garnered significant attention in the field of biomaterials due to their exceptional ability to bond with bone tissue. Following the pioneering work of Larry Hench and the development of 45S5 bioglass, a variety of bioactive glass formulations have been explored. Among these, phosphate-based bioactive glasses are of particular interest for drug delivery applications, owing to their higher solubility. In this research, two novel phosphate-based bioactive glasses with compositions of P_2O_5–CaO–$Ca(OH)_2$–KF–Na_2O–TiO_2 and P_2O_5–CaO–$Ca(OH)_2$–ZnO–KF–TiO_2 were synthesized by melt-quenching method. The bioglasses were additionally doped with 500 ppm or 2000 ppm of $HAuCl_4 \cdot 3H_2O$ to impart radiopaque properties and potentially enhance contrast for diagnostic imaging applications such as X-ray and CT scans after material's implantation. The crystallization behaviour of these glasses was analysed using DSC, revealing a characteristic crystallization temperature. Upon heating above this temperature, the glasses partially crystallized, what leads to the formation of bioactive glass-ceramics. Materials characterization using FT-IR revealed the presence of key bioactive structural units, while XRD analysis confirmed the formation of crystalline phases, including β-pyrophosphate. The $KAuF_4$ phase was detected in bioactive glass-ceramics doped with 2000 ppm of $HAuCl_4 \cdot 3H_2O$, which may confer radiopaque properties, potentially enhancing the material's visibility in medical imaging and making it a promising candidate for diagnostic applications, particularly in visualizing implants or monitoring tissue regeneration.

The bioactivity of the glass-ceramics was evaluated by immersion in Simulated Body Fluid (SBF), which led to the formation of an apatite-like layer on the surface of the P_2O_5–CaO–$Ca(OH)_2$–KF–Na_2O–TiO_2 glass-ceramics. This material was selected for further investigation. The influence of the bioglass composition, the presence of specific structural units, and the bioglass-ceramic phase composition on *in vitro* bioactivity was examined.

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Effects of Combining Quercetin and Curcumin on Viability, Morphology and Migration of L929 Fibroblasts and Macrophages Viability

Flavonoids, such as quercetin (QE) and curcumin (CUR), are phenolic, bioactive compounds with the potential to accelerate chronic wound healing due to their anti-inflammatory, antimicrobial and antioxidant properties [1]. Our aim was to investigate the effect of combining QE and CUR in different mass ratios on the viability, morphology and migration of L929 cells and viability of macrophages for potential use in chronic wound treatment.

Cell viability was tested in contact with L929 fibroblasts by resazurin reduction assay and by live/dead fluorescent staining. Cell migration and morphology were evaluated by scratch test. QE and CUR were sterilized by exposure to UV radiation. Tests were performed after 24 h cell incubation in medium (DMEM supplemented with 1% fetal bovine serum, 1% penicillin/streptomycin and 1% dimethyl sulfoxide) with QE, CUR, QE:CUR (1:1), QE:CUR (1:3) and QE:CUR (3:1); total additives concentration was 7.5 µg/mL. Primary human monocytes were isolated from buffy coats and differentiated to macrophages by macrophage colony-stimulating factor (M-CSF). LDH assay was performed on supernatants after cells in contact with QE and CUR (4.5 µg/mL) for 24 h.

Fibroblasts viability increased (*$p < 0.05$) for the QE:CUR (1:1) and QE:CUR (1:3) samples compared to the control (cells not submitted to additives). Moreover, the combination of CUR and QE had a better effect on cell viability than when used separately, suggesting potential synergy between them. The use of QE and CUR at this concentration did not affect cell morphology. The strongest migration was observed for QE:CUR (1:1). For the rest of the samples, the migration results were below those for the control. Macrophages viability after 24 h of incubation with QE and CUR did not change compared to the control.

We conducted *in vitro* studies of fibroblasts and macrophages in contact with QE and CUR, tested cell viability, morphology and migration. We have found that combining QE and CUR in particular ratios may be beneficial in chronic wound management. In the following studies, hydrogel matrices with QE and CUR will be prepared and their activity will be evaluated.

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Effect of Engineered Surface Features on Flow Dynamics and Endothelial Cell Response in a Biomimetic Vessel Model

The success of vascular implants depends on rapid and stable endothelialisation, essential for reducing thrombosis, inflammation, and implant failure [1]. Traditional surface modifications often rely on biochemical coatings; however, recent research highlights the potential of physical surface cues - such as micro- and nano topographies - to modulate endothelial cell behaviour, including adhesion, orientation, and proliferation [2], [3]. However, the relationship between geometric parameters and biological response remains complex and difficult to generalize. Integrating machine learning into biomaterial design offers a promising approach to predict and optimize cell-surface interactions based on structural features, enabling more efficient, data-driven development of vascular biomaterials [4]. This study focused on the development of a PDMS microfluidic vessel incorporating engineered surface topographies to promote endothelial cell response. Two cubic-pattern variants were investigated, differing in curvature: Variant 1 (height 0.6 mm, radius 0.5 mm, fillet 0.15 mm) and Variant 2 (height 0.6 mm, radius 0.4 mm, fillet 0.11 mm). CAD models of the molds were developed in Fusion360 and fabricated using SLA 3D printing to ensure high-fidelity reproduction of surface features. In this proof-of-concept stage, both the channel dimensions and topographic elements were intentionally upscaled to facilitate observation of fluid flow behaviour and molecule distribution under controlled conditions. After surface quality assessment, the optimized variant was used to produce PDMS channels via soft lithography. Fluorescently labelled molecules were introduced into the system to visualize and assess flow behaviour. Preliminary results suggest increased local accumulation in regions with surface features, indicating potential topography-driven interaction. Future work will focus on downscaling the topographic design to biologically relevant dimensions and seeding endothelial cells within the microchannels to assess adhesion, alignment, and monolayer formation under flow. Additionally, the integration of machine learning models will be explored to predict cellular responses based on geometric parameters, enabling data-driven optimization of surface design.

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3D/4D-Printed Functional Hydrogels as Transdermal Platforms for Targeted Skin Cancer Therapy

Skin cancer is one amongst the most commonly diagnosed malignancies worldwide and its incidences continue to rise due to factors such as exposure to UV radiation, aging population and lifestyle changes. Despite significant advances in early diagnosis and treatment, surgical excision still remains the standard treatment method, often requiring adjuvant therapy to prevent reocurrence and improve therapy outcomes. Commonly used chemotherapy, despite its effectiveness also causes serious side effects and poor selectivity. Encountered clinical complications highlight the need to develop innovative, local drug delivery systems that will maximize therapeutic efficacy while also avoiding systemic toxicity.

The aim of the project is to develop functional, transdermal systems based on biocompatible hydrogels, capable of releasing encapsulated cytostatics in a continuous and controlled manner - directly at the site of contact with the tumor. Hydrogels will be manufactured using 3D and 4D printing technologies intended for targeted skin cancer therapy. Using the capabilities of 3D printing, it will be possible to precisely control the geometry, porosity and mechanical properties of the created hydrogel matrices. This will enable to design personalized therapeutic platforms tailored to the individual patient's needs. Additionally, the integration of 4D printing will enable the creation of more complex systems which, responding to the patient's biological parameters will be able to adjust the drug release profile.

A hierarchical approach will be applied to implement the project. In the first stage, methods for synthesizing and modifying hydrogels with appropriate rheological, mechanical and drug-loading properties will be developed using natural and synthetic polymers. Subsequently, 3D/4D printing parameters will be optimized to enable the fabrication of reproducible and structurally well-defined hydrogel constructs. In the next stage, the physicochemical and morphological properties of the hydrogels will be characterized using SEM, FTIR spectroscopy and 3D profilometry. The drug release profile will be assessed in-vitro using Franz diffusion cells in combination with UV-Vis and HPLC analysis. Finally, the biological evaluation of the developed hydrogels will be performed, including cytotoxicity, biocompatibility and antitumor activity assays on selected skin cancer cell lines.

The solution being developed aims to complement existing surgical interventions by providing physicians with a selective, controlled and personalized drug delivery platform. This platform could help reduce cancer reocurrence rates and improve patient's quality of life. By conducting interdisciplinary research - utilizing the latest advances in materials science, bioengineering and nanomedicine - this project could contribute to the development of new solutions for precision oncology, which could find a place in everyday clinical practice one day.

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Sustainable Synthesis of Silver Nanoparticles with Antioxidant Activity for Potential Biomedical Applications

Accumulation of reactive oxygen species in cells leads to oxidative stress. This stress is correlated with many diseases. For these reasons antioxidant molecules have attracted a lot of attention. One such molecule is tannic acid, which is additionally obtained from natural sources [1], [2]. On the other hand, it is important for biomedical materials to exhibit antibacterial properties without the use of antibiotics, which can contribute to the growth of antibiotic-resistant bacteria. In this context, special attention is directed toward silver nanoparticles [3].

In this study synthesis of Ag nanoparticles using tannic acid (TA) as reducing and stabilizing agent was carried out. Following the synthesis, the nanoparticle surfaces were further modified through coordination of TA with Fe(III) or Cu(II) ions. As a result, novel metal-organic hybrid nanostructures (Ag@TA_Fe(III) and Ag@TA_Cu(II), respectively) were obtained. Then the resulting materials were characterized by UV-Vis spectroscopy, dynamic light scattering and electron microscopy. Next, the catalytic activity of the obtained nanocolloids was analyzed. The total radical scavenging activity was determined using the DPPH (1,1-diphenyl-2-picrylhydrazyl) radical [1], while antioxidant activity related to scavenging of H_2O_2 and generation of $^{\bullet}OH$ radicals was analyzed by terephthalic acid (TFA) assay[4]. Then, antibacterial activity was tested *in vitro* on two selected Gram-(-) and Gram-(+) bacteria strains (*E. coli*, *B. paramycoides*).

Presented herein preliminary studies are promising and envision various potential applications in biomedical sector. The obtained materials fall within the realm of sustainable chemistry, adding to their appeal. However, further research is needed, especially in terms of biological activities (i.e., cytotoxicity *in vitro* and *in vivo*).

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Drug-Loaded κ-Carrageenan and HP-β-Cyclodextrin Hydrogel Films: A Potential Approach for Diabetic Foot Treatment

Carrageenan is a natural polysaccharide from red algae, crosslinked with ions such as potassium to form stable gels, and valued in biomedical applications. Cyclodextrins are cyclic oligosaccharides that encapsulate poorly soluble drugs, enhancing their solubility and stability. β-Cyclodextrin (β-CD) is well studied but limited by low solubility and toxicity, while its derivative hydroxypropyl-β-cyclodextrin (HP-β-CD) is safer and more soluble. Diabetic foot is a serious complication of diabetes, marked by neuropathy, vascular problems, impaired immunity, and poor healing, which cause frequent infections and high amputation risk. Hydrogels support its treatment by keeping wounds moist, mimicking the extracellular matrix, and delivering bioactive agents.

This study aimed to develop carrageenan/HP-β-CD hydrogel films with an optimized drug mixture to improve delivery, antimicrobial activity, and biocompatibility in diabetic foot therapy.

Hydrogel films based on κ-carrageenan and hydroxypropyl-β-cyclodextrin (HP-β-CD) were prepared following the protocol of Wang et al. [1]. Solutions of HP-β-CD at concentrations of 1%, 2%, 3%, 4%, and 5% were heated in a water bath, after which κ-carrageenan powder and KCl were added. The mixtures were cooled to room temperature and stored at 4 °C for 24 h to allow film formation. These drug-free films were subjected to qualitative evaluation, which revealed no visible differences among concentrations; therefore, 5% HP-β-CD films, also identified as optimal in the reference study, were selected for further work. In the next stage, new hydrogel films were prepared using 5% HP-β-CD solutions loaded with an optimized mixture of Ciprofloxacin and Verapamil, following the same preparation procedure as above. These films were then evaluated for antimicrobial activity against *Staphylococcus aureus* using the serial dilution colony-counting method and for cytocompatibility of HaCaT cells via the MTT assay.

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Surface Functionalization of Polymers with Ibuprofen Nanoparticles

Polymeric implants are increasingly recognized as versatile platforms for biomedical applications, due to their mechanical properties, chemical adaptability, and high biocompatibility [1, 2]. Polyurethane and parylene C are especially notable among commonly used polymers because of their advantageous physical properties and their suitability for surface modifications that enhance therapeutic performance [3, 4].A major research direction involves equipping these materials with therapeutic functions by embedding bioactive agents. Ibuprofen, a widely used nonsteroidal anti-inflammatory drug, is particularly attractive for incorporation into polymer-based implants, as it enables localized and sustained release that reduces systemic side effects. However, efficient loading and controlled release are heavily dependent on the physicochemical characteristics of the polymer surface.

In this work, polyurethane and parylene C films were used as representative polymeric substrates. Ibuprofen nanoparticles were synthesized using a sonochemical approach, yielding stable dispersions with sizes in the 50–300 nm range. These nanoparticles were subsequently immobilized on polymeric surfaces, both pristine and oxygen plasma-modified, where plasma treatment was employed to introduce oxygen-containing functional groups (–OH, C=O). The chemical modifications of the substrates and the successful attachment of ibuprofen nanoparticles were confirmed by a range of analytical methods. Atomic Force Microscopy (AFM) revealed changes in surface topography and particle distribution, while X-ray Photoelectron Spectroscopy (XPS) and ATR-IR spectroscopy provided evidence of oxygenated groups and ibuprofen presence on the surfaces. Even unmodified polyurethane exhibited some affinity toward ibuprofen nanoparticles, but plasma-functionalized surfaces demonstrated markedly higher loading efficiency.

These results highlight the potential of combining sonochemistry with plasma-assisted surface functionalization to create polymeric implants with embedded ibuprofen nanoparticles. Such systems open promising perspectives for localized anti-inflammatory therapy, offering implants with enhanced therapeutic performance, optimized loading capacity, and controlled release kinetics.

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Janus Nanoparticles – Research into Active Substance Carriers in Targeted Skin Cancer Therapy

The development of modern biomaterials opens new possibilities in the treatment of skin cancers, including melanoma. One of the most promising areas of research is Janus nanoparticles, characterized by a bipolar structure in which each surface has different chemical properties. This unique architecture allows for the combination of different functions, such as the transport of hydrophilic and hydrophobic active substances, the integration of imaging systems, and precision targeting of cancer cells.

The use of Janus nanoparticles in targeted skin therapy allows for increased drug bioavailability, reduced side effects, and improved selectivity of action against cancer cells. Of particular interest is the possibility of functionalizing their surface with ligands that recognize markers characteristic of skin cancers. In addition, the potential of these systems includes the synergistic use of chemotherapy, photodynamic therapy, and in vivo imaging techniques.

The aim of the research is to provide theoretical and experimental validation of the superiority of Janus nanoparticles over conventional drug carriers and to highlight their role as a platform in personalized dermatological oncology. The development of such systems may significantly contribute to improving the therapy of skin cancer, being an important step towards the clinical implementation of nanomedicine.

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Sustainable Extraction Techniques for Functional Biopolymers with Improved Antibacterial Features

The extraction of biopolymers using natural deep eutectic solvents (NADES) offers a promising approach for developing sustainable and biocompatible materials for biomedical applications. In this study, we investigated the extraction of chitin and chitosan from organic Agaricus bisporus mushrooms using NADES, a method known for its sustainability and environmental friendliness (Figure 1). The structural, and physicochemical properties were evaluated in detail by various characterization techniques such as by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), thermogravimetric (DTG/TGA) analysis, scanning electron microscopy (SEM), atomic force microscopy (AFM), and nuclear magnetic resonance (1H NMR) techniques. By optimizing the NADES extraction conditions, high-purity chitin and chitosan were achieved, surpassing the purity levels achieved by traditional chemical methods.

Additionally, NADES- extracted chitosan exhibited a remarkable degree of deacetylation (DD%), and a crystallinity index (CrI) of up to 61.77 %, highlighting its enhanced functionality for biomedical applications. Importantly, the extracted chitosan exhibited significant antibacterial activity at a low concentration of 0.625 mg/mL against both Escherichia coli (E. Coli) and Staphylococcus aureus (S. Aureus), alongside enhanced biocompatibility and antioxidant activity, making it a promising candidate for wound healing and other antibacterial applications. As a result, NADES-extracted chitosan is a valid alternative to commercial chitosan for antibacterial and biomedical applications.

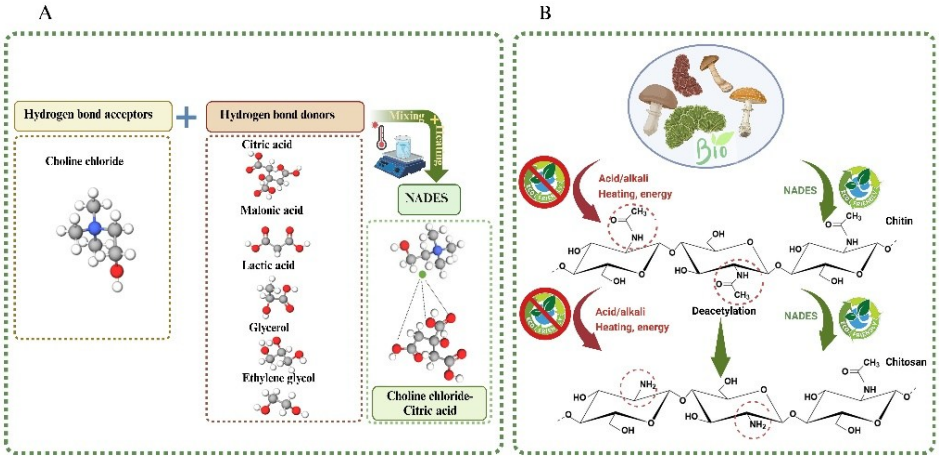

Figure 1. (A) Schematic for the preparation of NADES using various HBA and HBD (B) From forest to function: a green pathway to chitin and chitosan extraction.

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Effect of Processing Conditions on The Degree of Hyaluronic Acid Oxidation and Biological Tests on Hyaluronic-Acid Based Hydrogels

Articular cartilage exhibits very limited self-repair due to its avascular and aneural nature, rendering spontaneous regeneration inefficient. Current treatments mainly address symptoms, such as pain relief and joint mobility, but fail to restore the native tissue architecture and biomechanics, often resulting in total joint replacement in severe cases [1]. Hydrogels have emerged as attractive biomaterials for cartilage engineering because they mimic the extracellular matrix, possess tunable mechanical properties, and are highly hydrated. Among natural polymers, hyaluronic acid (HA) stands out due to its biocompatibility and bioactivity, yet its native structure lacks reactive groups necessary for covalent crosslinking. Chemical modification via periodate oxidation introduces aldehyde groups, allowing crosslinking with bifunctional hydrazides like adipic acid dihydrazide (ADH) under mild aqueous conditions [2] [3]. This study aimed to optimize HA oxidation conditions and evaluate the resulting oxi-HA/ADH hydrogels for their structural, physicochemical, and biological properties.

HA was oxidized with sodium periodate under controlled conditions, followed by reaction termination with ethylene glycol, dialysis, and lyophilization to produce oxidized HA (oxi-HA). Hydrogels were formed by mixing oxi-HA and ADH in PBS (4:1 ratio), casting into molds, gelation, and freeze-drying. Swelling behavior was assessed, and FTIR spectroscopy confirmed the introduction of aldehyde groups and formation of hydrazone crosslinks. Biological evaluation was performed using MG-63 osteoblast-like cells to assess cytocompatibility and potential cytotoxicity.

FTIR analysis confirmed both successful HA oxidation and hydrazone bond formation. TNBS assays identified the optimal oxidation conditions for efficient crosslinking. Cytocompatibility tests demonstrated high cell viability at extract concentrations up to 1%, with minimal cytotoxic effects, indicating the hydrogels' safety for cellular contact. These findings suggest that the materials are suitable for further development as injectable systems.

Optimizing the HA:ADH molar ratio enhanced crosslinking efficiency, while higher HA concentrations or shorter reaction times negatively impacted hydrogel formation. The presence of dynamic hydrazone linkages provides self-healing properties, highlighting the potential of these hydrogels for injectable cartilage repair applications, including microgel-based systems. Future studies will focus on evaluating injectability, mechanical performance, and in vivo efficacy.

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Novel Photocurable Resin with High-Density Packing of Bimodal Zirconia Particles for 3D Printing of Bone-Mimetic Scaffolds

Light-activated photochemical reactions and polymerization processes play a central role in materials science, with photopolymerization being extensively applied across fields such as biomedical engineering, automotive production, and dentistry. These technologies are advancing rapidly, particularly with the emergence of light-based additive manufacturing techniques like 3D printing.

One of the most promising approaches is Digital Light Processing (DLP), a high-resolution and fast photopolymerization method that enables precise fabrication of polymer-based structures. In recent years, DLP has been increasingly explored for the development of nanocomposites by incorporating functional nanopowders into liquid photopolymer resins. This strategy allows for tailoring the mechanical, thermal, and biological properties of printed materials, which is especially valuable for biomedical applications.

In particular, the integration of zirconium dioxide (ZrO_2) powder into 3D-printed polymer scaffolds has attracted significant attention for bone tissue repair. Zirconia nanoparticles not only enhance hydrophilicity and biocompatibility but also provide high strength, stiffness, and excellent osseointegration properties, making them ideal for bone regeneration. These improvements help scaffolds meet the demanding requirements of bone substitutes, both in terms of structural integrity and biological performance.

Bio-inspired ceramic-polymer scaffolds fabricated with this approach hold great potential in regenerative medicine and tissue engineering. The combination of DLP technology with zirconia-based nanocomposites enables the production of patient-specific, mechanically robust scaffolds with enhanced biological functionality. In this context, the 3D printer Lumen X (Cellink) was used to manufacture 3D structures, and their properties were characterized using advanced techniques such as scanning electron microscopy (SEM) and mechanical testing to assess microstructure, composition, and strength.

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New Generation of Drug Carriers: Transfersomes in Dermato-Oncology Therapy

Skin cancers are among the most frequently diagnosed malignancies worldwide, and their treatment with conventional methods (surgery, radiotherapy, chemotherapy) remains associated with limited efficacy and a high risk of adverse effects. Therefore, innovative drug delivery systems are being sought to increase therapeutic effectiveness while reducing toxicity toward healthy tissues [2].

Transfersomes are flexible lipid nanocarriers with a unique ability to overcome the skin barrier. Owing to the presence of so-called edge activators, they exhibit greater deformability than conventional liposomes, enabling penetration into deeper skin layers and precise delivery of active substances [1]. Studies have shown that transfersomes can provide several-fold higher drug penetration and retention in the skin compared to traditional formulations [1,2].

The application of transfersomes in dermato-oncology opens the possibility not only for the administration of cytostatics or kinase inhibitors but also of natural bioactive compounds, such as ginsenosides, whose bioavailability is significantly enhanced in nano- and microcarrier systems [4]. Similar solutions have also been successfully employed in other skin diseases, such as atopic dermatitis, where nanocarriers improved penetration and controlled drug release [3].

In summary, transfersomes represent a new generation of transdermal drug delivery systems, offering a synergistic combination of efficacy, safety, and the potential for personalized therapy in skin cancer treatment.

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Chitosan-Templated Biomimetic Mineralization of Calcium Phosphate: Theoretical vs. Experimental Studies

Chitosan (CS) promotes cell adhesion and can support the deposition of calcium phosphate (CaP) under biomimetic conditions. However, the mechanisms of early CaP nucleation on CS and their translation into mineralization protocols remain insufficiently understood. Here, molecular dynamics (MD) simulations combined with experimental validation were used to examine how CS influences CaP precipitation and to define conditions for CS–CaP hybrids as coatings for polymer scaffolds, with potential to enhance osteointegration.

MD simulations were conducted to examine ionic assemblies between Ca^{2+} and phosphate species (HPO_4^{2-}, $H_2PO_4^-$) in the presence of protonated CS at pH 7.4, 8.0, and 9.0. Mean square displacement (MSD) and Ca^{2+}– HPO_4^{2-} interaction energy (IE) were evaluated to identify conditions favoring ion assembly, which then guided mineralization experiments. CaP deposition was performed in the presence of CS, with pH values derived from MD results. The influence of CS molecular weight (5,000; 20,000; 100,000–300,000 g/mol) on CaP crystallinity (XRD) and morphology (SEM) was also assessed.

Simulations showed that at pH 8.0, CS stabilizes Ca^{2+}– HPO_4^{2-} assemblies, promoting nucleation and the formation of Posner clusters. Experimentally, under similar conditions in the presence of CS with a molecular weight of 20,000 g/mol, CaP precipitated mainly as carbonate-substituted hydroxyapatite (CHA) and octacalcium phosphate (OCP), both precursors of apatite. The CS–CaP hybrid exhibited uniformly distributed crystalline domains resembling bone mineral.

Guided by MD and confirmed experimentally, CaP precipitation in the presence of CS yields hybrids of potential relevance for scaffold coatings, with CS acting as a template that stabilizes prenucleation clusters, regulates crystal growth, and promotes homogeneous particle distribution.

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