SUMMER CONFERENCE OF CROATIAN CHEMICAL SOCIETY RIJEKA – PULA 2025

Ljetna konferencija Hrvatskog kemijskog društva Rijeka – Pula 2025

10 – 11 July 2025, Faculty of Biotechnology and Drug
Development, University of Rijeka, Rijeka, Croatia

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BOOK OF ABSTRACTS

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10 – 11 July 2025, Faculty of Biotechnology and
Drug Development, University of Rijeka, Croatia

BOOK OF ABSTRACTS

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Rijeka-Pula 2025, 10 – 11 July 2025

CHAIR WELCOME ☺

Dear colleagues,

It is our great pleasure to welcome you to the RiChem2025 Summer Conference of the Croatian Chemical Society. Building on the momentum of previous gatherings, this conference brings together researchers, educators, and professionals from all areas of chemistry to exchange ideas, present their latest findings, and foster new collaborations.

In addition to a broad scientific program, RiChem2025 places a special focus on chemistry education, offering a platform for dialogue between high school and university educators on the evolving challenges and opportunities in teaching modern chemistry.

With its relaxed coastal setting and rich cultural backdrop, the Conference also offers a chance to connect informally and enjoy the unique atmosphere of the Adriatic region. We invite you to explore this Book of Abstracts as a preview of the exciting work to be shared and discussed during our time together.

We look forward to a productive and inspiring few days.

Warm regards,

Mirna Petković Didović

Mirna Petković Didović
(on behalf of the Organizing Committee)

PROGRAM

THURSDAY

DAY 1 10 July

8:30 – 9:00	**REGISTRATION**
9:00 – 9:15	Opening addresses

Hall 029

Chair: Vladislav Tomišić

9:15 – 10:00	**Branka Miljević** (Queensland University of Technology, Brisbane, Australia) *Southern ocean aerosols: Climate impacts and the power of real-time chemical sensing*
10:00 – 10:30	**Davor Kovačević** (Faculty of Science, Zagreb) *Polyelectrolyte multilayers as versatile coatings: from dental materials to apples*
10:30 – 11:00	**Vanda Juranić Lisnić** (Faculty of Medicine, University of Rijeka) *Cytomegalovirus is a master manipulator of protein-protein interactions.*
11:00 – 11:15	**Monika Šabić Runjavec** (Faculty of Chemical Engineering and Technology, Zagreb) *Remediation of antibiotic contaminated water with indigenous microbial strain*
11:15-11:25	**Keith Racman** (Mettler Toledo)
11:25 -11:45	***Coffee break***

Hall 029 Chair: Nela Malatesti		Hall 269 Chair: Orjen Petković	
11:45 – 12:30	**Nikola Basarić** (Ruđer Bošković Institute, Zagreb) *Development of photocages for the applications in chemistry and biology*	11:45 – 12:30	**Ernest Meštrović** (Faculty of Chemical Engineering and Technology, Zagreb) *Brucoši pod povećalom: Što otkrivaju njihove pogreške u kemijskom računu*
12:30 – 13:00	**Nermina Malanović** (University of Graz, Austria) *Targeting Bugs, Cancer, and Inflammation: A Multifunctional Peptide-Based Strategy*	12:30 – 13:00	**Ivana Salajić** (Gimnazija Petra Preradovića, Virovitica) *Gdje se kemija i fizika dodiruju?*
13.00 – 13.15	**Ana-Marija Milisav** (Ruđer Bošković Institute, Zagreb) *Effects of pH on Mineralization of Bulk Alginate Hydrogels Containing Metal or Metal Oxide Nanoparticles*	13.00 – 13.30	**Lana Šojat** (VII. Gimnazija, Zagreb) *Metodičko znanje – što bi trebalo znati da bi mogli bolje poučavati*

PROGRAM

THURSDAY

DAY 1 10 July

	Hall 029		Hall 269
	Chair: Nela Malatesti		**Chair: Orjen Petković**
13.15 – 13.30	**Iva Zokić** (Faculty of Chemical Engineering and Technology, Zagreb) *Improving Ceritinib Solubility and Release using Deep Eutectic Solvents*		**Lana Šojat** (VII. Gimnazija, Zagreb) *Metodičko znanje – što bi trebalo znati da bi mogli bolje poučavati*
13.30 – 13.45	**Suzana Inkret** (Ruđer Bošković Institute, Zagreb) *Calcium phosphates/silver nanoparticles composite coatings on the titanium surface – properties and antibacterial activity*	13.30 – 14:00	**Orjen Petković** (Scuola media superiore italiana Fiume) *Zadatci s učestalo niskom rješivošću na državnim maturama iz kemije: u čemu je problem*

14:00 – 15:00 ***Lunch break****

Hall 029

Chair: Ernest Meštrović

15:00 – 15:30 **Andrea Usenik and Vladislav Tomišić** (Faculty of Science, Zagreb)
Acceleration of ions in solution under the influence of an electric field: What is observed macroscopically vs. what is happening microscopically

15:30 – 17:30 **ROUNDTABLE DISCUSSION**
Moderna nastava kemije i komunikacija nastavnika na obrazovnoj vertikali

Terrace of the Kampus restaurant

Chair: Dean Marković

18:30 – 19:30 Tomislav Pavlešić (Faculty of Biotechnology and Drug Development, Rijeka)
Autohtona vina Kvarnera – kako ih kušati (uz kušanje vina)

20:00 ***Conference dinner at the Kampus restaurant***

PROGRAM

FRIDAY

Day 2 11 July

8:30 – 9:00 **REGISTRATION**

Hall 029

Chair: Marina Šekutor

9:00 – 9:45 **Ivan Halasz** (Ruđer Bošković Institute, Zagreb)
In situ powder X-ray diffraction and Raman spectroscopy for monitoring of ball-milling mechanochemistry

9:45 – 10:15 **Marija Jozanović** (Department of Chemistry, University of Osijek)
Quaternary ammonium salts as selective potentiometric sensor materials and efficient antimicrobial agents

10:15 – 10:45 **Josip Požar** (Faculty of Science, Zagreb)
Thermodynamics of Hydrophobically Driven Inclusion Reactions; the Binding of Aliphatic and Aromatic Guest with Cyclodextrins and Cucurbiturils

10:45 – 11:00 **Elizabeta Forjan** (Faculty of Chemical Engineering and Technology, Zagreb)
Integrated Sol-Gel pH Sensors for Non-Invasive Tracking of Saponification in Microreactors

11:00 – 11:10 **Ahmed Dhifaoui** (JEOL)

11:10 – 11:35 ***Coffee break***

Hall 029

Chair: Leo Štefan

11:35 – 12:20 **Zdravka Knežević** (Jadran galenski laboratorij, Rijeka)
Technical, regulatory and IP aspects of innovations in pharmaceutical R&D process

12:20 – 12:50 **Adrijana Vinter** (Selvita, Zagreb)
Better Inputs, smarter outputs: why ePSA belongs in the drug discovery data pipeline?

12:50 – 13:20 **Domagoj Vrsaljko** (Faculty of Chemical Engineering and Technology, Zagreb)
Fabrication of 3D printed microfluidic systems for flow chemistry

13:20 – 13:35 **Sabino Sepčić** (Jadran galenski laboratorij, Rijeka)
Extractables and leachables from container closure systems

13:35 – 14:35 ***Lunch break****

Main hall

14:35 – 15:4 **Poster session**

PROGRAM

FRIDAY

Day 2 11 July

Chair: Maria Kolympadi Markovic

15:45 – 16:00	**Helena Biljanić** (Ruđer Bošković Institute, Zagreb) *Surface functionalization of stainless steel implants with fatty acid-based nanocoatings*
16:00 – 16:15	**Donna Danijela Dragun** (Faculty of Chemical Engineering and Technology, Zagreb) *Electrospinning for medical application and drug delivery systems*
16:15 – 16:30	**Marijan-Pere Marković** (Faculty of Chemical Engineering and Technology, Zagreb) *Development and Optimization of 3D Printed Reactors for Photochemical Reactions*
16:30 – 16:40	**Petra Glagolić** (Faculty of Chemical Engineering and Technology, Zagreb) *Optimization of Copper Nanoparticle-Based Antimicrobial Materials and Fabrication of PCL Nanostructures via Electrospinning*
16:40 – 16:50	**Sven Marinac** (Faculty of Science, Zagreb) *Experimental and Computational Studies of Solvent Molecule Inclusion within a Calix[4]arene Hydrophobic Cavity*
16:50 – 17:00	**Ana Boltek** (Faculty of Chemical Engineering and Technology, Zagreb) *Bioremediation of wastewater with indigenous bacterial cultures from biowaste*
17:00 – 17:10	**Marta Jerneić** (Faculty of Chemical Engineering and Technology, Zagreb) *Bioaugmentation of highly organically loaded waste stream with thermophilic bacterial cultures*
17:10 – 17:20	**Andrea Pleić** (Faculty of Chemical Engineering and Technology, Zagreb) *Mebendazole removal efficiency and ecotoxic effect*
17:20 – 17:30	**Josip Gudelj** (Faculty of Chemical Engineering and Technology, Zagreb) *Analysis of technologies for green hydrogen production*
17:30 – 17:40	**Ana Coban** (Faculty of Chemical Engineering and Technology, Zagreb) *Determination of the ecotoxicity of silver nanoparticles, chitosan, titanium dioxide and thymol with Vibrio fischeri, Chlorella sp. and Lemna minor*

Hall 029

17:40 – 18:00	***Best Poster Award and Closing Ceremony***

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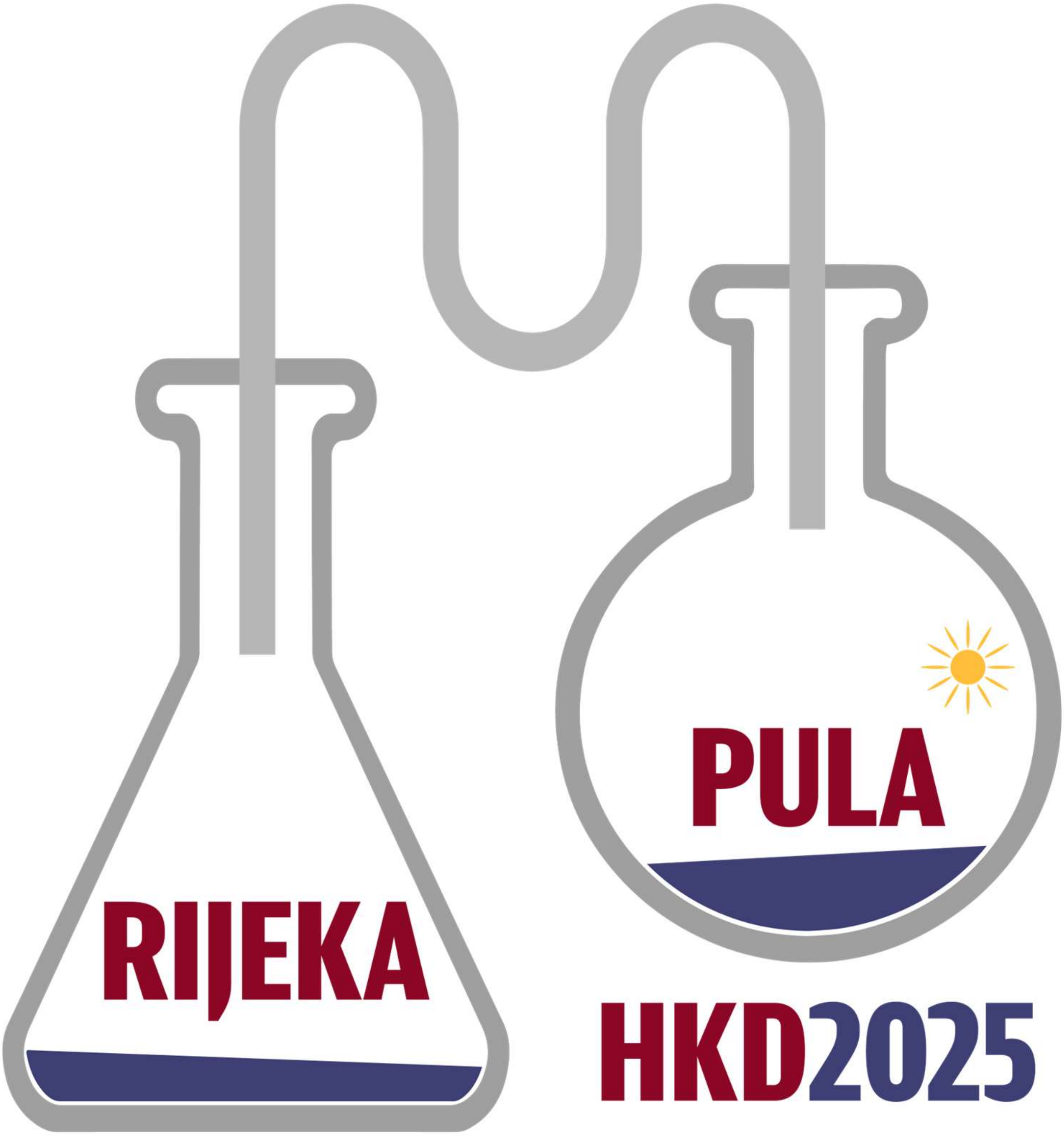
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LECTURES

PREDAVANJA

Southern Ocean aerosols: Climate impacts and the power of real-time chemical sensing

Branka Miljević
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The Southern Ocean is a region of the world where climate and weather models perform particularly poorly. They persistently overpredict the amount of sunlight reaching the Earth's surface over the Southern Ocean, causing an overprediction of sea surface temperatures. Robust prediction of human-induced global warming and future climate requires these models to be more accurate. One of the main sources of uncertainty in climate models are aerosols and their impact on cloud formation and properties. Production of aerosols in the Southern Ocean atmosphere occurs via two main pathways: 1) wave breaking and bubble bursting, which results in primary particles composed largely of sea salt, and 2) sea-air exchange of gaseous compounds produced by marine microorganisms (phytoplankton, algae), in particular dimethyl sulphide (DMS), and the subsequent secondary particle formation from atmospheric oxidation of these gaseous precursors. The processes controlling Southern Ocean new particle formation and their growth to sizes where they can act as seeds for clouds are not yet fully understood.

This talk will briefly introduce atmospheric aerosols and specifically Southern Ocean aerosols and showcase Australian research capabilities and activities in this space focusing on recent Southern Ocean voyages onboard the Australian research vessels. It will demonstrate how real-time mass spectrometry is advancing knowledge in this field by outlining results from a recent Southern Ocean voyages related to aerosol composition and aerosol gaseous precursors.

Polyelectrolyte multilayers as versatile coatings: from dental materials to apples

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Polyelectrolyte multilayers (PEMs) are very well-known surface coatings which could be prepared by alternating deposition of positively and negatively charged polyelectrolytes (polycations and polyanions) on a solid surface. In recent years we have developed new PEM strategies which could be valuable for designing soft nanomaterials whose properties can be finely adjusted according to the requirements of specific applications, especially in the field of biomedicine and food science and technology. The emphasis in our studies was in the application of PEMs for the prevention of bacterial adhesion to various surfaces. We investigated the influence of polyelectrolyte multilayer properties on bacterial adhesion capacity at the surface of airborne-particle abraded zirconia-based dental materials and showed that PEMs have significantly reduced adhered bacteria [1]. The specimens with negatively charged poly(acrylic acid) as a terminating polyanion layer have displayed the best performance. We also applied this PEM strategy for coating apples [2]. The influence of various experimental conditions on PEM formation was examined and it was shown that the PEM build-up and properties such as thickness and hydrophobicity strongly depend on the applied experimental conditions (e.g. pH of the polyelectrolyte solutions). Moreover, for the first time we showed that the PEM build-up on apples could be verified using contact angle measurements. The most dominant zigzag pattern on both silica and apple surfaces at pH(CS) = 5.0 and pH(CMC) = 3.0 highlights the optimal conditions for multilayer formation and suggests that this process can be effectively monitored using contact angle measurements. All the obtained results obtained could serve as a basis for obtaining tuned biocompatible transparent polyelectrolyte multilayers on apples with optimized physicochemical properties which could lead to the enhanced applications of the PEMs in the field of food technology.

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Cytomegalovirus is a master manipulator of protein-protein interactions

Magdalena Medved, Jelena Železnjak, Stipan Jonjić, Ilija Brizić, Berislav Lisnić,
Vanda Juranić Lisnić
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Cytomegalovirus (CMV) is a herpesvirus that infects a significant portion of the human population. Related animal CMVs infect nearly every vertebrate species. All cause life-long persistent infections interrupted by occasional reactivations, making them dangerous opportunistic pathogens in individuals with weakened or immature immune systems. They owe their success to numerous immunoevasive strategies targeting every arm of our immune system.

Murine CMV (MCMV) has successfully been used for decades in mouse models of CMV disease, pathogenesis and immune-evasion. In fact, MCMV has spearheaded numerous research venues that were subsequently successfully translated to human CMV treatment.

Our lab was among the first to demonstrate that MCMV downregulates MHC I molecules. Downregulation of MHC I protects the virus-infected cells from cytotoxic T cells but renders them sensitive to NK-cells. We have previously also uncovered an elaborate scheme in which two MCMV proteins – m04/gp34 and MATp1 collaborate to return certain MHC I molecules alleles to the cell surface and strengthen their interaction with inhibitory Ly49 NK cell receptors to prevent killing of infected cells. In addition to m04 and MATp1, the virus has also developed an MHC-I-like molecule m157 that can also engage inhibitory Ly49 receptors.

However, during co-evolution between virus and host, mice have evolved activating Ly49 receptors which specifically recognize virus-modified MHC-I molecules or virally encoded m157 decoy protein. In MCMV-susceptible mouse strains, inhibitory signals still predominate, but in MCMV-resistant mouse strain C57Bl/6, the activating receptor Ly49H recognizes the MCMV protein m157 and activates the NK cells. Using a panel of in vitro assays with reporter cells and in vivo infection data as well as multicolour flow cytometry, we now demonstrate that MATp1, independently of m04, interferes with this m157-Ly49 recognition. This interaction has a dampening effect on the interaction between m157 and its receptors – Ly49I and Ly49H. m157-Ly49H interaction is very strong and has been the main model for researching memory NK cells in an animal model. This complex interaction is a wonderful demonstration that viruses are fantastic tools to study cell biology and biochemistry.

Remediation of antibiotic contaminated water with indigenous microbial strain

Monika Šabić Runjavec, Martina Sudar, Ernest Meštrović, Zvjezdana Findrik Blažević,
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Antibiotics are pharmaceuticals used to treat infections caused by microorganisms, specifically bacteria. They are defined as organic compounds that can completely stop bacterial growth or reproduction, causing the decline of the bacterial number cells [1]. As biologically active molecules, antibiotics in the aquatic environment pose a significant threat to the health of the ecosystem and contribute to the emergence of antibiotic-resistant bacteria and genes. Resistance is the natural ability of microorganisms to resist a compound that attempts to inhibit their growth. Microorganisms achieve antibiotic resistance through mechanisms such as avoiding interactions with the antibiotics, effluxing antibiotics from the cell through efflux pumps and modifying antibiotics and their metabolites through enzymatic reactions [2].

In this study, the potential of an indigenous microbial strain for the remediation of water contaminated with antibiotics was investigated. The microbial strain was isolated from the industrial waste stream and identified as rod-shaped, motile, Gram negative bacteria. Batch experiments showed that the bacterial isolate degraded 33.2±1.4% of the tested antibiotic within 72 hours under submerged conditions (25±1°C). Bacterial growth, determined as total suspended solids, increased by 295±45 mg/L, while the number of living bacterial cells reached the value of 2.4×10^{7} CFU/ml.

These results demonstrate the promise of indigenous microbes for environmentally friendly and cost-effective strategies to remove antibiotic contaminants from the aquatic environment. Further research is needed to evaluate performance in complex wastewater systems.

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Development of photocages for the applications in chemistry and biology

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Photocleavable Protective Groups (PPGs), also known as Photocages, have become widely explored for the use in chemistry [1] and biology [2], particularly with the development of PPG chromophores that absorb visible light [3]. However, an ideal universal PPG for the use in different applications has still not been discovered. Therefore, researchers try to develop new PPGs characterized by better properties and reactivity, which can be selectively cleaved off by use of light of different wavelengths [4] in the processes with spatial and temporal control.

In our research group at the Ruđer Bošković Institut (RBI), we try to develop PPGs that are benzyl derivatives and base their photoreactivity on the *meta*-effect in photochemistry [5]. Over last decade we investigated the photoreactivity of anilines [6], aminonaphthalenes [7-9], and aminobiphenyl photocages. The photoelimination mechanism was investigated by fluorescence spectroscopy and transient absorption spectroscopy, which allowed for the detection of reactive intermediates in the decaging reactions including carbocations and free radicals [6-9]. Furthermore, we demonstrated the applications of photocages for the release of different aliphatic and aromatic alcohols and carboxylic acids, including carbohydrates and nonsteroidal anti-inflammatory drugs. Moreover, we have recently extended our investigation on the decaging reactions from BODIPY derivatives (Figure 1), which release the payload upon irradiation with visible light in a heterolytic cleavage taking place on the boron atom [10]. The scope of the decaging from the BODIPY was investigated for different phenols, alcohols and alkyl derivatives to develop applications in organic synthesis and biology.

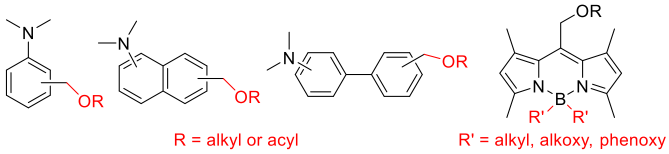

Fig. 1: Different photocages developed at the RBI

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Targeting bugs, cancer, and inflammation: A multifunctional peptide-based strategy

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Bacterial infections (BI) and cancer remain two of the leading causes of death worldwide, worsened by limited treatment options and increasing drug resistance. Both represent major global health challenges that share a common feature: disruption of the immune system. Bacterial infections can affect multiple organs and become life-threatening when bacteria enter the bloodstream, triggering sepsis—a rapid and often fatal organ failure driven by the immune response to bacterial components such as lipopolysaccharide (LPS). Sepsis is notoriously difficult to diagnose and treat, with each untreated hour reducing patient survival by up to 8 %.

Recent research has revealed a surprising connection between bacteria and cancer, challenging long-held views in oncology. Bacteria and their products can promote cancer development and metastasis by suppressing immune responses, supporting tumor growth, and preventing immune cells from attacking cancer effectively.

To tackle these complex challenges, we have developed novel peptide-based active ingredients as part of the NERA peptide platform. These next-generation NERA peptides demonstrate a significant increase in therapeutic potential, offering a unique mechanism of action that combines antimicrobial, anti-inflammatory, and anticancer activities. This innovative approach represents a promising new therapeutic avenue with the potential to address urgent health threats posed by both bacterial infections and cancer.

Effects of pH on mineralization of bulk alginate hydrogels containing metal or metal oxide nanoparticles

Ana-Marija Milisav,[1] Vida Strasser,[1] Andrea Marfoglia,[2,3,4] Krunoslav Bojanić,[1] Ina Erceg,[1,5]
Silke Christiansen,[5,6] Maja Ivanić,[1] Željka Fiket,[1] Sophie Cazalbou,[3] Maja Dutour Sikirić[1]
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Bone tissue defects affect millions of people worldwide, and with the increasing population, there is a rising demand for bone-like materials. One of the promising approaches to promote bone growth and healing is the development of innovative bone-mimicking materials [1]. For this purpose, alginate hydrogels were used in our research given their ability to mimic the extracellular matrix. To further improve their properties, the alginate hydrogels were biomimetically mineralized with calcium phosphates as described in our previous work [2]. The aim of this research was to optimize the conditions for the preparation of both non-mineralized and mineralized alginate hydrogels with incorporated nanoparticles (NPs) such as silver (AgNPs), copper oxide (CuONPs) and zinc oxide (ZnONPs). The addition of NPs was intended to minimize the risk of bacterial infection, and their incorporation into the matrices addressed potential cytotoxicity risks [3]. Mineralization of the hydrogels was carried out at pH 7.4 or 9.0, with the phosphate added to the alginate and calcium as the crosslinking agent. Characterization included Fourier-transform infrared spectroscopy (FTIR), powder X-ray diffraction (PXRD), scanning electron microscopy (SEM), inductively coupled plasma mass spectrometry (ICP-MS), rheological measurements and antibacterial assays. PXRD and FTIR confirmed the formation of calcium-deficient hydroxyapatite at pH 7.4 and amorphous calcium phosphate at pH 9.0. The incorporation of NPs influenced the morphology of the mineral phases. Early network breakdown was observed in mineralized hydrogels, with critical strain and ion release depending on pH and NP type. *Staphylococcus aureus* was inhibited with hydrogels prepared at pH 9.0, except for hydrogels with incorporated CuONPs. Overall, these results indicate the promising potential of biomimetic mineralization of alginate hydrogels and their use as controlled release systems, which could be of interest for bone tissue engineering.

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Improving ceritinib solubility and release using deep eutectic solvents

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One of the main challenges facing the pharmaceutical industry today is the low solubility of active pharmaceutical ingredients (APIs) in water, which is present in a significant number of drugs available on the market (up to 40%) and drug candidates in development (70-90%), leading to low bioavailability, reduced therapeutic efficacy, and the need for higher drug doses [1,2]. Consequently, solubility is a key parameter in the development and fabrication of pharmaceutical products, and new formulation technologies should be explored. One promising alternative is the use of deep eutectic solvents (DESs), environmentally friendly solvents prepared by combining hydrogen bond donors and acceptors in specific molar ratios to yield a stable liquid. Dissolving active ingredients in DESs results in API-DES systems that can be used to improve solubility and drug delivery [2-4].

Six DESs were prepared by mixing various components, and their formation was confirmed by Fourier transform infrared spectrophotometry (FTIR). The density, viscosity, and pH values of the prepared solvents were determined, and their toxicity to the bacterium *Vibrio fischeri* was tested. By adding ceritinib, an API used in the treatment of non-small cell lung cancer, to the prepared DESs, API-DES systems were obtained. The maximum solubility of pure ceritinib and prepared API-DESs in water was determined. The release profiles of pure ceritinib and ceritinib from API-DES were determined and compared, as well as the permeability and the diffusion coefficient. It was found that the preparation of the API-DES system increased the solubility of ceritinib, making the first step in improving the delivery of this drug and the potential development of a new formulation.

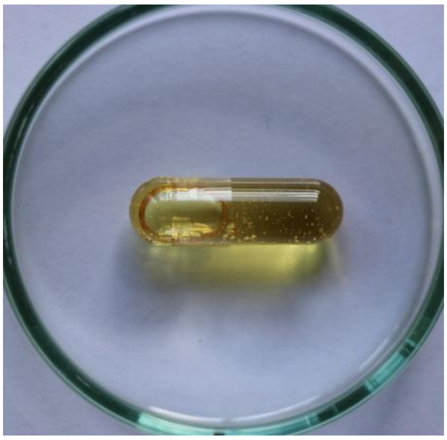

Fig. 1: Prepared capsule containing the API-DES system.

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Calcium phosphates/silver nanoparticles composite coatings on the titanium surface – properties and antibacterial activity

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Calcium phosphates (CaP) combined with antimicrobial metal/metal oxide nanoparticles and/or biomacromolecules are emerging as a promising alternative to antibiotic therapy in implant-related infections, thereby enhancing their biological properties.[1,2] In addition, they are a promising coating material for titanium orthopedic implants, which are widely used due to their excellent mechanical properties, but are biologically inert.[3]

For this reason, in this study composite coatings of calcium phosphates and silver nanoparticles (CaP/AgNP) were prepared on differently etched titanium surfaces. The influence of different etching methods and the influence of silver nanoparticles on the preparation and properties of these coatings, as well as the influence on their antibacterial activity, were investigated. To determine the influence of the etching method, two different etching methods were employed: one using hydrochloric acid [4] and other utilizing a mixture of sulfuric and hydrochloric acid.[5] The etching of the surfaces alters their surface properties, such as roughness and wettability, as demonstrated by AFM and contact angle measurements. The morphology of the CaP/AgNP composites formed on different surfaces varied depending on the etching method, as indicated by SEM characterization. The difference was also evident in the uniformity of the coatings and the surface coverage. The influence of silver nanoparticles was evident in the lower aggregation of CaPs and improved wettability of the surfaces, which also depended on the etching method used. Different antibacterial activity was observed for the differently etched and coated titanium surfaces. Etching with HCl/H_2SO_4 led to weaker S*. aureur and P. aeruginosa* biofilm formation. In addition, CaPs coating significantly reduced biofilm formation for both surfaces, while the addition of AgNPs reduced it even further.

In conclusion, surface modification of titanium is an important step in the process of coating titanium with functional materials such as CaP/AgNP composites, as it changes the surface properties and thus influences the deposition of coatings. Furthermore, etching and coating contribute to the reduction of biofilm formation, but further studies are needed to improve antimicrobial activity.

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In situ powder X-ray diffraction and Raman spectroscopy for monitoring of ball-milling mechanochemistry

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In situ monitoring of mechanochemical reactions using powder X-ray diffraction (PXRD) has matured into a routine technique and is now widely implemented at several synchrotron beamlines across Europe. Currently, it stands as the preferred method for elucidating the transformations of bulk crystalline materials, albeit with a time resolution typically limited to a few seconds and with significant sample averaging. This methodology requires access to a synchrotron radiation source—ideally one capable of delivering high-energy photons.[1]

When coupled with Raman spectroscopy, PXRD enables complementary molecular-level insights, enhancing the analytical power of mechanochemical studies.[2] In this presentation, we will explore various approaches and setups for in situ PXRD and showcase some of the most significant findings achieved through its application over the past decade. Notably, we have uncovered a surprisingly dynamic reaction environment: reactions on the 1 mmol scale often complete within minutes; intermediates are frequently observed; and new phases and polymorphs can be selectively and controllably synthesized.

Furthermore, we are now able to derive detailed reaction profiles from both PXRD and Raman data, allowing us to investigate the role of liquid additives, probe solid-state catalysis, and map reaction sequences by analyzing the energy landscapes of the reacting solids.[3] We will also discuss recent advancements in the chemical isotope labeling of solids, which have revealed how milling can overcome the inherently slow diffusion in the solid state.[4] Finally, we will demonstrate how varying the solid forms of starting materials offers a strategy to modulate the kinetics and mechanisms of mechanochemical transformations.[5]

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Quaternary ammonium salts as selective potentiometric sensor materials and efficient antimicrobial agents

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Potentiometric surfactant sensors are typically composed of an ion pair embedded within a plasticized PVC membrane. To improve their analytical performance, the development of novel ionophores is essential. In this study, a series of nitrogen containing heterocycles containing long alkyl or polyalkyl chains were synthesized as quaternary ammonium compounds (QACs) using a one-step method. The newly synthesized compounds were both theoretically evaluated and experimentally tested as ionophores in surfactant-selective sensors. These sensors demonstrated reliable performance in detecting both anionic and cationic surfactants across a broad pH range, with consistent and accurate responses in both pure and complex sample matrices. Additionally, new sensors tailored for disinfectants and antiseptics, especially those used in COVID-19 formulations, were successfully developed, offering a cost-effective alternative to current surfactant detection methods. Beyond their role as ionophores, QACs are also recognized for their pronounced antimicrobial properties. Several of the synthesized QACs exhibited significant antibacterial and antifungal activity. Among them, 3-hexadecyl-1-vinyl-1*H*-imidazol-3-ium bromide against yeasts. For molds, the most effective compounds were 3-octadecyl-1-vinyl-1*H*-imidazol-3-ium and 1,3-didecyl-2-methyl-1*H*-imidazol-3-ium bromide. Notably, vinyl-imidazolium based QACs containing two long alkyl chains (12-18 C-atoms) achieved complete microbial inhibition (MIC) against several Gram-negative bacteria: *E. coli*, *K. pneumoniae*, and *P. aeruginosa*. Furthermore, 3-decyl-1-vinyl-1*H*-imidazol-3-ium bromide, 1-benzyl-3-octadecyl-1*H*-imidazol-3-ium bromide, and 1-benzyl-2-methyl-3-octadecyl-1*H*-imidazol-3-ium bromide exhibited complete inhibition against Gram-negative bacterium *E. coli* and Gram-positive bacterium *S. aureus*. These results underscore the potential of QACs as dual function agents serving both as ionophores in advanced sensor technology and as effective antimicrobial agents. Further investigation into their chemical structures and mechanisms of action is warranted to fully exploit their capabilities in analytical and biomedical applications.

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Electrospinning for medical application and drug delivery systems

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Electrospinning is a versatile technique for fabricating nanofibrous membranes with controlled morphology, high surface area, and interconnected porosity – features essential for biomedical, environmental, and energy applications. Beyond its structural adaptability, electrospinning enables the direct incorporation of functional agents into fibers, facilitating the development of responsive, bioactive materials [1].

This study explores the electrospinning of polycaprolactone (PCL) membranes as a sustainable strategy for valorizing polymer waste. Using a custom-designed electrospinning setup, the central composite design (CCD) and response surface methodology (RSM) were employed to systematically optimize processing parameters – voltage, flow rate, and tip-to-collector distance to fine-tune membrane properties such as thickness, uniformity, and wettability [2]. To enhance biomedical functionality, indomethacin, a model anti-inflammatory drug, was incorporated into the PCL solution prior to electrospinning. Thermogravimetric analysis confirmed successful drug encapsulation, while SEM and optical microscopy revealed uniform fiber morphology, with drug loading having no adverse effect on fiber formation. Further characterization by FTIR spectroscopy and droplet absorption testing showed that voltage and collector distance significantly influenced fiber architecture, while flow rate had a comparatively minor impact.

The resulting membranes exhibit strong potential for wound healing and localized drug delivery. This work positions electrospinning not only as a powerful fabrication technique, but also as a platform for advancing medical material solutions – transforming polymers into functional materials aligned with World health organization goals for fighting antimicrobial resistance.

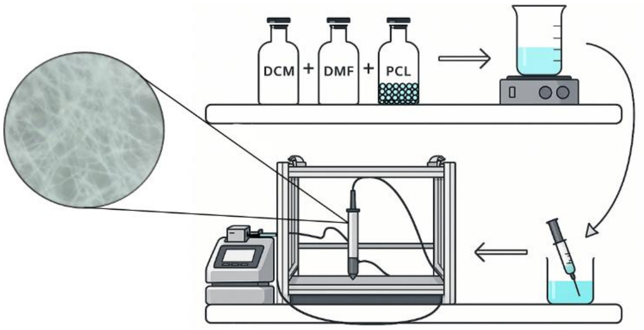

Fig. 1: Schematic representation of the electrospinning process.

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Development and optimization of 3D printed reactors for photochemical reactions

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Additive manufacturing (AM) has enabled the fabrication of complex structures with tailored properties, offering new possibilities for chemical and photochemical applications. This study explores the potential of 3D printed reactors for conducting photochemical reactions, focusing on material selection, chemical compatibility, and reactor design and performance. Stereolithography (SLA), digital light processing (DLP), and fused filament fabrication (FFF) technologies were used to fabricate test plates and reactor prototypes from various polymeric materials, including polyacrylates, epoxy, polypropylene (PP), and polyethylene terephthalate glycol (PETG).

Material suitability was assessed through swelling tests in organic solvents to evaluate chemical resistance. Based on the swelling test results, a polymer exhibiting the lowest degree of swelling is the most suitable material for photochemical applications.

Photochemical reactions were conducted in a controlled reactor setup, wherein the reactant streams were irradiated through optically transparent glass and polymeric windows of the microreactors. Custom-designed 3D printed microreactors featuring varied internal geometries were employed to investigate their influence on photoreaction efficiency. Reaction outcomes were analyzed using ultra-high-performance liquid chromatography (UHPLC).

This research highlights the potential of AM for fabricating chemically resistant photoreactors, paving the way for further optimization in continuous-flow photochemistry. Future work will focus on refining reactor designs and expanding the range of compatible photochemical transformations.

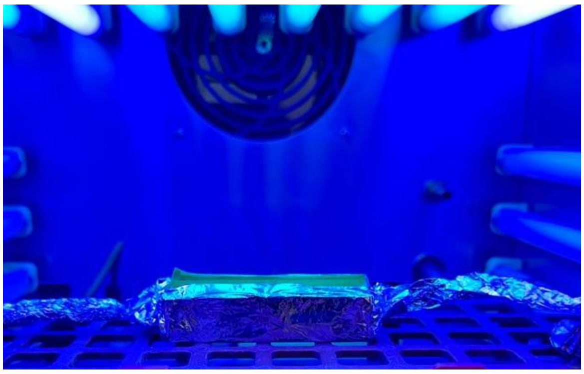

Fig. 1: Photochemical reactions in 3D printed microreactor

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Integrated sol-gel pH sensors for non-invasive tracking of saponification in microreactors

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Advances in additive manufacturing have enabled the development of customizable, low-cost microfluidic devices with seamlessly integrated sensing functionalities. A novel method was developed for incorporating sol-gel based pH sensor films into 3D printed microreactors, enabling non-invasive, real-time monitoring of chemical reactions. Microreactors were fabricated from polyethylene terephthalate glycol (PETG) using fused filament fabrication (FFF), chosen for its accessibility, rapid turnaround and suitability for producing complex, application-specific designs. A pH-sensitive sol-gel film was applied to the microchannel walls, forming an optically responsive interface capable of detecting pH fluctuations during reaction processes. Unlike traditional metrology techniques, which typically measure pH at specific points in time, sol-gel sensors provide continuous, real-time data, allowing for more dynamic and accurate tracking of reaction conditions.

The system was validated using saponification of sunflower oil with sodium hydroxide, a base catalyzed ester hydrolysis reaction that produces soap and glycerol. This reaction was chosen to demonstrate the system's capabilities because it involves pH changes over the course of conversion, making it suitable for evaluating *in situ* pH sensing within microfluidic environment.

This work highlights the potential of combining additive manufacturing with integrated chemical sensing to create intelligent microreactor platforms. This approach offers promising applications in process monitoring, green chemistry and continuous-flow synthesis. It provides a scalable and efficient alternative to conventional methods.

Fig. 1: 3D-printed microfluidic channel incorporating sol-gel pH sensing film.

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Technical, regulatory and IP aspects of innovations in pharmaceutical R&D process

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The pharmaceutical industry is an important part of the health care system. It focuses on key aspects of pharmaceutical and medicinal products R&D, manufacturing and access to patients and consumers. While the size, expertise and operational geography of different companies may differ, there is always ambition- to innovate and offer differentiated products, processes, and services as a prerequisite for sustainable business models. Pharmaceutical innovations[1] may be radical/ major ("breakthrough") and/or may be incremental ("smaller but meaningful")- both requiring strategy direction, cultural build, organizational support, and various expertise to advance the challenging and risky path: from idea to commercial solution. Innovation is essential in the pharmaceutical R&D process—vital for improving patient outcomes and sustaining industry growth. However, key stakeholders view innovation through different lenses.

R&D teams focus[2] is on the technical feasibility, therapeutic value, and process improvements. Regulators emphasize the enlarged regulations and the need for extensive data to demonstrate safety, efficacy, and quality. Meanwhile, IP professionals and patent offices[3] assess whether an innovation meets strict criteria: it must be novel, inventive, and industrially applicable, what is often a high hurdle in a competitive patent landscape.

When these differing perspectives are successfully aligned[4], companies can achieve significant outcomes: regulatory approval of new or improved products, exclusivity data granted by authorities, and patent protection ensuring market and commercial exclusivity.

These incentives are not only rewards, but they are also strategic drivers. They enable return on investment and support the next cycle of meaningful innovation, creating a new circle where science, regulation, and intellectual property intersect to bring value to patients, healthcare systems, and industry alike.

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Better Inputs, smarter outputs: Why ePSA belongs in the drug discovery data pipeline?

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In an era of data-driven drug discovery, the quality and context of input data critically determine the reliability of downstream predictions and decisions. The effective polar surface area (ePSA) is an experimentally derived descriptor that offers a more nuanced and context-relevant measure of molecular polarity than traditional calculated PSA. This talk explores the integration of ePSA into the drug discovery data pipeline, illustrating how its inclusion enhances model accuracy, informs permeability and absorption predictions, and bridges the gap between in silico and in vitro workflows. Through examples, it will be demonstrated that ePSA provides more biologically meaningful inputs, leading to smarter, more actionable outputs in both early screening and lead optimization. Ultimately, embracing ePSA is not just about refining data, it's about making better decisions across the discovery process.

Fabrication of 3D printed microfluidic systems for flow chemistry

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The use of additive manufacturing for microfluidic system development represents a major advancement in flow chemistry, offering precise control over reaction parameters, enhanced mixing efficiency, and seamless integration of functional components such as sensors and catalysts. Traditional fabrication techniques, including soft lithography and micromachining, often involve complex processes and require specialized facilities. In contrast, additive manufacturing provides a cost-effective, rapid, and highly customizable alternative.

This research is conducted within the framework of the HRZZ INDIGO project, which aims to develop 3D printing methods for manufacturing complex microsystems, such as microreactors and separators, for use in flow chemistry. Continuous chemical processes require real-time monitoring using *in situ* sensors, whereas conventional batch processes typically rely on post-reaction analysis. With the increasing adoption of flow chemistry, the demand for on-line *in situ* measurements is growing. This study focuses on the design, fabrication, and optimization of pH sensors, surface coatings, and reactor channels to incorporate FTIR sondes for improved process control. By refining digital light processing (DLP) and fused filament fabrication (FFF) techniques, the project aims to enhance material properties, improve chemical compatibility, and ensure greater mechanical stability of printed devices. New systems with integrated probes for on-line *in situ* measurements will be designed and 3D printed, enabling more efficient monitoring and control of flow chemistry processes. The ultimate objective is to develop robust and efficient microfluidic platforms suitable for both academic research and industrial applications.

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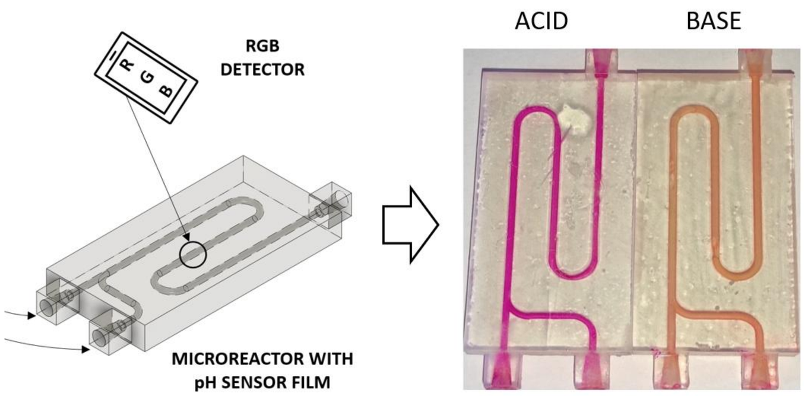

Fig. 1: Scheme of the pH test in microreactor and RGB color detection.

Extractables and leachables from container closure systems

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Extractables and leachables are critical components of pharmaceutical development. They are tested in pharmaceuticals to ensure patient safety by identifying and assessing potentially harmful substances that can migrate from container components into the drug product. Extractables are organic and inorganic chemical substances that can be extracted from a container under laboratory conditions. Extractables, or substances derived from them, have the potential to migrate into a drug product during shelf life, and thus become leachables. Using multiple extraction media with varying properties such as polarity, pH, ionic strength and extracting power is recommended to simulate a worst-case leachables profile [1]. Following extraction, the chemical composition of the extract should be characterized. Multiple analytical techniques should be employed to analyze the vast array of possible substances with different properties; and the most routinely used for the identification and quantification of substances are high-performance liquid chromatography (HPLC) and gas chromatography (GC) [1]. A safety threshold should be established based on several risk factors such as the duration of treatment, daily exposure and route of administration. This threshold is then converted into a concentration-based analytical threshold, which guides the interpretation of analytical results [2]. If the results of the extractable study demonstrate that the concentrations are toxicologically safe, leachable testing does not need to be performed. Otherwise, leachables should be monitored through the entire shelf life of the product [3].

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Surface functionalization of stainless steel implants with fatty acid-based nanocoatings

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Medical grade stainless steel is often used in biomedical implants due to its favorable mechanical properties and inherent biocompatibility. However, prolonged exposure to physiological environment can lead to corrosion, which may compromise the structural integrity and performance of the material. To mitigate this issue and improve the durability and functionality of stainless steel implants, surface functionalization is essential.

Fatty acids, **due to their** biocompatibility and **amphiphilic nature,** have the ability to form self-assembled monolayers (SAMs) on metal surfaces, offering an initial protective barrier against corrosion. This makes them promising candidates for the functionalization of stainless steel surfaces. However, their long-term stability is limited by their tendency to gradual desorption from the metal surface over time. To overcome this limitation, fatty acid SAMs can be cross-linked using gamma irradiation, resulting in the formation of polymer nanocoatings (PNCs). These ultrathin, covalently bonded layers retain the nanoscale thickness of a monolayer **while** significantly improving the stability of the coating and providing long-term corrosion resistance.

The aim of this research was to systematically investigate and optimize the conditions for the functionalization of 316L medical grade stainless steel using behenic acid SAMs. Gamma irradiation was employed to induce cross-linking of the SAMs, resulting in the formation of robust PNCs. The corrosion resistance of the functionalized stainless steel was evaluated using electrochemical techniques, including potentiodynamic polarization and electrochemical impedance spectroscopy (EIS), while contact angle measurements were used to characterize surface energy and wettability.

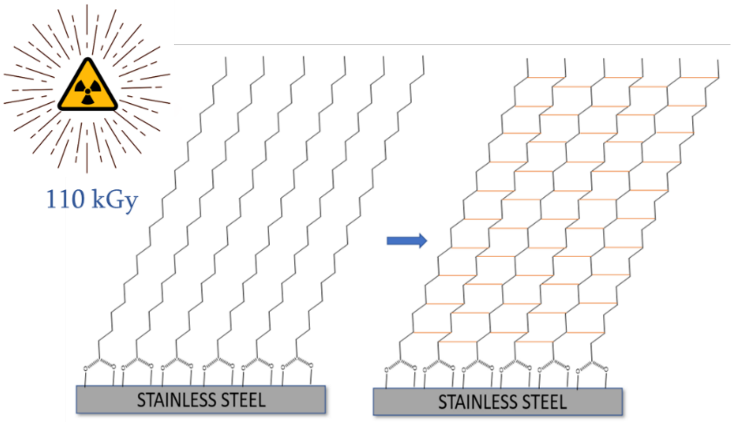

Fig. 1: Radiation cross-linking of behenic acid on stainless steel surface.

Acknowledgements

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Determination of the ecotoxicity of silver nanoparticles, chitosan, titanium dioxide and thymol with *Vibrio fischeri*, *Chlorella* sp. and *Lemna minor*

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Biopolymers, such as chitosan, represent a promising alternative to conventional plastics due to their biodegradability and reduced environmental impact. To enhance their functional properties, various additives such as silver nanoparticles (AgNPs), titanium dioxide (TiO_2), and thymol are commonly incorporated into biopolymer matrices. However, the increasing use of these additives raises concerns about their potential ecotoxic effects once released into the environment. In this study, the ecotoxic potential of AgNPs, chitosan, TiO_2, and thymol was evaluated using standard aquatic test organisms: *Vibrio fischeri*, *Chlorella sp.*, and *Lemna minor*. Tested concentration ranges were as follows: AgNPs at 1, 3, 5, 7, and 10 g/L; chitosan and TiO_2 at 0.1, 0.3, 0.5, 0.7, and 1.0 g/L; and thymol at 10, 30, 50, 70, and 100 g/L. Effective concentration values (EC_x) were calculated via linear interpolation. In the *Vibrio fischeri* bioluminescence inhibition assay, estimated EC values were: $EC_{20,\text{chitosan}}$ = 0.016 g/L; $EC_{50,\text{chitosan}}$ = 0.049 g/L; $EC_{20,\text{thymol}}$ = 0.016 g/L; $EC_{50,\text{thymol}}$ = 0.035 g/L. Based on these results, both chitosan and thymol were classified as weakly ecotoxic. For TiO_2, a maximum bioluminescence inhibition of 14.82% was recorded, which was insufficient for EC value estimation. In the *Chlorella sp.* growth inhibition test, the following EC values were determined: $EC_{50,\text{chitosan}}$ = 0.413 g/L, $EC_{50,\text{thymol}}$ = 8.845 g/L, EC_{20,TiO_2} = 0.169 g/L; EC_{50,TiO_2} = 0.357 g/L. Notably, microscopic observation revealed significant aggregation between TiO_2 particles and algal cells, indicating potential morphological and physiological stress in *Chlorella sp.* In the *Lemna minor* assay, EC values could not be established due to data variability; however, the observed toxicological effects followed the trend: Thymol (most toxic) > AgNPs > Chitosan> TiO_2. Thymol and AgNPs caused complete inhibition of frond and root development, with associated reductions in chlorophyll content of 56.98% and 91.16%, respectively. In contrast, TiO_2 and chitosan exhibited negligible phytotoxicity, with growth inhibition values of only 5.23% and 16.69%, respectively.

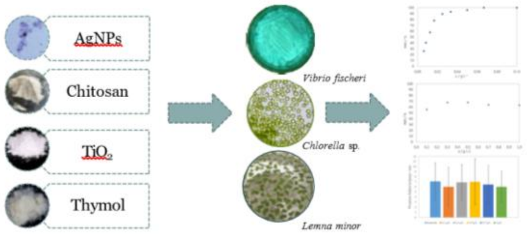

Fig. 1: Illustration of application of AgNPs, chitosan, TiO_2 and thymol on tested microorganisms, along with the assessment of their biological responses.

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Analysis of technologies for green hydrogen production

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Abstract:

Global dependence on fossil fuels has led to serious environmental challenges, including greenhouse gas emissions and climate change. In response, the European Union has implemented strict policies and guidelines aimed at establishing a sustainable and carbon-neutral society. Hydrogen production via electrolysis stands out as a key solution in this transition, offering a clean alternative for energy storage, transportation, and industrial applications.

This paper compares the key technologies for green hydrogen production:

1. Proton exchange membrane (PEM) electrolysis uses a solid polymer electrolyte and operates at relatively low temperatures. It's known for high efficiency and fast response times, making it suitable for dynamic environments where renewable energy supply fluctuates.
2. Anion exchange membrane (AEM) electrolysis is similar to PEM but uses an anion exchange membrane, allowing for the use of cheaper catalysts and potentially lower costs.
3. Alkaline electrolysis (AE) is one of the oldest technologies, uses liquid electrolytes and operates at higher efficiencies at larger scales, but slower in response to energy supply changes compared to PEM.
4. Solid oxide electrolysis (SOE): operates at high temperatures, which improves efficiency by utilizing heat as energy. It is best suited for stable, high-heat environments.

Efficiency, scalability, and economic viability are analyzed for each of technologies explained, along with real-world examples of hydrogen production systems. Finally, the paper highlights the contribution of green hydrogen production to decarbonization strategies (European Climate Law), energy security (due the current political situation for Croatia and EU), and integration with renewable energy sources (as a battery energy storage systems).

Key words: green hydrogen, electrolysis, energy transition

Mebendazole removal efficiency and ecotoxic effect

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Mebendazole belongs to a group of antiparasitic drugs with anthelmintic activity used for treating various parasitic infections. In nature, we increasingly find such substances in aquatic environments, where they enter through sewage systems containing biological secretions from living organisms. The increasing presence of such synthetic chemicals and compounds in aquatic environments has emerged as a significant threat to water quality and biodiversity. This concern has driven growing interest in sustainable and innovative methods for mitigating the impact of these pollutants on ecosystems. In this study, we explored the effectiveness of an advanced oxidation process method that uses hydrogen peroxide (H_2O_2) in combination with the use of simulated solar radiation for decomposition purposes. This approach is used for investigating the removal of mebendazole from aquatic solutions in varying pH-levels and H_2O_2 concentrations (Fig. 1.). Experiments were conducted using H_2O_2 both in the presence and absence of simulated solar radiation. Samples for removal efficiency analysis were collected over a period of 5 hours and analyzed using HPLC-DAD analysis. The results showed that removal efficiency increased under simulated solar radiation and H_2O_2 concentration has a more significant influence on removal than pH-value. Ecotoxicity of the solutions was determined using the bacterial culture *Vibrio fischeri* before and after photolytic treatment. The samples do not show ecotoxic effects before or after degradation, indicating that no toxic by-products were formed during the decomposition process.

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NATO OTAN *This publication is supported by:* The NATO Science for Peace and Security Programme

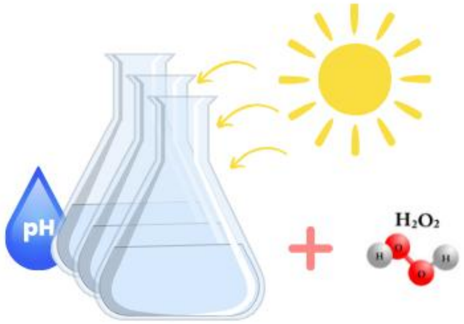

Fig. 1.: Simplified process scheme

Optimization of Copper Nanoparticle-Based Antimicrobial Materials and Fabrication of PCL Nanostructures via Electrospinning

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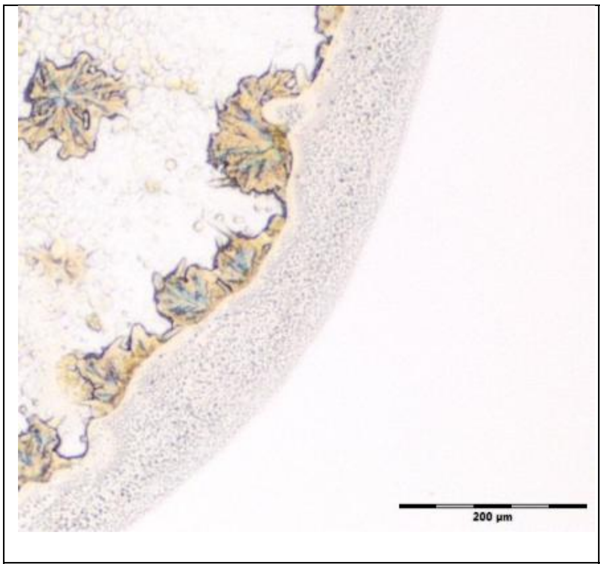
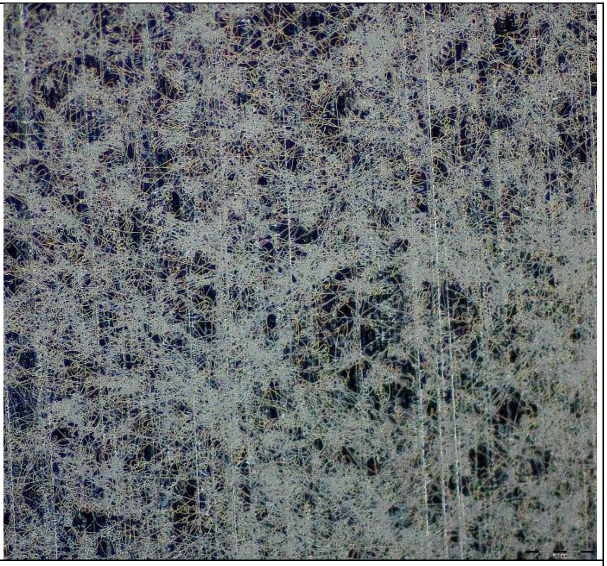
Antimicrobial and antiviral properties of materials play a crucial role in preventing infections and limiting pathogen transmission, particularly in medical and industrial settings. [1]. This study explores the green synthesis of copper nanoparticles (CuNPs) using environmentally friendly reagents via various synthetic routes, and their effect on surface hydrophobicity, aiming to enhance antimicrobial efficiency. Various synthesis methods were employed to produce stable CuNP dispersions, followed by detailed chemical characterization, including particle size, solution stability, and deposition behaviour in order to improve antimicrobial properties and hydrophobicity of the materials. Surface analysis included contact angle measurements to determine hydrophobicity, spectroscopy to confirm nanoparticle presence, and microscopy to observe coffee-ring effects and particle distribution. Results indicate that increased surface hydrophobicity significantly reduces microbial adhesion, thus enhancing the material's antimicrobial performance and extending the durability of protective coatings [2].

In addition, CuNPs were successfully incorporated into polycaprolactone (PCL) matrices and processed into nanostructured fibers using the electrospinning technique. This approach yielded uniform, porous materials with large surface areas, further boosting its antimicrobial potential. The integration of copper nanoparticles into PCL nanofibers represents a promising strategy for developing advanced antimicrobial surfaces suitable for sustainable and scalable use in healthcare and industrial environments, aligned with green chemistry principles.

 200 µm	
Figure 1. Coffee fing effect of CuNPs	Figure 2. Microphotography od PCL porous material

***Acknowledgments**: This paper was funded by the Croatian Science Foundation through the project IP-2024-05-4339 entitled " Coffee ring' effect in 'Lab on a Chip' environments in the development of new drug formulations." leader prof. Ernest Meštrović.*

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Experimental and Computational Studies of Solvent Molecule Inclusion within a Calix[4]arene Hydrophobic Cavity

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Calixarenes bearing electron-donating groups at the lower rim exhibit a high affinity towards first- and second-group metal cations. The inclusion of solvent molecule into the calixarene hydrophobic *basket* plays an important role in determining the extent of cation complexation reactions [1]. However, the thermodynamic and structural aspects of this process involving alkaline earth metal cation complexes have been seldom explored in detail.

In the present work, we have determined the thermodynamic reaction parameters for complexation of alkaline earth metal cations by calixarene derivative **L** (Figure 1) by means of several experimental methods (UV absorption spectrometry, fluorimetry, and isothermal titration calorimetry) and compared them with those corresponding to alkali metal cations [2]. The solvent effect, specifically that of the solvent molecule inclusion in the calixarene *cone* was addressed from the structural and thermodynamic points of view. The ligand-solvent and complex-solvent adduct structures were investigated by NMR spectroscopy, classical molecular dynamics simulations, and DFT calculations. The main difference between the adducts of alkali and alkaline earth metal cation complexes was in the orientation of the solvent molecule inside the calixarene cavity (Figure 1). In the latter case, cations were additionally coordinated by the solvent -CN/-OH group, which significantly affected the thermodynamic stability of the complexes. The solvent inclusion process was also quantitatively investigated by UV spectrometry and ITC.

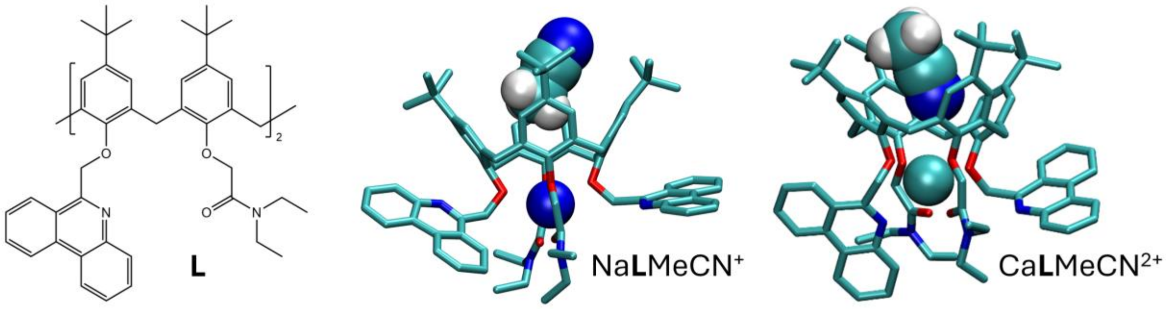

Fig. 1: Structures of calixarene derivative **L** and acetonitrile adducts of Na**L**$^+$ and Ca**L**$^{2+}$ complexes obtained by MD simulations.

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Bioremediation of wastewater with indigenous bacterial cultures from biowaste

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Wastewater contains a wide range of pollutants that must be treated before discharge. Bioremediation represents an environmentally friendly solution, as it relies on naturally occurring processes without the emission of harmful substances or the use of chemicals. This process is carried out with the help of microorganisms, which, through their metabolic capabilities, degrade or transform toxic pollutants into less toxic forms. The use of microorganisms in bioremediation plays a key role in maintaining and preserving ecological balance.[1] The main techniques applied in bioremediation are bioaugmentation and biostimulation. Their application enhances the efficiency of wastewater treatment while supporting sustainable environmental practices.

In this study, bioremediation of wastewater from biowaste was carried out using the biostimulation technique under batch, submerged, and aerobic conditions at 25±1°C over 5 days. The chemical oxygen demand (COD), pH value and dissolved oxygen concentration (DO) were determined in the experiment. The results showed a 57% reduction in COD and a 46% reduction in DO concentration, indicating increased microbial activity. The obtained pH values were in the neutral to slightly alkaline range. Bioremediation is considered a modern and effective approach to remediating contaminated areas because it uses biological processes to break down and remove pollutants from the environment.

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Bioaugmentation of highly organically loaded waste stream with thermophilic bacterial cultures

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Considering the increasingly pronounced water stress, wastewater treatment is becoming a key element of strategies to achieve sustainable development. In this context, increasing emphasis is placed on the use of environmentally friendly and economically acceptable processes that enable the effective degradation of pollutants contained in wastewater. One of the techniques that stands out in this area is bioaugmentation. This technique involves the inoculation of microorganisms into the polluted area, whereby the microorganisms, due to their metabolic activity, break down the pollutants present into less harmful metabolites such as H_2O and CO_2. Thermophilic bacterial cultures can be used as inoculum in bioaugmentation. They are of great importance for biotechnological development due to their enzymes, which remain stable even at high temperatures.

In this work, the efficacy of bioaugmented thermophilic microorganisms in the bioremediation of highly loaded wastewater was investigated, in batch and submerged conditions at room temperature for 8 days. Bacterial cultures used for bioaugmentation were isolated from the thermophilic phase of the composting process. In the experiment, the following was determined: biochemical oxygen demand (BOD), chemical oxygen demand (COD), total solids (TS), volatile solids (VS), optical density (OD), pH and total number of living cells (CFU). The initial values of the ratio BOD_5/COD and VS/TS were 0.73 and 0.82, respectively. The process of biodegradation was observed throughout the microscopic analysis of the system. By using bioaugmentation, the bioremediation of wastewater was successfully carried out, as indicated by the BOD_5/COD value, which was 0.24 on day 8, and the appearance of activated sludge flocs.

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EDUCATIONAL SECTION

EDUKACIJSKA SEKCIJA

"Freshmen Under the Microscope: What Their Mistakes in Chemical Calculations Reveal"/ *Brucoši pod povećalom: Što otkrivaju njihove pogreške u kemijskom računu*

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During the first year of studies in Applied Chemistry and Chemical Engineering, students face a range of challenges that often expose gaps in their prior knowledge. This lecture analyzes those mistakes—not as weaknesses, but as valuable indicators of areas in secondary education that require systematic strengthening. Drawing on real student responses from the courses *General and Inorganic Chemistry*, the lecture highlights the most common types of errors: from misunderstanding basic units and quantities, to imprecise stoichiometric calculations, and confusion when working with concentrations and pH values. Special emphasis is placed on foundational concepts that students may have formally learned, but not truly understood—an issue that later complicates the solving of more complex problems. This lecture is intended for high school chemistry teachers, with the aim of raising awareness about the educational gap between secondary school and university-level approaches to chemistry. In addition to analyzing specific mistakes, the lecture offers suggestions on how to prevent them through teaching—by placing greater focus on conceptual understanding, interconnection of ideas, and the development of computational skills in a chemical context. The goal is shared: to prepare students not only for exams, but for a genuine understanding of chemistry as the language through which science communicates with the world.

Tijekom prve godine studija primjenjene kemije i kemijskog inženjerstva, studenti se suočavaju s nizom izazova koji često otkrivaju pukotine u prethodno usvojenom znanju. Ovo predavanje analizira upravo te pogreške – ne kao slabosti, već kao dragocjene pokazatelje onoga što treba sustavno jačati u srednjoškolskom obrazovanju. Na temelju stvarnih studentskih odgovora iz kolegija Opća kemija, te Opća i anoganska kemija prikazuju se najčešći tipovi pogrešaka: od nerazumijevanja osnovnih jedinica i veličina, preko nepreciznih stehiometrijskih izračuna, do konfuzije u radu s koncentracijama i pH vrijednostima. Poseban naglasak stavlja se na temeljne koncepte koji se često formalno svladaju, ali ne i suštinski razumiju – što kasnije značajno otežava rad na složenijim problemima. Predavanje je namijenjeno profesorima kemije u srednjim školama, s ciljem osvješćivanja obrazovnog jaza između srednjoškolskog i fakultetskog pristupa kemiji. Uz analizu konkretnih pogrešaka, nude se prijedlozi kako ih prevenirati kroz nastavu – kroz veći naglasak na razumijevanje, povezivanje pojmova i razvoj računalnih vještina u kemijskom kontekstu. Cilj je zajednički: pripremiti učenike ne samo za ispite, već i za stvarno razumijevanje kemije kao jezika kojim znanost komunicira sa svijetom.

The Intersection of Chemistry and Physics
Gdje se kemija i fizika dodiruju?

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This presentation explores the interrelationship between physics and chemistry—two fundamental natural sciences that, while differing in focus (physics studies the fundamental laws of nature, and chemistry examines the structure and transformations of matter), share numerous points of connection both in scientific methodology and in educational practice. Through an analysis of the high school curriculum, the presentation identifies specific areas of overlap, such as thermodynamics, gas laws, electromagnetism, atomic and quantum theory, spectroscopy, and radioactivity. Special emphasis is placed on the similarities and differences in how these concepts are approached in each discipline—for example, the definitions of work and energy in physics versus chemistry—which can often lead to conceptual confusion among students. The role of physical chemistry is highlighted as a bridge between the two sciences, along with the importance of conceptual understanding that transcends subject boundaries. Using practical classroom examples, the presentation examines opportunities for better content alignment and enhanced interdisciplinary collaboration, ultimately promoting more integrated and functional student knowledge. The aim is to encourage reflection on approaches to teaching complex content, the value of cross-curricular connections, and the development of scientific literacy as a cornerstone of modern education.

U ovom izlaganju razmatra se međuodnos fizike i kemije, dviju temeljnih prirodnih znanosti koje, iako imaju različite fokuse – fizika proučava temeljne zakone prirode, a kemija strukturu i promjene tvari – dijele niz dodirnih točaka, kako u znanstvenoj metodologiji, tako i u nastavnoj praksi. Kroz analizu kurikuluma gimnazijskog obrazovanja, identificiraju se konkretna područja preklapanja, poput termodinamike, plinskih zakona, elektromagnetizma, atomske i kvantne teorije, spektroskopije te radioaktivnosti. Poseban naglasak stavlja se na razlike i sličnosti u pristupima pojedinim pojmovima, primjerice definiranju rada i energije u fizici i kemiji, što često može dovesti do pojmovne nejasnoće kod učenika. Također se ističe uloga fizikalne kemije kao mosta između dviju znanosti, kao i važnost konceptualnog razumijevanja fenomena koje nadilazi granice pojedinog predmeta. Kroz primjere iz nastavne prakse, analiziraju se mogućnosti boljeg usklađivanja sadržaja te jačanja međupredmetne suradnje, čime se potiče cjelovito i funkcionalno znanje učenika. Izlaganje ima za cilj potaknuti refleksiju o pristupima poučavanju kompleksnih sadržaja, važnosti međupredmetnih poveznica i razvoju prirodoslovne pismenosti kao temelja suvremenog obrazovanja.

Pedagogical Content Knowledge – the knowledge behind effective teaching that makes a difference

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Pedagogical Content Knowledge (PCK) plays a critical role in effective chemistry education, as it bridges the gap between subject matter expertise and pedagogical strategies that support student understanding. In chemistry education, PCK includes knowing how to explain abstract concepts, address misconceptions, design experiments and create learning environments that foster inquiry and curiosity.

In the Croatian context, where the curriculum increasingly prioritises competencies, critical thinking, and real-world applications, PCK is more important than ever. Stronger collaboration between university educators and high school teachers is needed. University educators must integrate more pedagogical practice and reflection into chemistry programs, while experienced high school teachers can offer real-world classroom insights. This bidirectional exchange could be facilitated through joint workshops, teaching practicums, and continuous professional development sessions. Joint teacher development initiatives, mentoring programs, and practice-based learning can help bridge the gap between theory and practice.

A detailed examination of Croatian pre-service chemistry teachers reveals important insights into their pedagogical content knowledge (PCK), teaching beliefs, and the challenges they face in translating subject knowledge into effective classroom practice. While these future educators often possess a solid conceptual grasp of chemistry, they frequently struggle to adapt their knowledge to suit the cognitive needs of secondary school students. Many enter the profession with traditional, teacher-centred perspectives that can limit their ability to implement contemporary, student-oriented, and inquiry-based teaching methods. This gap between content mastery and pedagogical application can hinder lesson design, weaken classroom interactions, and reduce student engagement with complex scientific concepts.

To summarise, improving chemistry education in Croatia requires systemic support for PCK development, aligned university curricula, and structured cooperation between academic and school-based educators. Such efforts can lead to more effective, engaging, and relevant chemistry teaching that supports student understanding and curiosity.

Challenges in Chemistry Tasks with Low Solvability on the National Matura: Where Lies the Problem?/ *Zadatci s učestalo niskom rješivošću na državnim maturama iz kemije: U čemu je problem*

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The implementation of the national chemistry exam (Matura) serves as an important indicator of students' interest in the natural sciences and their readiness to pursue related fields of study. As an elective subject, chemistry provides insight into candidates' preparedness and competencies, while also reflecting the challenges involved in test design. Expert working groups face the complex task of creating exams that must meet clearly defined cognitive levels, balanced representation of curriculum content, and an appropriate degree of task complexity. fter sixteen years of administering the national Matura, available analyses from the National Centre for External Evaluation of Education (NCVVO) offer valuable insights into educational trends, while also highlighting certain persistent challenges. A notable proportion of students leave specific questions partially or entirely unanswered, with certain types of tasks repeatedly emerging as particularly problematic. These are most often tasks requiring interdisciplinary connections with mathematics and physics, graph interpretation, analysis of laboratory diagrams, and comprehension of situational problems. This presentation analyzes concrete examples of both high- and low-performing tasks, with an effort to identify the root causes of weaker performance. In addition, it offers practical guidelines and suggestions to support teachers in preparing students for more complex tasks during regular chemistry instruction. Emphasis is placed on the importance of developing analytical thinking, functional knowledge, and skills that go beyond rote memorization—competencies essential for successfully tackling the more demanding components of the national chemistry exam.

Provođenje ispita državne mature iz kemije predstavlja važan indikator interesa učenika za prirodoslovna područja i nastavak obrazovanja na povezanim studijima. Kao izborni predmet, kemija pruža uvid u spremnost i kompetencije pristupnika, ali i izazove koji prate oblikovanje ispita. Stručne radne skupine suočene su sa zahtjevnim zadatkom izrade ispita koji mora zadovoljiti jasno definirane parametre kognitivnih razina, uravnoteženu zastupljenost obrazovnih sadržaja i odgovarajuću razinu složenosti zadataka.Nakon šesnaest godina provedbe državne mature, dostupne analize Nacionalnog centra za vanjsko vrednovanje obrazovanja (NCVVO) omogućuju uvid u obrazovne trendove, ali i ukazuju na određene izazove. Značajan broj učenika ostavlja pojedine zadatke djelomično ili potpuno neriješenima, a pritom se uočavaju specifični tipovi zadataka koji se redovito pokazuju problematičnima. Riječ je ponajprije o zadacima koji zahtijevaju međupredmetno povezivanje s matematikom i fizikom, interpretaciju grafova, analizu laboratorijskih shema te razumijevanje situacijskih problema. U izlaganju su analizirani konkretni primjeri zadataka s visokim i niskim postotkom riješenosti, uz pokušaj identifikacije temeljnih uzroka slabijeg uspjeha. Također, ponuđene su smjernice i prijedlozi koji bi mogli pomoći nastavnicima u pripremi učenika za složenije zadatke tijekom redovne nastave kemije. Naglasak je stavljen na važnost razvijanja analitičkog mišljenja, funkcionalnog znanja i vještina koje nadilaze puko memoriranje sadržaja, a koje su ključne za uspješno rješavanje zahtjevnijih zadataka na državnoj maturi iz kemije.

Acceleration of ions in solution under the influence of an electric field: What is observed macroscopically vs. what is happening microscopically

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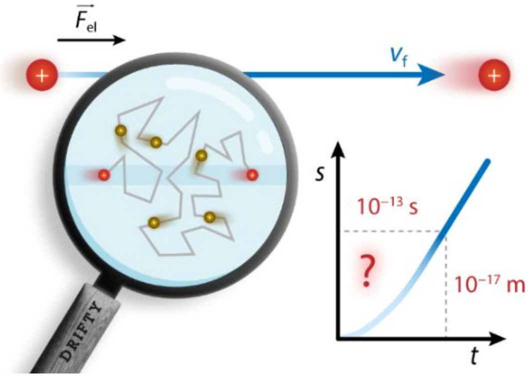
The challenge in teaching phenomena related to conductivity of electrolyte solutions, particularly that of ionic motion under the influence of an electric field, lies in balancing macroscopic and microscopic perspectives. With this respect, traditional macroscopic approach can lead to misunderstanding of what happens at the submicroscopic scale.[1,2] In this talk, an approach to teaching macroscopic and microscopic views on the motion of ions in solution will be presented. Through setting and solving the appropriate equations, followed by discussion of the obtained results, it will be shown that the macroscopic model cannot be applied to describe particle behavior at the submicroscopic level.[2] An interactive simulation (free for download: https://pubs.acs.org/doi/10.1021/acs.jchemed.4c00365)[2] is proposed for use in teaching the migration of ions in solution. It allows users to simulate Brownian motion of ions without the applied electric field and that when the component resulting from the action of the electric force is superimposed to the completely random motion. The simulation is envisaged for implementation in teaching ionic motion in high schools and universities by visualizing the fact that averaging of movements of many ions in solution results in the macroscopically observed properties corresponding to uniform motion of ions through solution. The described approach enhances students' understanding of the relation between the macro- and microscopic properties of the moving charged particles and is suggested to be applied in teaching the conductivity of electrolyte solutions as well as transport phenomena in general.



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ROUND TABLE

OKRUGLI STOL

Round table:

Contemporary Chemistry Education and Vertical Communication Among Educators

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In an era of rapidly evolving scientific knowledge and educational technologies, the need for coherent, aligned, and communicative chemistry teaching across all educational levels has never been more pressing. This round table brings together educators from secondary schools, universities, and teacher training institutions to explore the challenges and opportunities of modern chemistry instruction within a vertically integrated educational system.

Key discussion points will include: the alignment of learning outcomes between secondary and tertiary chemistry curricula; the role of conceptual understanding versus procedural knowledge; the use of digital tools and modern pedagogical approaches; and the importance of consistent communication among educators at different stages of the educational pathway. Participants will share experiences, identify systemic gaps, and propose actionable strategies for improving continuity in chemistry education—from high school foundations to university-level complexity.

Special attention will be given to how interdisciplinary competencies, problem-solving skills, and scientific literacy can be nurtured through better collaboration and feedback loops among teachers at different levels. By fostering a dialogue between secondary and higher education professionals, this round table aims to contribute to a more unified and effective chemistry education framework—better preparing students for academic success and real-world scientific challenges.

POSTERS

POSTERI

Synthesis of a methylcellulose based polymeric pharmaceutical dispersants in the green solvent Cyrene™

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Cancer is a rising problem in modern times. New therapies are being discovered with targeted therapies gaining more and more attention. Many innovative therapies for cancer consist of large molecules which are poorly soluble in water.[1] One approach to combat this problem is to use the amorphous form of the drug, which has a crystal lattice energy of nearly zero.[2] The drug in this form is unstable and prone to crystallization. Therefore, the drug is dispersed in an appropriate carrier which inhibits the crystallization. Many dispersants are used, such as various methacrylates, poly(*N*-vinyl pyrrolidone), PEG, as well as various cellulose derivatives.[3] Our goal is to create a polymeric dispersant based on hydroxypropyl methylcellulose grafted with different monomers as to tailor the cellulose's properties. The synthesis was carried out in the green solvent Cyrene™ (dihydrolevoglucosenone) which is a novel, "practically non-toxic",[4] solvent derived from waste biomass.[5] The synthesized material was characterized with FTIR, ^{1}H-NMR, GPC, TGA and DSC. Additionally, we have conducted a solubility test of naproxen as a model drug in the material by DSC via melting-point depression study.

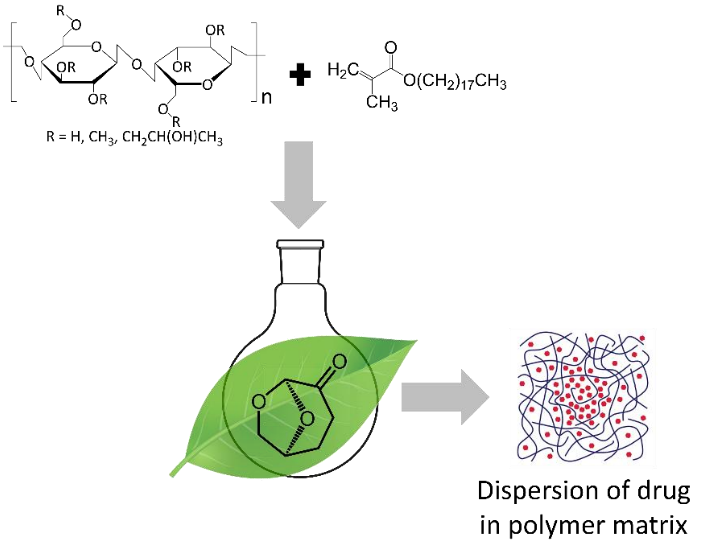

Fig. 1: The synthesis of the polymeric carrier is conducted in Cyrene. Naproxen is dispersed in the polymer matrix after polymer's isolation.

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DPP3 knockdown reveals a negative regulatory role in CDKN1/p21 expression in HeLa and SCC-25 Cells

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Dipeptidyl peptidase 3 (DPP3) is a zinc-dependent metallopeptidase involved in peptide degradation and cellular stress responses.[1] Although DPP3 has been implicated in oxidative stress regulation and KEAP1-NRF2 signaling, its role in cell cycle regulation remains unclear. In this study, we explored the consequences of DPP3 knockdown on the expression of CDKN1 (also known as p21), a cyclin-dependent kinase inhibitor that plays a central role in cell cycle arrest and tumor suppression.[2,3]

Using siRNA-mediated silencing of DPP3 in HeLa (cervical carcinoma) and SCC-25 (oral squamous cell carcinoma) cells, we observed an increase in CDKN1 expression at both the transcript (qPCR) and protein (western blot) levels. The upregulation of CDKN1 suggests that DPP3 may function as a negative regulator of p21 expression in epithelial cancer cells, potentially affecting cellular proliferation and tumorigenic potential. These findings offer new insights into the molecular interplay between peptidase activity and cell cycle control and raise the possibility that DPP3 contributes to oncogenic processes by suppressing key cell cycle checkpoints. Ongoing work is focused on elucidating the downstream effects of elevated CDKN1 on cell cycle progression and assessing whether this regulatory relationship is conserved in other cancer models.

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Functional triarylboranes as molecular sensors: from synthesis to protein targeting

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Triarylboranes are a class of compounds in which a boron atom is bonded to three aromatic rings. Owing to their electron-deficient nature, ability to coordinate with nucleophiles (e.g., oxygen, nitrogen), and remarkable optical properties they have emerged as promising building blocks in the development of molecular sensors. Furthermore, their polyaromatic and hydrophobic characteristics allow for interactions with hydrophobic pockets in proteins such as bovine serum albumin (BSA) [1-2].

In this study, lysine-functionalized bis-triarylborane derivatives were synthesized and characterized (Fig. 1.). Spectroscopic investigations revealed a pronounced solvatochromic effect, dependent on the solvent used for spectral acquisition. Binding interactions with BSA and liposomes were evaluated via titration experiments, and the binding constant with BSA was determined. Additionally, cytotoxicity was assessed using the MTT assay, demonstrating that the compounds exhibit no significant cytotoxic effects.

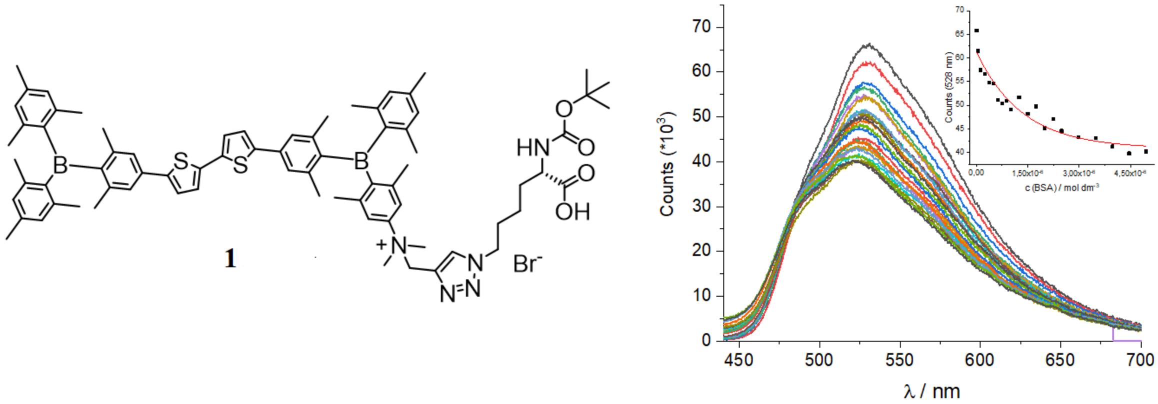

Fig. 1: Structure of TAB-compound and emission spectra of titration with BSA

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Thermal properties of the PLGA copolymers of different composition (lactide to glycolide molar ratio)

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Poly(lactic-*co*-glycolic acid) (PLGA) is a linear biodegradable copolymer with random distribution of the lactic and glycolic monomeric units (LA/GA ratio) along the copolymer chain. Owning to its biodegradability, good biocompatibility and ability to achieve extended drug release, PLGA has been widely used as a drug carrier. It is capable of delivering a wide range of molecules, from small hydrophilic and/or hydrophobic to large protein/peptide molecules such as leuprolide acetate, human growth hormone, buprenorphine and risperidone [1,2].

In this study, the thermal properties of PLGA copolymers with varying LA/GA ratios were investigated using thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). The thermal stability of the PLGA copolymers was studied by analysing mass loss temperatures from the TG curve, while DSC thermograms provided insights about glass transition temperatures. The glass transition temperature is a critical parameter influencing the copolymer's mechanical properties which plays a significant role in modulating drug release profile [3]. The results demonstrated that lowering the lactide content in the copolymer led to higher onset and end temperatures of thermal degradation (232.0 °C for 50 % PLA and 222.7 °C for 85 % PLA), as well as elevated glass transition temperatures (37.5 °C for 50 % PLA content and 39.4 °C for 85 % PLA).

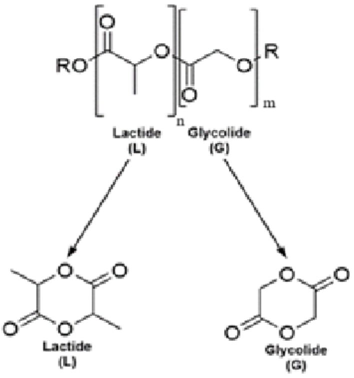

Fig. 1: Chemical structure of PLGA copolymer and its lactide / glycolide monomers.

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Antioxidant power of pumpkin seeds oil, flour and cake measured by ESR spectroscopy

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Pumpkin (*Cucurbita pepo* L.) seed products, including oil and flour as well as pumpkin seed cake as by-product, are an important source of natural antioxidants. Antioxidants neutralize free radicals which are harmful to human health. Radicals may be generated through human metabolism, introduced into the body by food or inhalation, or produced internally as a result of exposure to high-energy radiation (UV, X and γ). Electron spin resonance (ESR), an extremely sensitive spectroscopic technique used to measure the concentration of free unpaired electrons, was applied to measure the antioxidant power (AP) of pumpkin seed oil, flour and cake samples. The loss of the ESR signal of 2,2-diphenyl-1-picrylhydrazyl (DPPH), used as a scavenging object, was monitored over time after adding ethanol extract of pumpkin seed oil, flour and cake to DPPH ethanol solution. It is important to determine whether processing temperature (40 °C and 122 °C) and storage temperature of the samples (4 °C and 22 °C) affect their AP. It was found that above mentioned parameter affects AP of all investigated sample. Notably, the pumpkin seed cake, particularly from cold pressed seeds, exhibit surprisingly high AP values. This result supports its potential use as a valuable raw material for the food, pharmaceutical and cosmetic industries. In conclusion, the study indicates that both the oil production temperature and the storage temperature of seeds and oil as the final product might have a significant impact on their antioxidant power.

Effect of electrode substrate material on Methylene Blue adsorption and electrochemical determination

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Methylene Blue (MB) is the most commonly used redox reporter in aptamer sensors, albeit functionalized with alkyl thiols to form SAMs on gold substrates [1]. However, few works tackle direct electrochemical detection on bare electrode surfaces and are mostly based on chemically modified electrodes [2-5]. Achieving reliable electrochemical detection would facilitate and enable integrated tracking of Methylene Blue as the process throughput indicator in various applications, such as photodegradation studies or sensor applications. Its tendency to strongly adsorb on a wide variety of substrates, including gold and especially carbon nanomaterials, can be exploited to achieve reliable electrochemical sensing when paired with low-cost, flexible and easily fabricated printed electrode systems.

In this work, Methylene Blue (MB) was dissolved in phosphate buffer aqueous solutions (pH range 5-8) and its properties examined using square wave voltammetry, differential pulse voltammetry, linear sweep voltammetry and cyclic voltammetry. Due to pH dependence of the MB reduction potential, square wave voltammetry was conducted in phosphate buffer solutions of varying pH to determine the reduction potential change per pH unit. Optimization of method parameters was conducted in a 1 µM or 10 µM MB solution at pH 6. Gold and various carbon substrates were used, including Au and glassy carbon disk electrodes, as well as screen printed gold and carbon planar electrodes. Collected data will be used as a crucial reference point for further development of a microfluidic system with integrated printed electrodes for real-time continuous MB determination.

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Quantum chemical docking study of selective acetylcholinesterase inhibition by α-acylaminobenzamides

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Alzheimer's disease is a progressive neurodegenerative disorder that severely impairs individuals' cognitive abilities, leading to severe memory loss and difficulty performing everyday tasks [1,2]. This incurable disease ranks among the leading causes of death worldwide, highlighting its profound impact on public health. The cholinergic hypothesis suggests that an acetylcholine deficiency, a key neurotransmitter involved in learning, memory, and attention, plays a central role in the disease's progression. Acetylcholine acts by binding to specific receptors in the brain, with its signaling being terminated by cholinesterases, primarily acetylcholinesterase (AChE) and butyrylcholinesterase (BChE). In individuals with Alzheimer's disease, acetylcholine levels are significantly reduced due to neuronal degeneration and impaired synthesis, leading to the development of cholinesterase inhibitors as the primary treatment strategy.

This study focuses on finding selective inhibitors of AChE by semi-flexible quantum-chemical molecular docking. A newly developed parallelized Monte Carlo algorithm was used for structure generation, effectively sampling vast configurational spaces, while considering all translational, rotational, and torsional degrees of freedom [3]. To ensure physically realistic structures, a *smart structure generator* eliminated any configurations with atomic overlaps. Binding energies within the AChE's active site were estimated using single-point quantum chemical calculations with the PM7 hamiltonian [4]. The top 1000 local minima identified through this process were further refined through geometry optimization, clustered, and ranked based on binding energy. An automated hydrogen bond search module and visual inspection were used to analyze the resulting docked structures.

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The role of ERK signaling pathways in mitochondrial dysfunction

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Mitochondrial dysfunction plays a central role in the progression of different diseases by disrupting cellular energy balance and promoting epithelial degeneration, inflammation, and apoptosis. While mitochondria are key regulators of cellular stress responses, the effects of mitochondrial impairment on signaling pathway activation remain incompletely understood. Among these pathways, extracellular signal-regulated kinases (ERK) activity is implicated in regulating autophagy/mitophagy, oxidative stress, and apoptosis. However, their role in mitochondrial dysfunction is not yet fully investigated. Additionally, changes in mitochondrial membrane potential significantly affect mitogen-activated protein kinase (MAPK)-dependent mechanisms.

In this study, we investigated the impact of mitochondrial uncouplers – FCCP, CCCP, chloroquine (CQ), and oligomycin (OMY) – on ERK pathway activation in HEK293 (human embryonic kidney) and HK2 (human proximal tubule) cells. These cell lines were selected due to their distinct mitochondrial metabolic profiles: HEK293 cells rely predominantly on glycolysis, while HK2 cells exhibit higher oxidative phosphorylation (OXPHOS) activity, reflecting differences between embryonic and mature kidney epithelial cells.

We also investigated the role of ERK pathway inhibitors (U0126 and mirdametinib) in modulating mitochondrial function by monitoring mitochondrial membrane potential, and by assessing the expression and localization of key proteins involved in mitochondrial oxidative stress, apoptosis, autophagy, and oxidative phosphorylation. Our preliminary results imply that ERK activation is essential for the maintenance of mitochondrial population and regulation of glycolysis. Clarifying the exact function of ERK in mitochondrial dysfunction is crucial for understanding kidney disease pathophysiology and may aid in developing novel therapeutic approaches targeting these signaling pathways.

Quaternization of pyridine-4-aldoximes with substituted 2-bromoacetophenones

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The quaternization of pyridine with alkyl halides or related compounds is a prime example of the Menschutkin reaction, which is the most common method for preparing quaternary ammonium salts (QAS). These QAS exhibit a wide range of biocidal activities, including antibacterial, antifungal, antiparasitic, and antiviral properties. Pyridinium oximes, which carry a permanent positive charge from the quaternary nitrogen in the pyridinium ring, are among the most effective reactivators. They possess the potential for neuroprotection and efficacy against both nerve agents and insecticidal chemicals, suggesting promise for future development. Consequently, there is a need for the creation of new compounds with potential biological activity. In this context, quaternary salts of pyridine-4-aldoxime have been synthesized by quaternizing pyridine-4-aldoxime with substituted phenacyl bromides through conventional heating in ethanol.

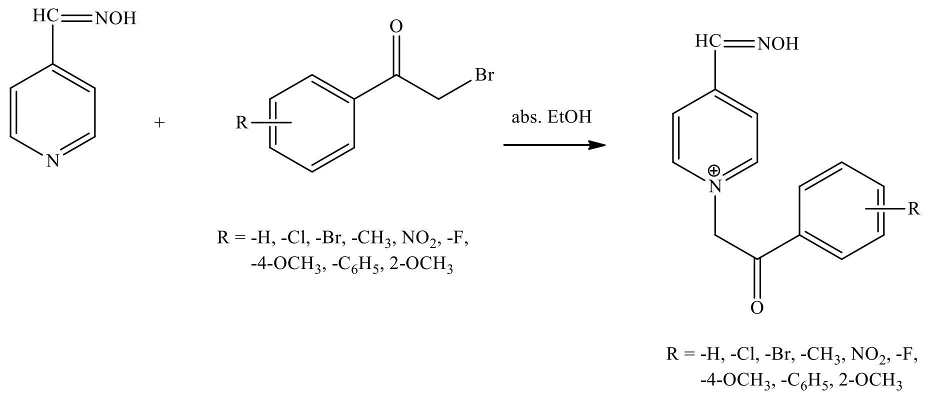

Fig. 1: Synthesis of quaternary salts

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Analysis of the surface morphology and chemical composition of orthodontic bands

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Bands are an essential component of fixed orthodontic appliances. They are usually made of stainless steel (SS) alloys. In the oral cavity, with its own physiological, thermal, microbiological and biochemical properties, the bands are exposed to an ideal corrosive medium. As a result of corrosion, many different metal ions are released, while morphological and chemical changes are observed on the surface of the bands [1].

In this work, the differences in the surface morphology and chemical composition of the bands were investigated when they were exposed individually or together with all parts of the fixed orthodontic appliance after their exposure to artificial saliva (AS) (T. Zucci receipt [1]). The morphological (Atomic Force Microscopy (AFM) and Scanning Electron Microscopy/Energy Dispersive X-ray Spectroscopy (SEM/EDX)) and chemical changes (Inductively Coupled Plasma Mass Spectrometry (ICP/MS) and X-ray Photoelectron Spectroscopy (XPS)) caused by immersion in AS during 3, 7, 14, and 28 days were determined. Possible correlations between the changes in surface morphology and ion release profiles were identified.

The SEM images of the SS bands, individually immersed, showed clear changes and a gradual formation of a protective layer whose formation starts already after 3 days and becomes more homogeneous with time. EDX analysis of the bands after immersion revealed gradually higher amounts of oxygen, indicating the formation of an oxide layer, which is consistent with the results of qualitative SEM analysis. EDX analysis also revealed the presence of metals not listed in the nominal composition of the bands, namely copper (Cu) [1]. Protective layer formation was also observed on the bands immersed with all other parts of orthodontic appliances, in approximately the same periods of time. AFM micrographs confirmed the formation of a thicker rough "wavy" layer while XPS identified that those surface deposits were mixed iron (Fe) and chromium (Cr) oxides or locally as pure Fe_2O_3. XPS results showed that Fe is present in the form of FeO and Fe_2O_3, Cr in the form of Cr_2O_3, and nickel (Ni) as NiO or $Ni(OH)_2$. Besides those oxides, oxygen could be a part of Na/K/Ca dihydrogen phosphates, phosphates, and carbonates. Standing alone, stainless steel bands released significant amounts of Fe, Ni, Cr and Mn with the highest release observed after 7 days of immersion. All parts together released Fe and Ni in the highest concentrations after 14 days. The concentrations of Cr began to decrease after 7 days, indicating the formation of a protective layer [2].

The results indicate that the released ions from the bands can have cytotoxic effects, particularly during the initial stages of immersion.

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Particulate matter at a background station on the island of Krk, Croatia

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Particulate matter in the ambient air poses a significant public health problem. While particulate matter is usually monitored at urban and industrial sites, background stations are important for understanding broader atmospheric processes. In this study, the first elemental analysis of particulate matter at a background station on the island of Krk in the northern Adriatic (Croatia) is presented. Sampling was conducted from June to December 2023 at the Ponikve station, the water reservoir. The samples were analyzed for 11 elements from S to Zn using energy dispersive X-ray fluorescence. In addition, microplastics were analyzed using fluorescence microscopy and scanning electron microscopy. The results show good air quality with occasional episodes of air quality deterioration, mainly in the winter months. These episodes are probably related to distant sources such as industrial areas or Saharan dust, although local influences, including soil dust and traffic, also contribute. The concentrations of microplastic particles detected showed no correlation with particulate matter pollution. An important contribution of this study is the placement of the sampler near the water reservoir, the main source of drinking water on the island. Understanding potential sources of pollution is critical to maintaining water quality. Continued monitoring at this site is essential to assess whether the episodes of poor air quality are isolated incidents or whether they are related to long-term sources of pollution.

Use of carbon dioxide for the synthesis of linear and cyclic organic carbonates

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Carbon dioxide (CO_2), an inert and non-toxic gas, plays a central role in the greenhouse effect — a natural process that maintains Earth's habitable temperature. However, human activities such as fossil fuel combustion and industrial processes have intensified this effect, leading to global warming. In the last decades, CO_2 has been also exploited as a reagent that can be transformed into fuels and industrial chemicals through catalytic processes [1].
Linear and cyclic organic carbonates are versatile, low-toxicity compounds used in fuels, batteries, and plastics, offering benefits in terms of efficiency and environmental sustainability. Their CO_2-based synthesis further supports environmental goals. These compounds can be successfully synthesized in catalyzed reactions of CO_2 and propagyl alcohols [2,3]. We synthesized allyl (1-(oct-1-yn-1-yl) cyclohexyl) carbonate (2) from 1-(oct-1-yn-1-yl)cyclohexan-1-ol (1) in three-component reactions (Fig. 1). Our aims are to optimize these catalytic processes by testing various reaction conditions and optimize the time of addition of allyl electrophile to achieve higher yields.

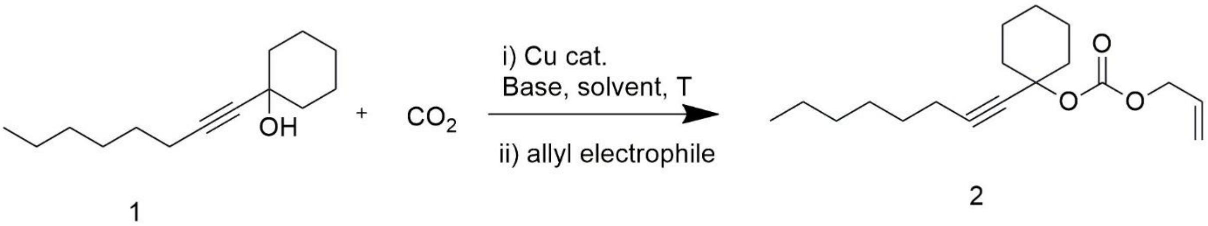

Fig. 1: General reaction for the synthesis of linear carbonate from CO_2.

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Dithienylethene-coumarin based photoswitches as sensors for metal cations

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Photoswitches are a class of compounds that can change their structures and properties under irradiation with UV or visible light. This type of compounds is of particular interest in the field of sensors, because of the potential to induce certain effects depending on the photoswitch form [1]. Additionally, many proteins functions as metalloproteins upon binding metal ions and it is known ions such as Cu^{2+} can alter DNA structure and function [2], [3].

In this work, a dithienylethene based photoswitch with coumarin moieties was synthesized and spectroscopically characterized in aqueous media and methanol. Compound **1** (Fig 1., left) showed reversible photochromism in methanol upon irradiation with UV light, while photocyclization did not occur in aqueous media. Since the triazole-coumarin moiety showed preference towards metal cation binding in previous studies [4], fluorimetric titrations with Cu^{2+} and Fe^{2+} cations were performed both in methanol and aqueous solution. Results show binding affinities in a biorelevant range (10 µM), with quenching of emission in methanol and increase of emission in aqueous solutions. Interestingly, with regard to expected difference in geometry of the closed and open form of **1** (Fig 1., right), both forms interact with Cu^{2+} and the photocyclization reaction is not hindered by complex formation, as shown by UV/Vis spectroscopy for methanolic solutions. These preliminary results show potential of compound to act as sensors for metal cations, and further studies will be performed to determine the effect of both compound and its metal complexes on binding to biomolecules.

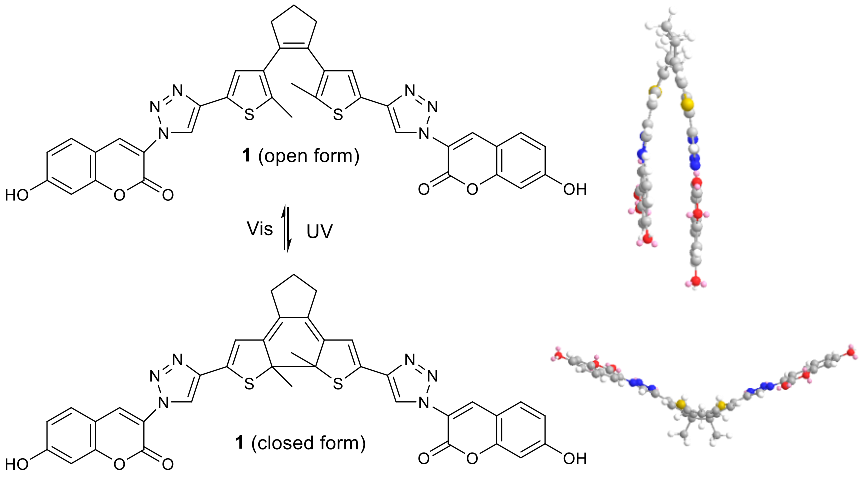

Fig. 1: Structures of open and closed form of **1** (left), expected geometries of open and closed form obtained by MM2 (right).

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Application of molecularly imprinted polymer for selective sorption of sulfamethoxazole, torasemide and procaine – kinetic study

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The increasing demand for the development of new and more effective treatments has led to the creation of a large number of new medicines. Increased production, consumption and inadequate disposal have led to their increased presence in the environment, where they are most commonly found water systems. Although they are used in relatively low concentrations, their biological activity and longevity in the environment pose a significant risk to entire ecosystems and human health. Conventional methods for their detection and removal are often ineffective, highlighting the urgent need to develop new approaches. With the aim of developing new sorbents that could contribute to the detection and eventual removal of pharmaceuticals, this study investigated the preparation of multi-molecularly imprinted polymers (MIPs), imprinted with three different template molecules: sulfamethoxazole, torasemide, and procaine. The sorption affinity of each pharmaceutical towards the polymer with three recognition sites; sulfamethoxazole, torasemide, and procaine - was studied separately. The effect of contact time was determined by performing the experiment at different time intervals over 24 hours. The pseudo-first-order model, the pseudo-second-order model, and the intraparticle diffusion model were used to describe the sorption kinetics. To evaluate the selectivity and efficiency of the MIP, the kinetic study was performed in parallel for non-imprinted polymer (NIP). The results showed similar kinetic sorption behavior but with improved selectivity when using the multi-molecularly imprinted polymer.

Acknowledgement

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Sustainable Hydrogen Production from Surplus Wind Energy Using PEM Water Electrolysis

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Abstract

The production of hydrogen using renewable energy sources plays a key role in reducing greenhouse gas emissions and achieving climate neutrality. As fossil fuel reserves dwindle and their environmental impact becomes increasingly unsustainable, hydrogen emerges as a clean energy carrier capable of storing and balancing electricity generated from intermittent renewable sources. One of the most promising methods for sustainable hydrogen production is water electrolysis using a PEM (proton exchange membrane) electrolyzer. This poster provides an overview of hydrogen production methods, with a focus on green hydrogen obtained through electrolysis powered by surplus electricity from renewable sources. Particular attention is given to the integration of PEM electrolysis with wind power. Due to fluctuations in electricity demand, wind farms are often forced to curtail production, leading to unused energy potential. By redirecting this excess electricity to electrolyzers, hydrogen can be produced and stored, effectively converting otherwise wasted energy into a valuable fuel. Using efficiency values obtained in laboratory conditions at FKIT, an estimation is made of the hydrogen yield from curtailed wind energy. The electrolyzer's construction, key components, and system requirements for safe operation and storage of produced gases are analyzed. A mathematical model is developed to predict the system's behavior, taking into account real-world constraints and necessary simplifications. Finally, a Matlab simulation is performed for a proposed electrolyzer design, comparing calculated performance metrics with manufacturer data to evaluate its feasibility for grid-balancing applications.

Keywords: Green hydrogen, PEM electrolysis, Sustainable energy, Wind power integration, Energy storage

Physicochemical insights into choline chloride-based deep eutectic solvents

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Deep eutectic solvents (DESs) are a class of green solvents formed by mixing a hydrogen bond acceptor (HBA) and a hydrogen bond donor (HBD), which results in a eutectic mixture with a melting point significantly lower than that of the individual components. Among various HBAs, choline chloride (ChCl) is one of the most commonly used due to its low toxicity, biodegradability, low cost, and availability. Choline chloride can be combined with a wide range of hydrogen bond donors, such as sugars, organic acids, alcohols, and amines, to form DESs with diverse physicochemical properties.

In this study, 17 different ChCl-based DESs were prepared by combining choline chloride with selected sugars, acids, alcohols, and amides. The prepared solvents were characterized by measuring their viscosity, polarity, and pH.

This parameters of the DESs were strongly affected by the nature of the hydrogen bond donor. DESs containing sugars and certain acids, such as citric and malic acid, exhibited markedly higher viscosity compared to those containing alcohols and amines. The polarity order from highest to lowest was found to be: ChCl : acids > ChCl : sugars > ChCl : alcohols > ChCl : amides. Similarly, pH values varied depending on the DES composition, with the following trend observed: ChCl : acids < ChCl : sugars < ChCl : alcohols < ChCl : amides.

These findings highlight the importance of physicochemical characterization in understanding DES systems. Knowledge of parameters such as viscosity, polarity, and pH are essential for assessing their potential application in various fields, including synthesis, extraction, and isolation processes.

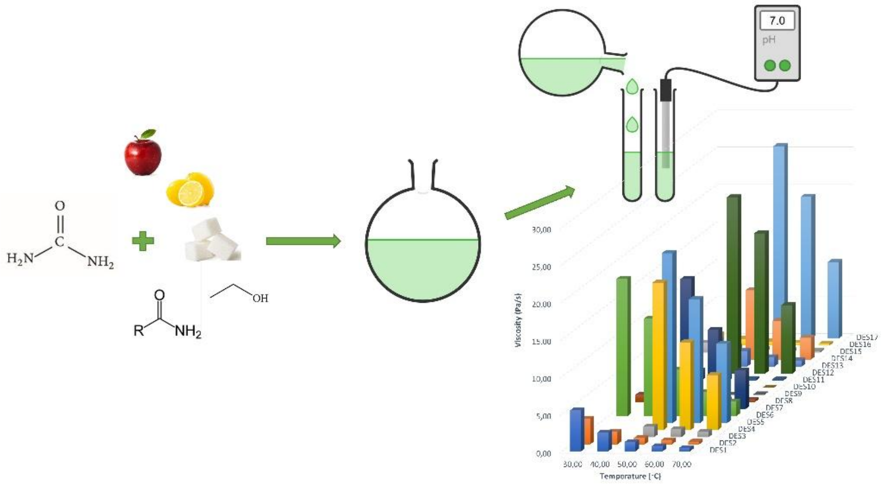

Fig. 1: Physicochemical characteristics of prepared choline chloride-based deep eutectic solvents

Investigation of metronidazole binding to TiO_2 coated PMMA surface for dental applications

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Polymethyl methacrylate (PMMA) is a synthetic polymer widely used in medicine due to its high biocompatibility. Since 1937, PMMA has been the primary material for manufacturing dental prostheses and implants [1]. However, its porosity and hydrophobicity make the surface susceptible to bacterial adhesion, particularly by *Candida albicans*. Attachment of the bacteria causes the formation of biofilms, a complex community of bacteria encased in a self-produced extracellular matrix. Biofilms exhibit increased resistance to antibiotics and can lead to various infections such as cavities, periodontitis and even systematic infections. Nanocoating of PMMA with TiO_2 using atomic layer deposition showed a significant decrease in the adhesion of *C. albicans*, as well as the reduction of bacteria adhesion in general [2]. Although promising, TiO_2 coating is not selective for all bacteria; it shows antibacterial property only on surface, and it must be activated *via* UV light. To overcome these limitations, functionalization with antibiotics is being investigated. One of the antibiotics most often used for bacterial infections in oral cavity is metronidazole. It is effective in treating infections of anaerobic bacteria and protozoa. Binding metronidazole to TiO_2-coated PMMA surface would allow localized and controlled release of the antibiotic, which leads to prevention of infections and reduces the risk of developing antimicrobial resistance [3].

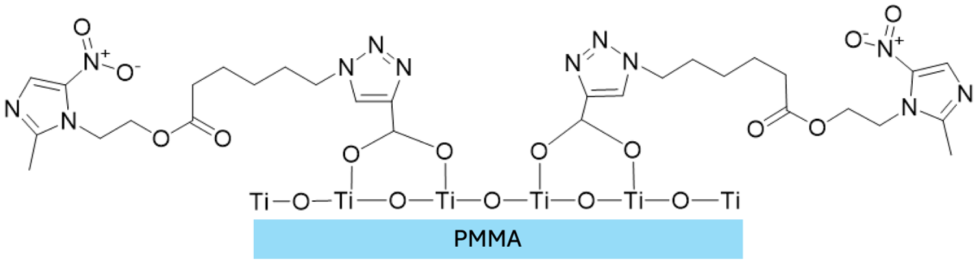

Fig. 1: Metronidazole binded to TiO_2 coated PMMA surface.

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Application of microchip electrophoresis for the determination of inorganic analytes in dietary supplements

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Dietary supplements are nutritional supplements made from concentrated sources of nutrients. Due to their easy availability on the market and the increase in the number of consumers, the need for their precise analysis has risen. Microchip electrophoresis (ME) was created by the miniaturization of capillary electrophoresis [1]. In ME, charged species are separated in the microchannel under the influence of an electric field. The presented investigation examines the possibility of fast determination and separation of potassium in dietary supplements. A C^{4}D detector was used for detection, and 0.5 mol/dm^3 acetic acid was used as the background electrolyte. The electropherogram of the dietary supplement shown in Fig. 1 shows a pronounced potassium peak at a retention time of 18 s. The results (peak height) are satisfactory with a correlation coefficient (R) of 0.9764 and a determination coefficient (R^2) of 0.9534. The selected method proved to be fast, efficient, and environmentally friendly for the separation of inorganic analytes, with analysis completed in less than one minute. In the near future, due to its easy portability and small size, microchip electrophoresis with a C^{4}D detector could be applied in pharmaceutical, food, and other industries and scientific fields. This work aims to investigate the possibility of potassium separation in complex samples of dietary supplements by microchip electrophoresis.

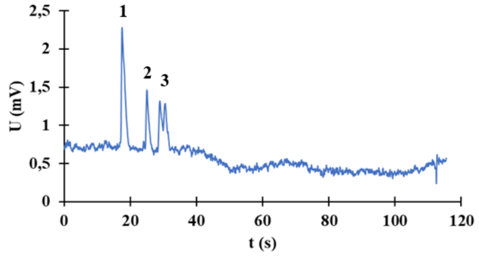

Fig. 1. ME electropherogram of the dietary supplement obtained in a background electrolyte of 0.5 mol/dm^3 acetic acid. Peak identification : 1, potassium; 2, unidentified; 3, unidentified.

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Eco-Friendly Solid-State Synthesis of Trisubstituted Guanidines

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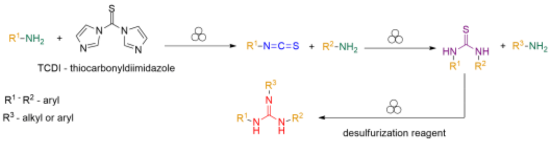
Through the application of mechanical force, mechanochemical synthesis—consistent with sustainable-chemistry goals—frequently achieves higher reaction yields and shorter reaction times than traditional solution-based methods [1, 2].

Mercury-based regents such as HgO and $HgCl_2$ have long been employed in the desulfurization step of guanidine synthesis. However, the adverse toxicological profile of mercury has prompted efforts to replace these reagents with safer transition metal salts, including $FeCl_3$, $CuSO_4$, and Ag_2O [3,4].

The present study investigates the mechanochemical route to trisubstituted guanidines using alternative, mercury-free desulfurization agents. Such guanidines are of notable interest for their prospective use as tripodal recpetors in anion-sensing applications [5].



Scheme 1. General reaction scheme.

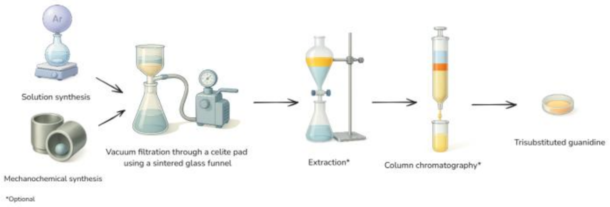


Fig 1. Schematic representation of the general synthetic procedure for the preparation of trisubstituted guanidines.

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Tumor-selective cytotoxicity of a vanadium(IV) complex with maltol as a carrier ligand

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Maltol (3-hydroxy-2-methyl-4*H*-pyran-4-one) is a naturally occurring hydroxypyranone widely used for its antioxidant properties, its non-toxicity and its remarkable ability to chelate metal ions. In addition to its industrial application as a flavor enhancer in foods, maltol has recently attracted considerable scientific interest as a bioactive ligand that can modulate the biological functions of metal ions, particularly in therapeutic contexts. Its ability to form stable, biologically available metal complexes makes it a promising candidate for the development of metal-based drugs. In this study, the vanadium(IV)-maltol complex — bis(maltolato) oxovanadium(IV) (BMOV) was synthesized using solution-based methods and subsequently tested for its cytotoxic potential against a group of seven human cell lines. These included one non-cancerous line (MRC-5) and six tumor-derived lines of different origins. Although BMOV is already well documented in the literature due to its insulin-mimetic properties and potential for diabetes therapy, the results presented here show its pronounced antiproliferative activity at a concentration of $2.5 \cdot 10^{-5}$ mol dm^{-3}. The most pronounced cytotoxic effect was observed in triple negative breast cancer cells (MDA-MB-231), where cell viability was reduced to 29.2%. This was followed by Hep G2 liver carcinoma cells (45.3%), KATO III gastric cancer cells (51.3%) and MRC-5 lung fibroblasts (47.2%). In contrast, the colorectal cancer cell lines (Caco-2 and HT-29) were the least responsive to treatment. In comparison, free maltol showed no cytotoxicity. The cell survival rate was above 80% for all tested lines, which underlines the crucial role of the vanadium center for the biological activity of BMOV. These results suggest that BMOV has dual therapeutic potential, both as an antitumor agent and as a metabolic modulator, highlighting the value of maltol as a carrier ligand in the design and development of vanadium-based drugs. The study opens up opportunities for further research into the mechanism of action of BMOV and its potential applications in oncology and in the treatment of metabolic diseases.[1–3]

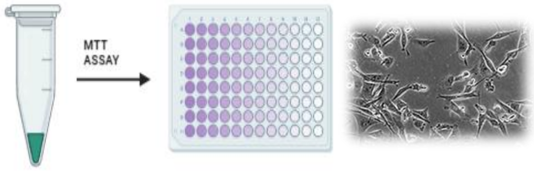

Fig. 1 : Citotoxicity of BMOV on malignant cell lines.

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Influence of fatty acids incorporation in lipid bilayer on anoplin-bilayer interaction

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Bacterial cell membranes consist of both zwitterionic and anionic phospholipids, whereby their ratio depends on the respective species [1]. Additionally, Gram-negative bacteria can regulate membrane fluidity by adjusting the ratio of saturated to unsaturated fatty acids (FA), which serves as a mechanism to control membrane permeability [2]. On the other hand, antimicrobial peptides have emerged as promising alternatives to conventional antibiotics because they act directly on the bacterial membrane. Anoplin (GLLKRIKTLL) is a decapeptide carrying four positive charges and has been shown to penetrate membranes, bind to bacterial DNA and inhibit ATP synthase. It is well-established that anoplin adopts an α-helical conformation in amphipathic environments, which is crucial for its membrane activity. However, in the presence of zwitterionic phosphatidylcholine vesicles, it predominantly adopts a disordered structure [3]. To better understand its interaction with bacterial membranes, we have prepared the latter using 1,2-dipalmitoyl-*sn*-glycero-3-phosphocholine (DPPC) as the zwitterionic and 1,2-dipalmitoyl-*sn*-glycero-3-phospho-rac-glycerol (DPPG) as the anionic phospholipid, along with stearic acid (SA) and linoleic acid (LA) to modulate membrane fluidity. The modification of their thermotropic properties was explored by differential scanning calorimetry (DSC).

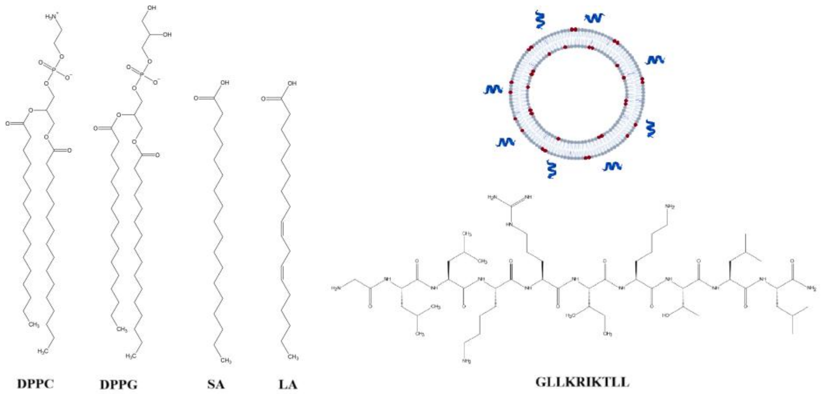

Fig. 1: Structural formulas of: DPPC, DPPG, SA, LA, anoplin and model membrane with anoplin.

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Application of metal-organic frameworks as solid-contact in all-solid-state ion-selective electrodes

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Potentiometric sensors are versatile probes that measure the activity of ions in aqueous samples. Their long-lasting development led to the characteristic solid-state design, where a transducer layer (solid-contact) is sandwiched between the electrode and the ion-selective membrane. The ideal solid contact should be highly conductive with high capacitance, but also hydrophobic enough to prevent accumulation of the electrolyte under the membrane (so called water layer) [1].

Metal-organic frameworks (MOF) are porous materials built up from metal ions and organic linkers in a repeating 3D network. High porosity and surface area reflect this structure, enabling their use in many applications, including gas storage, catalysis and sensing [2].

Herein, we compared the applicability of mechanochemically synthesized fullerene-intercalated cobalt-imidazolate MOFs as a transducer in potassium selective electrodes (K-ISE) before (C60@ZIF-67) and after pyrolysis (pyro-C60@ZIF-67). A significant water-contact angle increase from 133.5° to 161.7° was observed after pyrolysis, indicating superior hydrophobicity of pyro-C60@ZIF-67. This is a key property responsible for electrodes' long-term stability. Capacitance measurements using chronopotentiometry provided information on the efficiency of signal transduction; the higher the capacitance, the faster the ion-to-electron transfer. Pyrolysis induced a capacitance jump from 1.87 μF to 5.15 μF, which is a 176 % increase. These transducers' changes in properties were best reflected in prolonged measurements, including water-layer tests and a reversibility study. Both transducers gave electrodes with comparable analytical characteristics, including dynamic linear range in $c(\mathrm{K}^+) = 10^{-5} - 10^{-1}$ mol dm^{-3} and lower limit of K-ion detection $a(\mathrm{K}^+) = 10^{-5.4}$ mol dm^{-3}.

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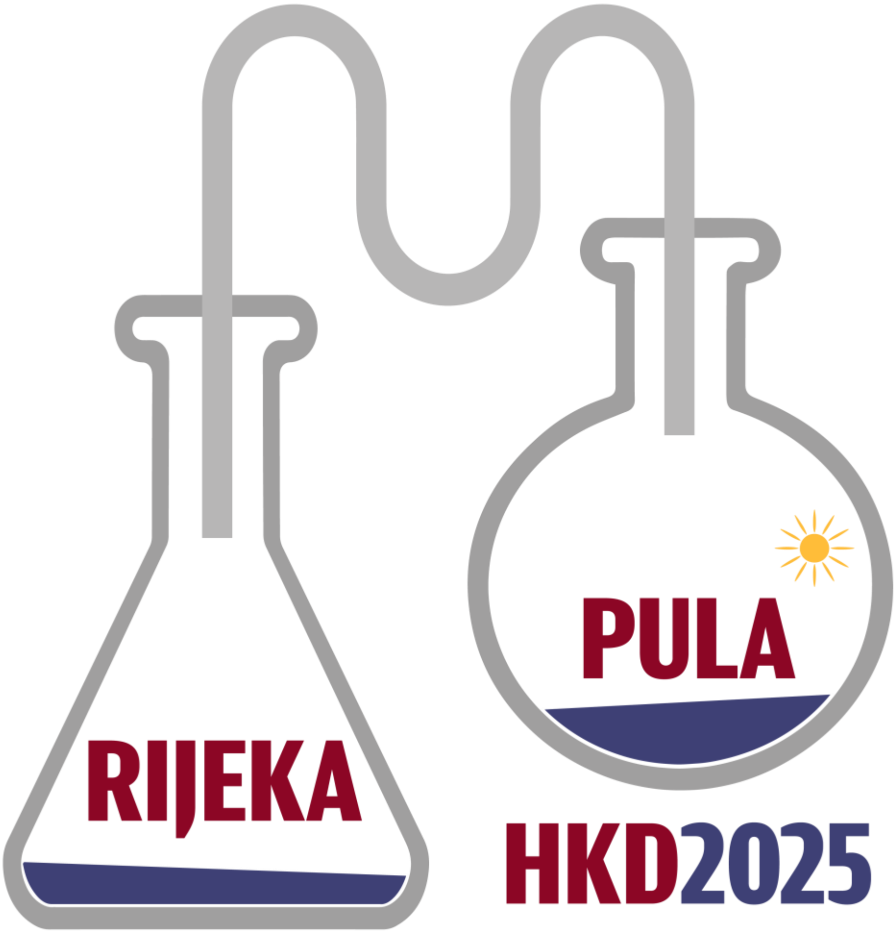
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DNA and RNA binding by bis-triarylborane dyes

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Bis-triarylborane dyes are a class of compounds known for their unique electronic properties, including strong fluorescence and the ability to interact with biomacromolecules such as nucleic acids and proteins. The tetracationic form of these dyes, in particular, has gained attention due to its potential to form stable, non-covalent complexes with DNA and RNA, enabling their applications in areas like biosensing and molecular diagnostics. Their high binding affinity and ability to stabilize nucleic acids make them valuable for investigating and understanding the interactions with biomacromolecules, which is essential for advancing bioorganic research. Moreover, the versatility of these dyes in binding different polynucleotides offers a wide range of opportunities for their use in various biotechnological and therapeutic applications [1].

In this study, we investigate the binding behavior of three novel bis-triarylborane tetracationic dyes with double-stranded DNA (ds-DNA) and RNA (ds-RNA) using a range of spectroscopic techniques, including UV-Vis absorption, fluorescence, thermal denaturation, and circular dichroism (CD). The dyes exhibit strong affinity toward both DNA and RNA, accompanied by slight bathochromic shifts in their UV-Vis spectra. CD spectroscopy indicates the formation of dye–polynucleotide complexes, correlated with changes in helicity. Thermal denaturation experiments show significant stabilization of DNA and RNA structures upon dye binding, with a stronger stabilizing effect observed for DNA. Furthermore, cytotoxicity assays in human lung cancer (A549) cells demonstrate negligible cytotoxicity across all tested concentrations.

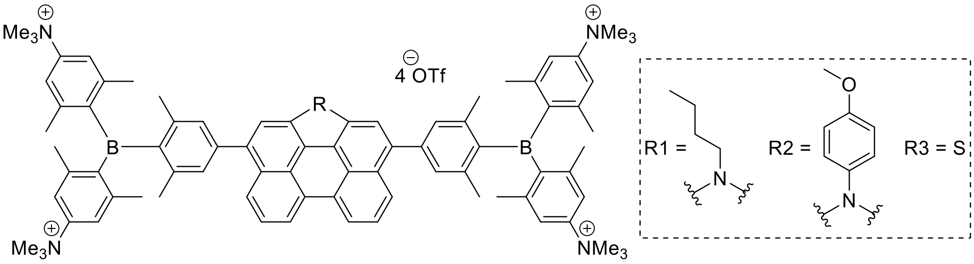

Fig. 1: Structures of new bis-triarylborane dyes C1, C2, and C3.

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Biocatalytic hirsutanonol production from biogenic oregonin

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Melanin pigmentation in human skin acts as a primary defence mechanism against ultraviolet (UV) radiation from sunlight. However, irregular pigmentation, including freckles and chloasma (such as liver spots and melasma), may present significant aesthetic and health concerns. The compound hirsutanonol proved to possess melanogenesis inhibitory activity [1]. Its enzymatic synthesis involves the hydrolysis of oregonin into hirsutanonol and xylose. The compound oregonin is a secondary metabolite of black elder tree and can be extracted from its bark. Due to utilization of natural resources for the efficient and environmentally friendly synthesis of valuable compounds, hirsutanonol can this way be labelled as "natural" and therefore can be readily offered to different markets and sectors [2]. Monte Carlo analysis (MCA) is a mathematical technique used to estimate the possible outcomes of an uncertain process by running many simulations using random inputs in order to understand the impact of risk and uncertainty in prediction and forecasting models [3]. In this study, the reaction of oregonin hydrolysis by RAPIDASE was observed. The kinetic parameters were estimated under the optimal conditions (T = 40 °C, ultra-pure water). To validate the developed mathematical model and estimated kinetic parameters, experiment was carried out in a batch reactor. Based on validated model, simulations were done and used for MCA.

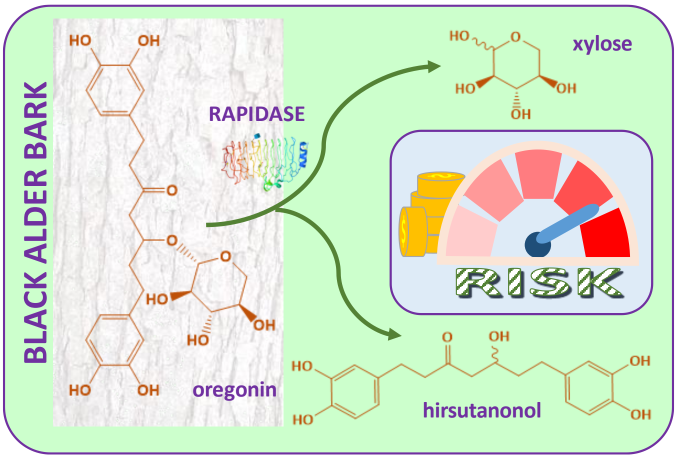

Fig. 1: Schematic overview of biocatalytic hirsutanonol production from the black elder secondary metabolite – oregonin.

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Optimization of a Vilsmeier reaction for the synthesis of oxime-forming stilbene intermediates

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In recent years, considerable attention has been directed toward the development of compounds for the treatment of neurological diseases such as Alzheimer's and Parkinson's, as well as organophosphate poisoning caused by pesticides and the misuse of nerve agents. Among these compounds, oximes have attracted significant interest due to their ability to reactivate the enzymes acetylcholinesterase and butyrylcholinesterase, the inhibition of which underlies these diseases. Biologically active oximes can be synthesized from stilbene derivatives by a two-step reaction in which a formyl group is introduced in the first step [1]. This formylation can be achieved via the Vilsmeier reaction, which employs a highly reactive and unstable Vilsmeier reagent that is usually formed in situ by mixing *N*,*N*-dimethylformamide (DMF) with phosphorus(V) oxychloride ($POCl_3$). The exothermic nature of the Vilsmeier reaction can lead to localized temperature spikes during batch processing and, in some cases, uncontrolled thermal degradation. To mitigate this risk, continuous millireactor systems are increasingly being considered as a sustainable alternative to conventional methods as they offer improved heat transfer efficiency [2]. In this study, the Vilsmeier formylation of a stilbene compound was investigated (Figure 1), as the resulting product serves as an intermediate for the synthesis of an oxime with proven bioactivity [3]. Reaction optimization was performed using Design of Experiments (DoE) in combination with Response Surface Methodology (RSM). After optimizing the yield, the reaction was carried out in a continuous millireactor to further improve heat transfer, productivity, and process control.

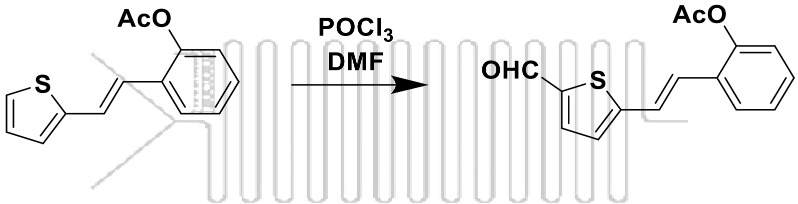

Fig. 1: Vilsmeier formylation of a stilbene compound.

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Development of FTIR method for molar ratio determination in PLGA copolymers

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In the past few decades, poly(lactide-*co*-glycolide) (PLGA) attracted much scientific and pharmaceutical attention owing to its biocompatibility and biodegradability, tunable mechanical properties and FDA approvement. In particular, it has been extensively studied for controlled delivery of small molecule drugs, proteins and other macromolecules in commercial use and research [1,2]. Moreover, parenteral PLGA-based drug delivery systems, which are excellent for controlled drug release, were studied in details [3]. Regarding its wide application, knowing chemical composition of PLGA is of paramount importance, for which various techniques could be utilized, including gel permeation chromatography (GPC) and mass spectrometry (MS), as well as nuclear magnetic resonance (NMR) and Fourier-transform infrared spectroscopy (FTIR) [4].

Although FTIR cannot give direct detailed information about molecular structure, it is often applied for the determination of polymers' composition owing to its simplicity, non-destructiveness, lesser equipment cost and reduced sample preparation. In the study, molar fractions of lactide and glycolide in the PLGA copolymers were determined in parallel using NMR and FTIR. Molar fractions obtained *via* FTIR and NMR were found to be within 2 % difference for all analyzed PLGA polymers. Hence, developed FTIR method could be utilized for the determination of lactide and glycolide molar fraction in PLGA copolymers (Figure 1).

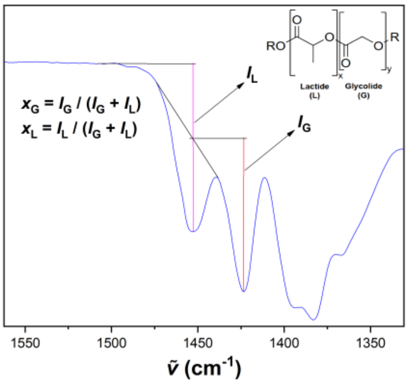

Fig. 1: Determination of glycolide and lactide molar fractions in PLGA polymers from FTIR spectrum.

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Effects of pH on mineralization of bulk alginate hydrogels containing metal or metal oxide nanoparticles

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Bone tissue defects affect millions of people worldwide, and with the increasing population, there is a rising demand for bone-like materials. One of the promising approaches to promote bone growth and healing is the development of innovative bone-mimicking materials [1]. For this purpose, alginate hydrogels were used in our research given their ability to mimic the extracellular matrix. To further improve their properties, the alginate hydrogels were biomimetically mineralized with calcium phosphates as described in our previous work [2]. The aim of this research was to optimize the conditions for the preparation of both non-mineralized and mineralized alginate hydrogels with incorporated nanoparticles (NPs) such as silver (AgNPs), copper oxide (CuONPs) and zinc oxide (ZnONPs). The addition of NPs was intended to minimize the risk of bacterial infection, and their incorporation into the matrices addressed potential cytotoxicity risks [3]. Mineralization of the hydrogels was carried out at pH 7.4 or 9.0, with the phosphate added to the alginate and calcium as the crosslinking agent. Characterization included Fourier-transform infrared spectroscopy (FTIR), powder X-ray diffraction (PXRD), scanning electron microscopy (SEM), inductively coupled plasma mass spectrometry (ICP-MS), rheological measurements and antibacterial assays. PXRD and FTIR confirmed the formation of calcium-deficient hydroxyapatite at pH 7.4 and amorphous calcium phosphate at pH 9.0. The incorporation of NPs influenced the morphology of the mineral phases. Early network breakdown was observed in mineralized hydrogels, with critical strain and ion release depending on pH and NP type. *Staphylococcus aureus* was inhibited with hydrogels prepared at pH 9.0, except for hydrogels with incorporated CuONPs. Overall, these results indicate the promising potential of biomimetic mineralization of alginate hydrogels and their use as controlled release systems, which could be of interest for bone tissue engineering.

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Biodegradable PBAT/PHBV blends: A path to sustainable food packaging

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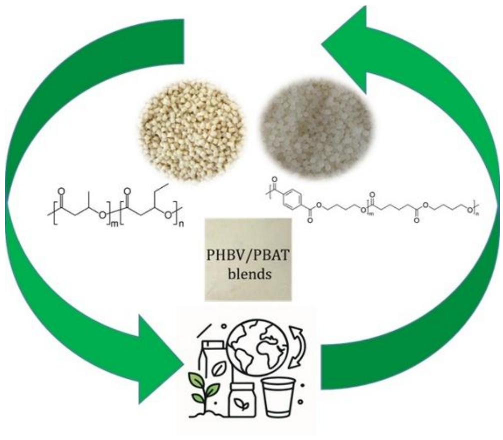
The increasing environmental impact of conventional plastics, especially in food packaging, is leading to an urgent need for biodegradable alternatives. Biodegradable blends based on poly(3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV) and poly(butylene adipate-co-terephthalate) (PBAT) are particularly promising as they combine the flexibility of PBAT with the commendable barrier and composting properties of PHBV. However, their immiscibility poses a challenge and compromises the mechanical, thermal, morphological and barrier properties. In this work, PHBV/PBAT blends were prepared in different ratios and subjected to thorough characterisation by thermal and morphological analyses, mechanical tests and gas and moisture permeability measurements. A higher PBAT content improved flexibility but slightly reduced heat resistance, while a higher PHBV content improved barrier properties, which is important for food safety. Morphological analysis showed how composition affects phase distribution and performance. This study highlights the relationships between composition, structure and properties of PHBV/PBAT blends and provides clear guidance for the development of biodegradable packaging tailored to food contact requirements. PHBV/PBAT blends have significant potential as sustainable food packaging materials. By adjusting the blend ratio, flexibility, barrier properties, and thermal properties can be customised without having to resort to petroleum-based plastics. The results support the development of environmentally friendly packaging solutions that meet current market requirements and comply with current EU regulations.



Acknowledgements*: This research was conducted as part of the project „Production and development of compostable packaging from waste biomass for the packaging of industrially processed food products” (NPOO.C3.2.R3-Il .04.0059) funded by National Recovery and Resilience Plan (funded by the EuropeanUnion, NextGenerationEU).*

TEMPO-containing smart nanoparticles for targeted induction of cancer cell death

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Cancer is one of the most important public health problems today. Classical anticancer drugs have numerous unwanted side effects such as cardiotoxicity, neurotoxicity, organ-specific toxicities and many others. Previous studies have shown that nitroxide radicals, such as 2,2,6,6-tetramethylpiperidin-1-oxyl (TEMPO), cause apoptosis of cancer cells and suppress tumor growth.[1] However, in *in vivo* conditions, these radicals accumulate non-specifically in normal tissue due to their low molecular weight and are rapidly excreted from the body.[2] We prepared a “smart” polymer nanoparticles with encapsulated nitroxide radicals and a pH-sensitive sensor that enables targeted induction of apoptosis in tumor cells. The pH-sensitive copolymer poly([*N*-(2-hydroxypropyl)]methacrylamide)-*b*-poly[2-(diisopropylamino)ethyl methacrylate] (PHPMA-*b*-PDPA) was synthesized and the corresponding nanoparticles containing encapsulated TEMPO radicals were prepared by using the microfluidic nanoprecipitation. The hydrodynamic radius of the nanoparticles was measured with dynamic light scattering. The shape and morphology of the nanoparticles were determined using cryo-transmission electron microscopy. *In vitro* research on the effect of nanoparticles was conducted on colorectal cancer cell lines (HCT 116) and non-cancer embryonic kidney cells (HEK 293). The effect of nanoparticles and pure nitroxide radicals on the viability of HCT 116 and HEK 293 was determined using XTT test. Protein expression of the molecular mechanisms involved in the induction of cytotoxicity of prepared nanoparticles on HCT 116 and HEK 293 was determined by Western blot analysis (LC3, p62, ATG-5, HO-1, SOD-1, GPX-1, PARP, casp-8, cl. casp-8, casp-9). This study is important to enable the targeted creation of nanoparticles for potential clinical application.

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Sorption of a pharmaceutical mixture onto molecularly imprinted polymer – kinetic study

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The development of the pharmaceutical industry has led to significant advances in the treatment of diseases, but at the same time to an increasing presence of pharmaceuticals in the environment, especially in soils and aquatic ecosystems. Apart from their primary therapeutic purpose, these compounds can disrupt the balance of ecosystems and pose a potential risk to human health. Therefore, it is of utmost importance to develop selective and efficient methods for their detection and removal from environmental matrices. In this study, a newly synthesized molecularly imprinted polymer (MIP) prepared from a mixture of three pharmaceuticals - procaine, sulfamethoxazole, and torasemide - was investigated as a selective sorbent for their detection and removal from environmental matrices. The sorption kinetics were analyzed at different time intervals at a constant concentration of pharmaceutical mixture to better understand the binding mechanism between the MIP and the target molecules. Based on the results obtained, it was found that the adsorption process most closely follows the pseudo-second-order kinetic model, suggesting that chemisorption is the dominant mechanism of removal. The optimum contact time for sorption was set at 24 hours. To ensure the reliability and comparability of the data regarding the efficiency of MIP in removing the target pharmaceuticals, a parallel kinetic analysis was performed using the corresponding non-imprinted polymer (NIP). As observed in previous studies, both materials exhibited similar sorption kinetics, while the MIP showed greater selectivity towards the target compounds. The results confirm that the new MIP, developed on the basis of a pharmaceutical mixture, is a promising solution for the effective simultaneous removal of multiple contaminants, an aspect that is particularly important in the context of complex environmental samples where different contaminants often co-occur.

Acknowledgement

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The use of TMS for determining absolute configuration of natural products bearing hydroxylic groups

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Compounds isolated from natural sources continue to make invaluable contributions across various fields of chemistry. Their elucidated structures often serve as starting points for the total synthesis of bioactive molecules. One of the most challenging steps in the painstaking process of separation and structural elucidation is the determination of absolute configuration. A method that can serve for this purpose is single-crystal X-ray diffraction (SCXRD) [1], but its key limitation is its dependence on the presence of heavier atoms to enhance anomalous dispersion, which is essential for unambiguous absolute configuration assignment.

In this work, we present a concept that combines a simple, robust, and selective molecular modification—silylation of hydroxylic groups using hexamethyldisilazane (HMDS) as a TMS source in nitromethane at room temperature, without additional catalysts [2] — with SCXRD. The introduction of the trimethylsilyl (TMS) group incorporates a silicon atom, which enhances anomalous scattering and improves the precision of structural refinement. This significantly increases the reliability of absolute configuration determination.

The method is broadly applicable to a wide range of compounds containing at least one hydroxylic group, encompassing a substantial portion of natural products. It offers a practical and general solution for improving absolute configuration determination in cases where suitable heavy atoms are otherwise absent.

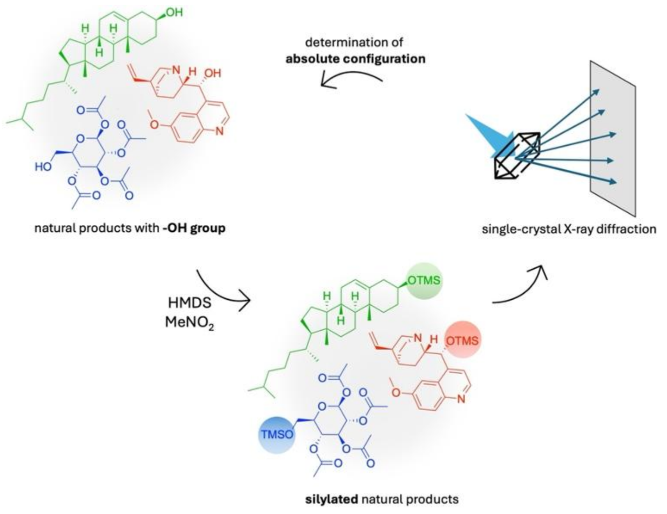

Fig. 1: Sylilation based method for absolute configuration determination using SCXRD.

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Sensor-integrated hydrogel simulating soft lung tissue for real-time monitoring in a lung-on-a-chip system

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Organs-on-chips offer a promising alternative to conventional *in vitro* and animal models by replicating the dynamic and structural complexity of human organs in microscale systems. Among them, the lung-on-a-chip stands out as a valuable platform for studying respiratory processes and testing inhalable drugs under physiologically relevant conditions. A critical component of such systems is the faithful replication of soft pulmonary tissue – particularly the alveolar region – where gas exchange and drug absorption occur.[1]

This study focuses on the development and evaluation of hydrogel-based materials designed to mimic the soft tissue of the lungs within a lung-on-a-chip device. Multiple hydrogel formulations were prepared and assessed to determine their suitability for simulating the biomechanical and functional characteristics of alveolar tissue. Key parameters were analyzed, including rheological properties to evaluate viscoelasticity and mechanical compliance, permeability to assess molecular transport, swelling behavior to capture hydration dynamics, and microscopic structure to verify morphological similarity to native tissue.

The goal was to identify a hydrogel that provides both structural fidelity and physiological relevance, thereby creating a more accurate *in vitro* environment for drug testing. Once optimized, a sensor for real-time monitoring of drug diffusion was incorporated into the selected hydrogel. As proof of concept, the integrated sensor was a flexible solid-state ion-selective electrode for pH determination, based on a plasticized PVC membrane. This sensor–hydrogel assembly was subsequently integrated into a lung-on-a-chip system, enabling simulation of the air-blood barrier and offering valuable insight into drug transport mechanisms following inhalation.

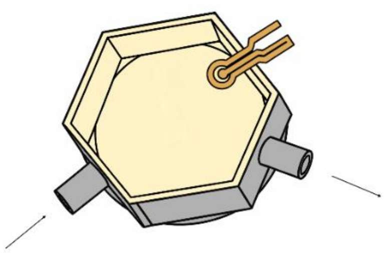

Fig. 1: Sensor-integrated hydrogel on a lung-on-a-chip system.

Acknowledgments: This work was funded by the Croatian Science Foundation through the project IP-2024-05-4339 entitled " *Coffee ring' effect in 'Lab on a Chip' environments in the development of new drug formulations.*" leader prof. Ernest Meštrović.

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Influence of API loading on the rheology of biodegradable polymer solutions

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Biodegradable copolymers are widely used in pharmaceutical applications, particularly valued for their tunable degradation profiles and excellent biocompatibility [1]. Understanding the rheological behavior of such polymer solutions is essential for optimizing processing methods including formulation of controlled release systems. The viscosity of polymer solutions is influenced by several key factors including the type of the solvent, polymer composition, its molecular weight and concentration level in the solution. In addition, the presence and the amount of an active pharmaceutical ingredient (API) can further affect the viscosity, by either increasing or decreasing it, depending on its interaction with the dissolved polymer in the solution [2]. Understanding these effects is essential for the formulation and optimization of polymer-based systems in pharmaceutical applications.

In this study, the focus is on evaluating how API incorporation affects the rheological behavior of polymer solutions. The presence of an API can modify polymer–solvent and polymer–polymer interactions influencing viscosity. Gaining insight into these effects is crucial for the development of robust and predictable drug delivery systems. This work aims to establish rheological analysis of API-loaded polymer solutions to support formulation optimization in pharmaceutical development [3].

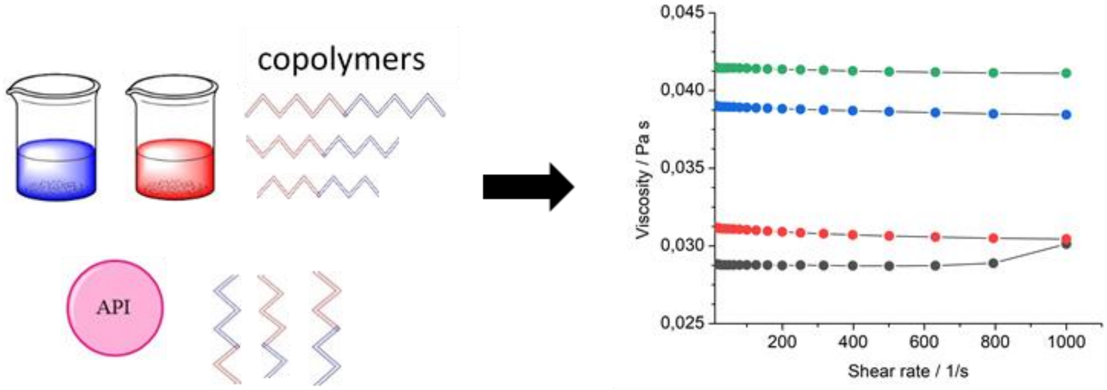

Fig. 1: Factors affecting the viscosity of a polymer solution – solvent, polymer composition, molecular weight and concentration in the solution (left). Viscosity vs. shear rate curves of different polymer solutions (right).

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Proximate Composition, Fatty Acid Profile and Trace Element Characterization of the Invasive Tunicate *Clavelina oblonga* in the Adriatic Sea

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Clavelina oblonga is an invasive tropical tunicate recently introduced into the Adriatic Sea, likely facilitated by anthropogenic influences and ongoing climate change [1]. Mussel aquaculture facilities offer highly favourable conditions for this colonial ascidian, where it has rapidly established itself as the predominant fouling species [2]. Its proliferation poses a competitive threat to mussels by monopolizing available substrate and food resources. Samples collected from January to December 2023 at the mussel farm in Lim Bay, Croatia, were analysed to gain a better insight into their biological properties, proximate composition, fatty acid profile and trace element characterisation. Proximate composition showed water (moisture) as the main component with 95.44%, followed by 39.2% proteins, 29.1% ash and 8.6% lipids [3]. The lower ash content compared to other tunicates could be related to the lower salinity of seawater caused by freshwater inflow in Lim Bay. The major fatty acids were palmitic acid, stearic acid and docosahexaenoic acid, followed by docosanoic acid, elaidic acid, linoleic acid and myristic acid. The three groups of fatty acids: saturated fatty acids (SFA), polyunsaturated fatty acids (PUFA) and monounsaturated fatty acids (MUFA) accounted for 51.37, 26.96 and 15.41%, respectively. Total unsaturated fatty acids (UFA) accounted for 42.37%. The proximate and fatty acid composition of *C. oblonga* suggests that it could be a valuable source of nutrients. The concentration (μg/g dry weight) of trace elements such as aluminium (Al), iron (Fe), strontium (Sr), titanium (Ti) and manganese (Mn) was found to be predominant and, as expected, exceeded the concentration found in seawater. *C. oblonga* had a lower concentration of arsenic (As) and a higher concentration of lead (Pb) than the mussels it fouls in Lim Bay. *C. oblonga* reaches its maximum dispersal and biomass in mid-autumn, although it could become permanently established in the Adriatic, which could initially have a significant impact on mussel farming and later on the local ecosystem. On the other hand, the results of this study suggest that *C. oblonga* could serve as a sustainable biomass and protein source for various feeds.

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Design of an Extended-Release Indomethacin Formulation using Crystal Engineering

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Indomethacin is a nonsteroidal anti-inflammatory drug used to relieve pain, inflammation, and stiffness associated with conditions such as osteoarthritis, rheumatoid arthritis, gout, and bursitis, as well as for the treatment of certain types of headaches. Despite its broad therapeutic applications, its use is limited due to serious side effects, including an increased risk of cardiovascular and cerebrovascular events, gastrointestinal issues such as ulcers, bleeding, or perforations of the stomach and intestines, and the need for frequent dosing due to its short elimination half-life. [1]

To improve the therapeutic profile of indomethacin and reduce the risk of side effects, research has focused on the development of an extended-release formulation based on the principles of crystal engineering and non-covalent interactions in combination with biodegradable polymers. The goal is to create a stable pharmaceutical formulation that enables controlled drug release and reduces dosing frequency.

Structural data analysis from the CCDC database identified key supramolecular synthons that support stable non-covalent interactions within the formulation. Based on these insights, indomethacin cocrystals were prepared with suitable coformers selected for their potential to form stable hydrogen bonds, π-π interactions, and other non-covalent forces.

Using mentioned formulations in our research, we can significantly improve the release profile of indomethacin, enabling better therapeutic control and reduced dosing frequency

This approach highlights the potential of crystal engineering as a modern and sustainable strategy in the development of extended-release drug formulations tailored to the needs of contemporary pharmacotherapy.

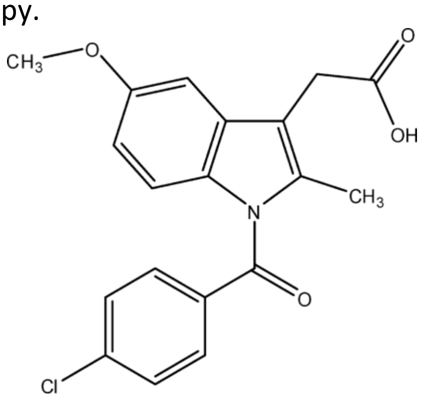

Fig. 1: Molecular structure of indomethacin

Acknowledgments: *This paper was funded by the Croatian Science Foundation through the project IP-2024-05-4339 entitled " Coffee ring' effect in 'Lab on a Chip' environments in the development of new drug formulations." leader prof. Ernest Meštrović.*

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Toward cyclic peptides: linear tetratyrosine precursor for chloride-templated cyclization

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Peptides are essential biomolecules whose diverse biological roles are often limited by their susceptibility to enzymatic degradation and poor structural stability. Cyclization offers a strategy to overcome these limitations, as cyclic peptides typically have improved metabolic stability, enhanced bioavailability, and greater target selectivity compared to their linear analogs. However, the cyclization of short peptides is often synthetically challenging due to conformational constraints, sequence-dependent inefficiencies and low yields [1,2]. It was previously demonstrated that chloride anions can act as templating agents by forming non-covalent interactions with nitrogen from backbone amides, thereby facilitating the alignment of peptide termini for efficient ring closure [2]. To demonstrate the method's applicability to amino acids with bulky side chains, a linear tetratyrosine precursor containing a *tert*-butyl (*t*Bu) side-chain protecting group was synthesized using solution-phase peptide synthesis. Through optimization of iterative coupling and deprotection reactions, the linear precursor was obtained and its structure was confirmed by ^{1}H and ^{13}C NMR spectroscopy. This peptide will serve as a precursor for the synthesis of linear penta- and hexatyrosines, as well as the foundation for testing the Cl$^-$-assisted macrocyclization strategy on tyrosine. Future work will focus on physicochemical characterization of cyclic tetra-, penta-, and hexatyrosines, as well as studies of their anion-binding properties using microcalorimetry and ^{1}H NMR titrations [3].

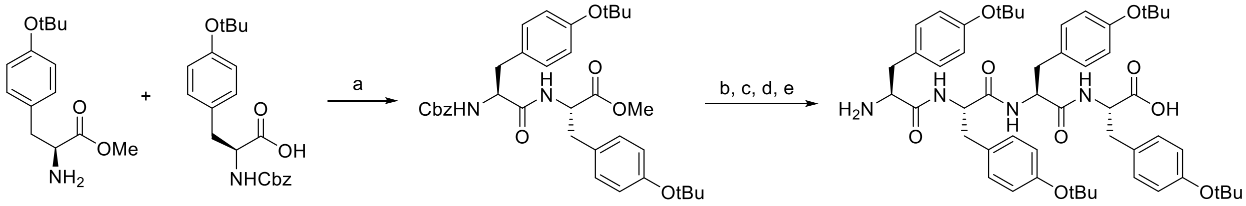

Fig. 1: Synthesis of linear tetratyrosine. (a) HOBt, HBTU, TEA, DMF; (b) LiOH, MeOH/H_2O; (c) Tyr(OtBu)-OMe, HOBt, HBTU, TEA, DMF; (d) NH_4HCO_2, Pd/C, MeOH; (e) Cbz-Tyr(OtBu)-OH, HOBt, HBTU, TEA, DMF. Steps d and e were repeated two times to obtain fully protected tetratyrosine. Subsequently, steps d and b were repeated to remove Cbz and methyl ester protecting groups, respectively.

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Synthesis of diamondoid pyrogallol derivatives

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Diamondoid [1] analogues have been in our continued focus due to their unique properties and highly symmetrical structures. For example, we studied them as photoactive molecules [2] and we also constructed their covalent assemblies [3] applicable in nanomaterial design. Now we turned our attention to the study of diamondoid scaffolds in micellar capsule architectures. It is known that capsule assembly of adamantane derivatives proceeds through the hydrophobic effect and van der Waals interactions, with a unique wide ranging host ability toward spherical molecules in water [4]. Our goal is therefore to prepare a series of diamantane-bearing analogues and test them for their ability to form micellar capsules.

The envisioned derivatives are composed of two hydrophobic diamantane moieties connected to a pyrogallol spacer. On the opposite side, the pyrogallol moiety bears three *N*,*N*-dimethylaminoethyl groups as hydrophilic pendants (Figure 1). The key difference between the two planned molecules is in the substitution position of the diamantane cage (apical *vs.* medial). Although the synthesis of the adamantane analogue has been reported [4], the synthesis of diamantane derivatives has proven to be quite demanding and new synthetic routes had to be developed. This nicely demonstrates different behavior in the synthesis for adamantane and diamantane cages, as well as the different reaction pathways of apical and medial positions of diamantane.

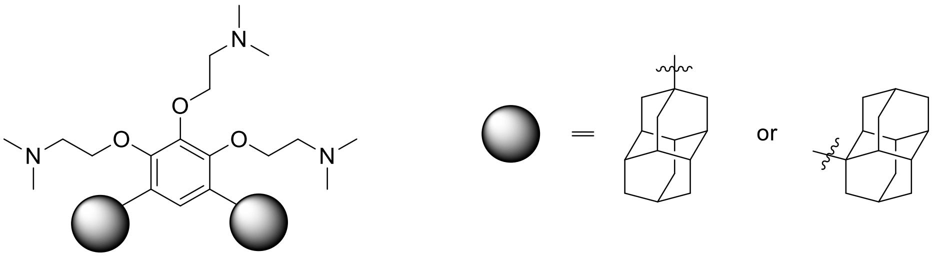

Fig. 1: Diamantane derivatives for use as micellar capsules.

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ERK signaling pathway involvement in free mitochondria transfer

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Mitochondria play an important role in metabolism, and their primary function is aerobic respiration and the creation of ATP to meet the energy needs important for cell survival. Mitochondrial dysfunction plays a key role in a wide range of diseases including tumors. Mitochondrial transfer is a novel and intriguing mechanism in intercellular communication and is a promising approach to achieving intercellular energy synchronization. The activity of extracellular signal-regulated kinases (ERK) is involved in various signaling pathways, and their role in mitochondrial transfer has not been investigated. Given that active ERK localizes to mitochondrial membranes and participates in cytoskeleton reorganization, modification of its activation could play a key role in creating effective mitochondrial transfer therapy in various diseases. We established *in vitro* models of mitochondrial transfer (HEK293, HK-2, and HeLa cells) and created ρ0 cell lines that lack mtDNA (HCT116, SW620, HK-2, HeLa) and are unable to support normal oxidative phosphorylation. ρ0 cell lines mtDNA content was determined by qPCR analysis. We monitored the success of mitochondrial transfer with modification of ERK activation in the mitochondrial transfers. Furthermore, glucose consumption and lactate production during a mitochondrial transfer protocol are determined which is crucial for several reasons, primarily related to assessing cellular metabolism, mitochondrial function, and the efficiency of the transfer process. Also, we monitored JC-1 (a mitochondrial membrane potential-sensitive dye) in mitochondrial transfers to assess whether the transferred mitochondria are functionally active, as a shift from red (aggregates, high $\Delta\Psi m$) to green fluorescence (monomers, low $\Delta\Psi m$) indicates loss of membrane potential and impaired mitochondrial health. We are still determining the transfer mechanism dependent on ERK by monitoring protein expressions (HSP-60, TOM20, p-ERK, ERK, TFAM, VDAC3, p-PDH, PDH, p-AMPK, Bcl-2, Bax). This research is of utmost importance to elucidate the mechanisms and develop safe and effective mitochondrial transfer approaches in clinical use.

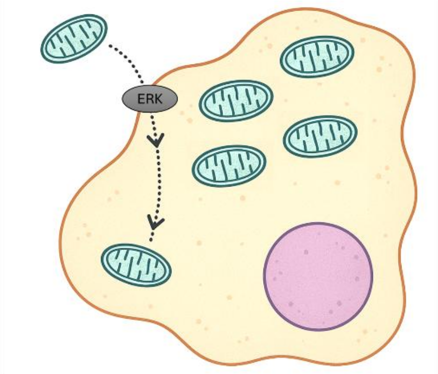

Fig. 1: This illustration depicts the process of free mitochondrial transfer into a cell and highlights the regulatory role of ERK (extracellular signal-regulated kinase). The image shows mitochondria entering the cell from the extracellular space.

Design and biological evaluation of a bipyridine-based copper(II) complex with enhanced cytotoxicity

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Coordination compounds of transition metals are increasingly recognized as key scaffolds for the development of new bioactive molecules due to their adaptable structures and tunable ligand environments. Among the most effective ligands, 2,2'-bipyridine (bipyridine; L1) is characterized by its strong chelating ability forming stable and planar complexes with various metal ions. This chelation not only determines the structural geometry but also modulates the electronic properties of the complex, allowing fine control over properties such as cytotoxicity, solubility and membrane permeability.[1-3] In this study, the cytotoxic activity of complex 1, a bipyridine-containing coordination compound, was investigated *in vitro* on the human liver carcinoma cell line Hep G2. The compound exhibited pronounced dose-dependent cytotoxicity with an average IC_{50} value of 15.28 µM, demonstrating notable antiproliferative potential. In contrast, the free ligand L1 showed reduced cytotoxicity (IC_{50} = 56.93 µM), while the corresponding metal salt, copper(II) nitrate trihydrate (S1), was substantially less active (IC_{50} = 438.60 µM). These differences underline the marked improvement in biological resulting from metal-ligand complexation.

Presented results emphasize the crucial role of bipyridine as both structural and electronic modulator in the rational design of metal-based therapeutics. Coordination with L1 in complex 1 significantly improved cytotoxicity against Hep G2 cells, highlighting its potential as a promising candidate for further pharmaceutical investigation. The comparative data support the utility of bipyridine in the development of potent and selective metal-based drugs.

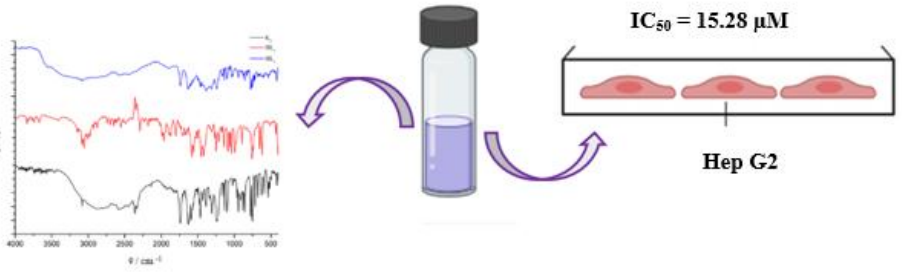

Fig. 1: Schematic representation of the cytotoxic evaluation of a bipyridine-based complex.

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The influence of desialylation on the binding of holo-transferrin and transferrin receptor investigated by microscale thermophoresis

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Terminal sialylation of N-glycans can exert significant influence on protein conformational dynamics and intermolecular interactions. Human serum transferrin (Tf) and its receptors (TfR1, TfR2) are extensively sialylated glycoproteins central to systemic iron transport. Upon binding diferric Tf (holo-Tf) at physiological pH, the holo-Tf–TfR1 complex undergoes clathrin-mediated endocytosis. Within endosomes, iron is released in response to acidic pH, and apo-Tf is recycled to the extracellular milieu [1]. While the iron- and protein-dependent features of this interaction are well characterized, the contribution of glycosylation, and particularly terminal sialylation, remains insufficiently defined.

Recent studies have demonstrated that enzymatic desialylation of Tf enhances Fe(III) affinity by three- to ten-fold, indicating a shift in conformational stability and iron release dynamics [2,3]. Although structural and thermodynamic analyses have mapped key binding determinants within the Tf–TfR1 complex, they have largely overlooked the potential role of glycans in modulating this interaction [4,5].

In this work, we employed microscale thermophoresis (MST) to quantify the binding of native and desialylated holo-Tf to recombinant His-tagged TfR1. Desialylation of holo-Tf was achieved using a commercial neuraminidase. MST measurements revealed that native holo-Tf binds TfR1 with a dissociation constant $K_D \approx 1$ μM. In contrast, no detectable binding was observed for desialylated holo-Tf, indicating that terminal sialic acid residues are critical for receptor recognition under near-physiological conditions.

These findings provide the first direct quantitative evidence that terminal sialylation significantly modulates holo-Tf–TfR1 binding affinity, likely by influencing local electrostatic interactions or glycan-mediated steric complementarity. This work highlights the importance of glycosylation in iron homeostasis and supports future strategies for glycoengineering Tf variants for therapeutic applications in iron dysregulation and targeted drug delivery.

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Rotational spectroscopy and computations of adamantyl esters and ethers

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Adamantane, the smallest diamondoid analogue,[1] can be a useful building block when designing new materials. However, to fully realize its potential of forming complex structural architectures, one needs to understand the molecular structure of its derivatives and gain insight into their structure-properties relationship. We have therefore investigated several classes of adamantyl covalent assemblies where the adamantane cage is bound to different heteroatoms/functional groups in order to determine exact experimental structures of the compounds and compare their properties as a function of the substituent. We have previously studied series of ether[2] and thioether[3] derivatives and now we turn our attention to esters[4]. By combining high-resolution rotational spectroscopy and computations we investigated five previously unexplored esters and ethers featuring an adamantyl group combined with alkyl substituents of increasing branching. The studied molecules are rigid with only one conformation predicted in the gas phase, resulting in relatively symmetric structures. The bond distances and angles determined experimentally showed an excellent agreement with those predicted by computations, thus advancing our knowledge of variously substituted adamantyl derivatives in the gas phase.

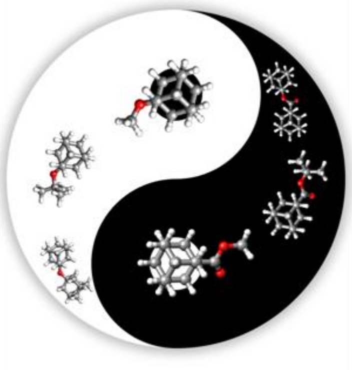

Fig. 1: Structural study of adamantyl esters *vs*. ethers.

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Expanding chloride-templated cyclization through ornithine-derived peptides

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Peptides are crucial biomolecules used as therapeutics due to their high selectivity and potent biological activity [1]. Among them, cyclic peptides show significant advantages over their linear analogues, such as better metabolic stability, higher bioavailability, and enhanced substrate-binding affinity [2]. However, despite their potential, the synthesis of cyclic peptides remains challenging due to low reaction yields, formation of undesired side products, and conformational constraints. According to our previous work, these limitations were addressed through a novel, efficient method that utilizes chloride anions for peptide head-to-tail cyclization, improving cyclization efficiency while minimizing epimerization and oligomerization [3]. The ultimate goal of this research is to synthesize cyclic tetra-, penta-, and hexapeptides containing L-ornithine to demonstrate that chloride-templated cyclization can be applied to a broader range of peptides. To accomplish this, linear tetraornithine with Boc-protected side chains was synthesized using solution-phase peptide synthesis. This peptide will act as a precursor both for tetrapeptide cyclization and for the preparation of linear penta- and hexaornithines. Successful cyclization of ornithine would demonstrate the applicability of this method to a broader variety of peptides containing diverse amino acid residues. Finally, the obtained cyclic peptides will be subjected to ^{1}H NMR and microcalorimetric titrations to gain deeper insight into their anion-binding behavior.

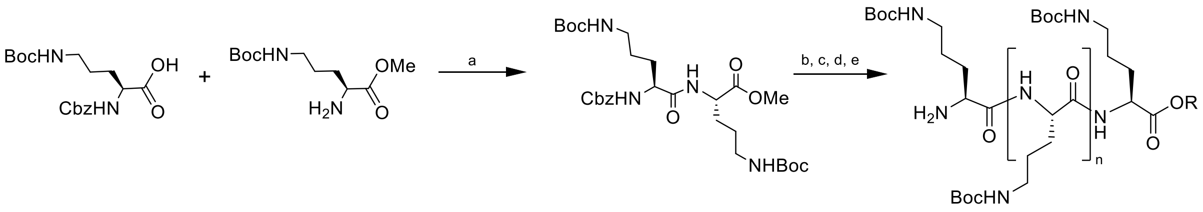

Fig. 1: Synthesis of linear L-ornithine tetrapeptide: (a) HOBt, HBTU, DMF, TEA; (b) LiOH, MeOH, H_2O; (c) Orn(Boc)-OMe, HOBt, HBTU, DMF, TEA; (d) NH_4HCO_2, Pd/C, MeOH; (e) Cbz-Orn(Boc)-OH, HOBt, HBTU, DMF, TEA. Steps d and e were repeated two times, followed by steps b and d in order to synthesize tetraorhnitine without Cbz and OMe.

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Natural allies against chemoresistance: oleanolic and betulinic acid in colorectal cancer cells HCT116

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Colorectal cancer remains one of the leading causes of cancer-related deaths worldwide. Despite the availability of chemotherapeutic agents such as 5-fluorouracil (5-FU), treatment efficacy is often compromised by chemoresistance, tumor recurrence, and adverse side effects. Natural compounds, particularly triterpenoids like oleanolic acid and betulinic acid, are emerging as promising candidates for enhancing cancer therapy. This study aimed to investigate the molecular mechanisms of oleanolic acid and betulinic acid in colorectal cancer treatment and to evaluate their ability to sensitize HCT116 cancer cells to 5-FU. *In vitro* experiments were performed using the HCT116 colorectal cancer cell line. Cell viability was assessed via XTT assay. Western blotting was used to analyze protein expression. Apoptosis, autophagy, and mitophagy were evaluated by fluorescence microscopy. Autophagy inhibitors were employed to explore the functional significance of autophagy in treatment response. Both oleanolic acid and betulinic acid exhibited significant cytotoxicity in HCT116 cells. Oleanolic acid triggered oxidative stress, apoptosis, and autophagy via activation of p38 MAPK and AMPK, alongside inhibition of mTOR. It also upregulated SIRT6 expression and promoted FOXO3a nuclear translocation. In contrast, betulinic acid primarily induced autophagy without initiating apoptosis and activated the Akt pathway. Notably, both compounds enhanced chemosensitivity to 5-FU, reducing cancer cell viability more effectively in combination treatment. Oleanolic acid exerts anticancer effects through the p38/FOXO3a/SIRT6 signaling axis, promoting both apoptosis and autophagy. Betulinic acid, while not proapoptotic, induces autophagy and engages survival pathways. These findings suggest that both compounds hold promise as adjuvants in colorectal cancer therapy by enhancing the efficacy of conventional chemotherapy.

Keywords: Colorectal cancer; 5-Fluorouracil; Oleanolic acid; Betulinic acid; Apoptosis; Autophagy; Chemosensitization

Quantum tunnelling in the low-lying water hexamer isomers

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Studying water clusters is of great importance because the behavioral essence of intermolecular forces between the water molecules mimics that of the bulk. The water hexamer is a particularly interesting water cluster to investigate both experimentally and theoretically because it is the smallest one with a 3D structure, often called the smallest water droplet. The energetically lowest structural isomers detected experimentally are prism, cage, and book [1]. Tunneling splittings (TSs) of these isomers are calculated using the modified WKB (Wentzel–Kramers–Brillouin), a semiclassical method based on instanton theory [2]. The method starts with finding the minimum action path, along which the semiclassical wavefunction is constructed and inserted into the Herring formula, yielding tunneling matrix elements. Finally, splittings are obtained by diagonalizing the tunneling matrix. TSs in the water hexamer prism are determined for a number of excited low-frequency vibrational modes. Internal rotation of a double-donor water monomer is identified as the mechanism that potentially plays a role in the appearance of the TS pattern in vibrationally excited states in addition to the mechanisms that shape the TS pattern in the ground state. The ground-state TSs of the water hexamer cage were found to form a doublet of doublets. The finer splitting is two orders of magnitude smaller due to a significant difference in the barrier heights for bifurcations of the water monomers at the two opposite vertices of the cage. First estimates of the ground-state TSs in the water hexamer book structure are also calculated. The TS pattern is again a doublet of doublets, caused by the monomer motions on one side of the book isomer. The wider doublet is of similar size to that in the cage and the narrower doublets an order of magnitude larger than that in the cage.

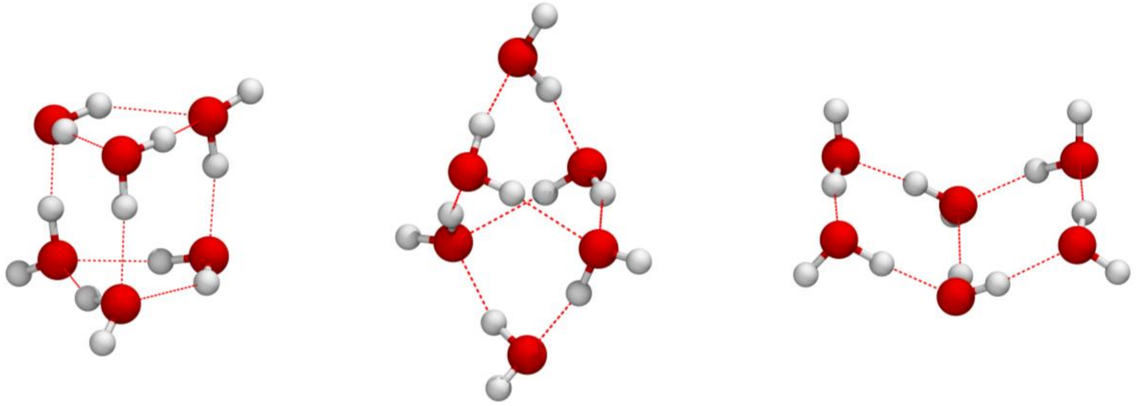

Fig. 1: The lowest-energy structural isomers of the water hexamer: prism (left), cage (middle) and book (right).

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Optimization of hydrogenase extraction from *Ralstonia eutropha* H16 cultivated on biodiesel-derived glycerol

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Glycerol is an important by-product of industrial biodiesel production, usually obtained by transesterification of vegetable oils and animal fats using chemical catalysts and alcohol.[1] Although crude glycerol is obtained in this process, the use of enzymatic catalysis instead of chemical catalysts offers a more environmentally friendly alternative and provides high-purity glycerol suitable for direct use in biotechnological processes.[2] One promising application of this glycerol is its use as a carbon source for the cultivation of bacteria that can produce the enzyme hydrogenase, a key enzyme in biohydrogen production.

The aim of this study is to utilize glycerol from different sources (chemical and enzymatic biodiesel production as well as commercial glycerol) for the cultivation *of Ralstonia eutropha* H16. A sustainable microbial process was developed and the extraction of the hydrogenase from the bacterial cells was optimized. Efficient extraction is crucial as unsuitable methods can compromise the integrity of the enzyme and reduce activity. For this reason, three strategies (permeabilization, ultrasonic treatment and their combination) were investigated for their effects on enzyme yield and biological activity.

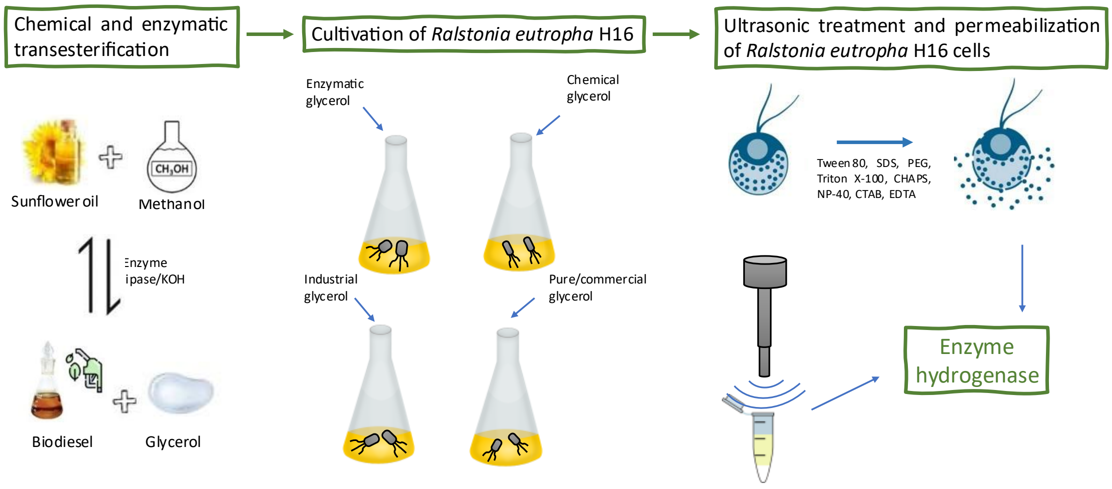

Fig. 1: Cultivation of *R. eutropha* H16 on different glycerol sources and optimization of hydrogenase extraction

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New trends in the sustainable treatment of highly contaminated wastewater

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The remediation of highly contaminated wastewater remains a major challenge for sustainable water management. Conventional physico-chemical methods are often costly, energy-intensive and generate secondary pollutants. Bioremediation represents a viable alternative by utilizing the metabolic potential of microorganisms to degrade contaminants and convert them into non-toxic forms [1]. In this study, an integrated bioremediation strategy combining biostimulation and bioaugmentation of indigenous microbial communities with advanced biotechnological tools was investigated. The focus is on the treatment of industrial wastewater using customized microbial consortia. Genetically enhanced microbial strains exhibit improved substrate specificity and degradation efficiency and show better performance with variable and heavy pollutant loads. The results emphasize the potential of combining natural microbial processes with synthetic approaches to improve treatment outcomes [2]. Integrated systems improve the efficiency and selectivity of pollutant removal and pave the way for more sustainable and robust solutions for the treatment of industrial wastewater.

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Predicting the outcome of thermal reactions by quantum-chemical calculations

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Computational methods [1] play a key role in modern chemistry, enabling detailed analysis and understanding of chemical reactions at the molecular level. Thanks to the rapid development of information technologies during the last few decades, computational chemistry [2] is becoming an equal and necessary collaborator of experimental research, which enables the calculation and prediction of almost all chemical and physical properties of molecules and their interactions [3], giving a deeper insight into the nature of the chemical process and the explanation of the obtained experimental data.

In order to obtain new polycyclic systems and provide a detailed insight into the reaction mechanism, as a part of this study, various thienyl and phenyl derivatives of *o*-divinylbenzene were synthesized and conducted to thermal reaction in acidic medium. Several derivatives led to cyclization products when heated under acidic conditions, while some were found to be non-reactive. The outcome of the thermal transformation is closely related to the structural modifications of the initial precursors and protonation position of the initial structures. DFT calculations have been used to predict the entry of protons, thus successfully predicting the outcome of the reaction itself.

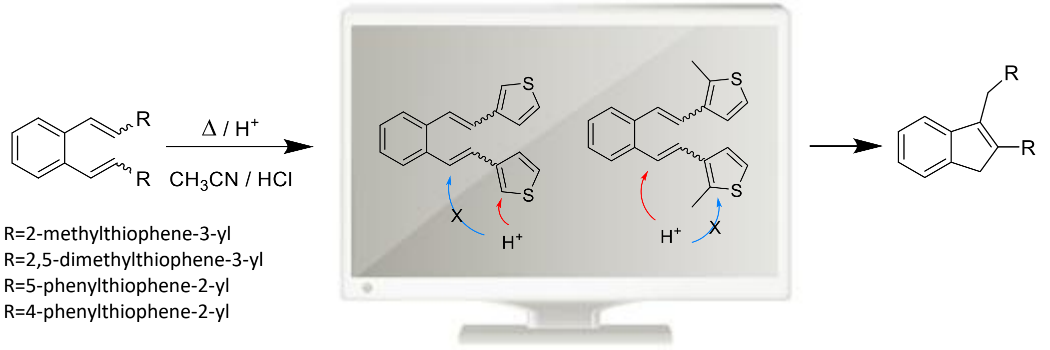

Fig. 1: Thermal transformations of *o*-divinylbenzene derivatives.

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Crystal structure and surface properties of azithromycin solvates: implications for taste prediction

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Azithromycin is a clinically relevant macrolide antibiotic; however, its pronounced bitterness, attributed to interactions between crystal surfaces and taste receptors, presents a major challenge in the development of palatable oral dosage forms, particularly for pediatric use. This study investigates a series of azithromycin crystalline solvates incorporating water and one of four organic solvents: cyclohexane, 1,4-dioxane, tetrahydrofuran (THF), or methyl tert-butyl ether (MTBE).

Single-crystal X-ray diffraction was employed to elucidate the crystal structures, revealing distinct solvent inclusion patterns, hydrogen-bonding networks, and packing motifs. To assess the impact of structural variation on surface properties, we analyzed the identity and spatial distribution of surface-exposed functional groups potentially involved in receptor interactions.

Predicted crystal morphologies, obtained using the Morphology module in Mercury based on the Bravais–Friedel–Donnay–Harker (BFDH) model, identified dominant crystal faces likely to be expressed during growth. These data provided insight into the anisotropic presentation of chemical functionalities, relative surface polarity, and wettability.

The results support a structure–property relationship whereby specific surface characteristics—shaped by crystal packing and solvent incorporation—may modulate taste perception. These findings provide a framework for rational taste-masking strategies via solid-form selection in the early stages of formulation development [1].

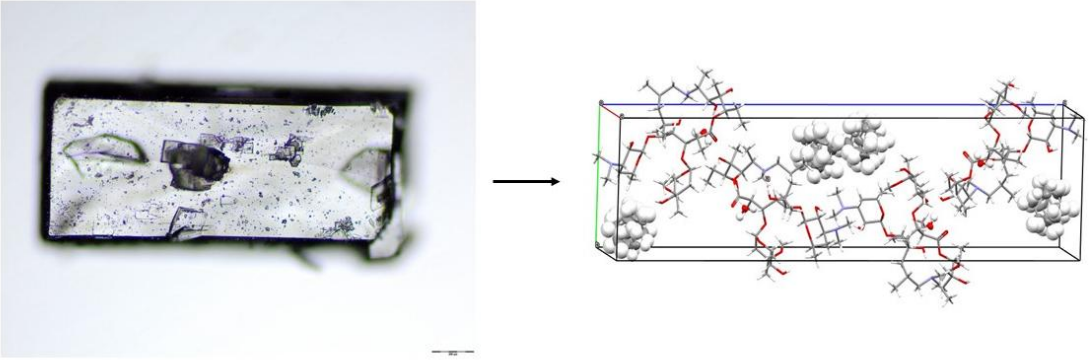

Fig. 1: Crystal of the cyclohexane solvate and its crystal structure.

Acknowledgments: *This paper was funded by the Croatian Science Foundation through the project IP-2024-05-4339 entitled " Coffee ring' effect in 'Lab on a Chip' environments in the development of new drug formulations." leader prof. Ernest Meštrović.*

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Evaluation of the ecotoxic effect of antivirals using the marine bacterium *Vibrio fischeri*

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Environmental contamination by pharmaceutical residues, particularly antiviral drugs, has emerged as a growing ecological concern due to their widespread use and resistance to degradation. These compounds are predominantly introduced into aquatic environments through domestic, hospital, and industrial wastewater. Owing to their complex chemical structures, antiviral drugs exhibit high persistence and are often inadequately removed by conventional wastewater treatment technologies, resulting in their accumulation in water bodies and sediments, with potential adverse effects on aquatic ecosystems. The surge in antiviral consumption during the COVID-19 pandemic has further underscored the urgency of evaluating their ecotoxicological impacts. [1,2] This study aimed to assess the ecotoxicity of four commonly used antiviral agents—ritonavir (RIT), lopinavir (LOP), remdesivir (REM), and daclatasvir (DAC)—using the marine bioluminescent bacterium *Vibrio fischeri* as a test organism. The tested concentrations were based on the maximum solubility of each drug in water: 0.0022 mM (RIT), 0.0025 mM (LOP), 0.0023 mM (REM), and 0.1000 mM (DAC). In addition to individual compounds, equimolar (50:50) binary mixtures were tested to explore potential synergistic or antagonistic interactions. The results demonstrated varying levels of toxicity, with the order of ecotoxic potency as follows: RIT > LOP > REM > DAC. Ritonavir exhibited the highest inhibition of bioluminescence (INH = 82.96%), with corresponding effective concentrations of EC_{20} = 0.00033 mM and EC_{50} = 0.00089 mM, indicating high acute toxicity. Daclatasvir showed the lowest toxic effect (INH = 22.69%, EC_{20} = 0.10114 mM). Furthermore, antagonistic interactions were observed in mixtures containing RIT, LOP, and REM, while DAC exhibited synergistic effects in combination. The most toxic binary mixture, based on the lowest EC_{50} value (0.0010 mM), was identified as the combination of LOP and REM.

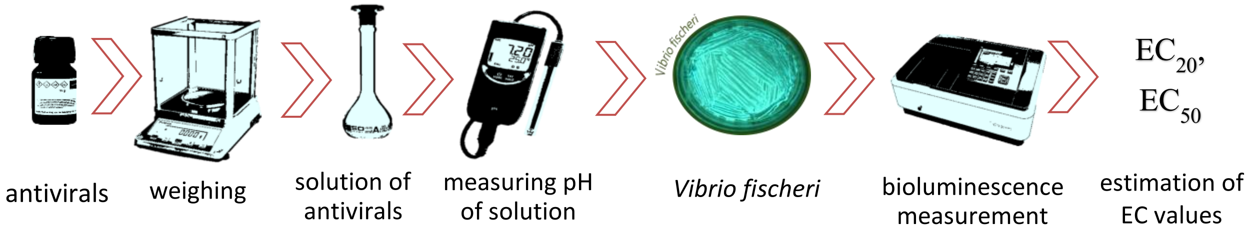

Fig. 1: Scheme of the ecotoxicity test with the bacterium *Vibrio fischeri*.

Acknowledgements: This work has been supported by the Croatian Science Foundation through the project entitled Environmental Aspects of SARS-CoV-2 Antiviral Substances (EnA-SARS, IP-2022-10-2822).

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Fluorimetric Studies of Cation-Binding Reactions of Calixarenes Lacking Fluorescent Substituents

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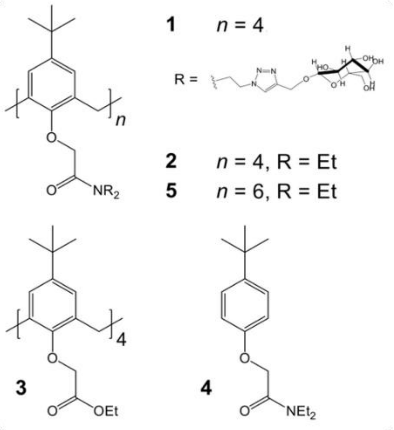
Calixarenes have been widely investigated as fluorescent sensors, [1] though their luminescent properties have traditionally been associated only with derivatives suitably functionalized with fluorescent groups. [2] In this study, the intrinsic fluorescence of several calix[4]- and calix[6]arenes without additionally introduced fluorophores was examined, along with the corresponding cation-binding induced fluorescence changes in water, acetonitrile, and methanol. Despite the low intrinsic luminescence of the studied compounds, a significant fluorescence enhancement was observed upon their complexation with alkali and alkaline earth metal cations. In contrast, for monomeric compound **4**, which constitutes tertiary-amide calixarene derivative **2**, an opposite trend was noticed. The results of excited-state lifetime measurements and quantum chemical calculations provided insight into the emission mechanisms and explained the differences between photophysical properties of the ligands and their cation complexes. Overall, the obtained findings highlight the potential of employing the intrinsic fluorescence of calixarenes for sensitive and quantitative monitoring of cation-complexation processes, enabling the use of rather low ligand concentrations and the determination of quite high complex stability constants by means of direct fluorimetric titrations.



Acknowledgements. This research was funded by Croatian Science Foundation projects CalixCORE (IP-2024-05-3012), POC-Sens-Bioact (IP-2022-10-9829), PhInMol (IP-2022-10-4658), MicroSynTotal (IP-2024-05-5352), NextGenerationEU program (NPOO.C3.2.R2-I1.06.0043), and the European Regional Development Fund infrastructural project CIuK, Grant No. KK.01.1.1.02.0016).

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Imagine-based analysis of the coffee ring effect to evaluate pantoprazole-excipient interactions

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The coffee ring effect, where particles migrate to the edges of an evaporating droplet forming ring-like deposits, offers a novel approach to study molecular interactions in pharmaceutical formulations. This work investigates whether the drying patterns of pantoprazole, a proton pump inhibitor, reveal stabilizing interactions when combined with different excipients. Pantoprazole solutions, alone and with excipients, were deposited on glass slides and dried under controlled conditions. The stains were imaged using light microscopy. Image analysis in Python - including grayscale conversion, radial profiling, contour detection, and feature extraction - was used to quantify morphology (e.g., ring radii, contour areas). Features were compiled into datasets for clustering to identify morphological classes correlating with excipient interactions (Fig. 1). Future work includes expanding the feature set with shape descriptors (circularity, eccentricity) and texture metrics (local entropy, Haralick features). Advanced machine learning models, such as convolutional neural networks and vision transformers, will be tested for automated pattern recognition and formulation behavior prediction. The methodology's generalizability will be evaluated using a wider range of active pharmaceutical ingredients and excipient combinations. Ultimately, this study aims to establish a scalable, reproducible, and low-cost image-based tool for early-stage pharmaceutical screening, helping accelerate drug development.

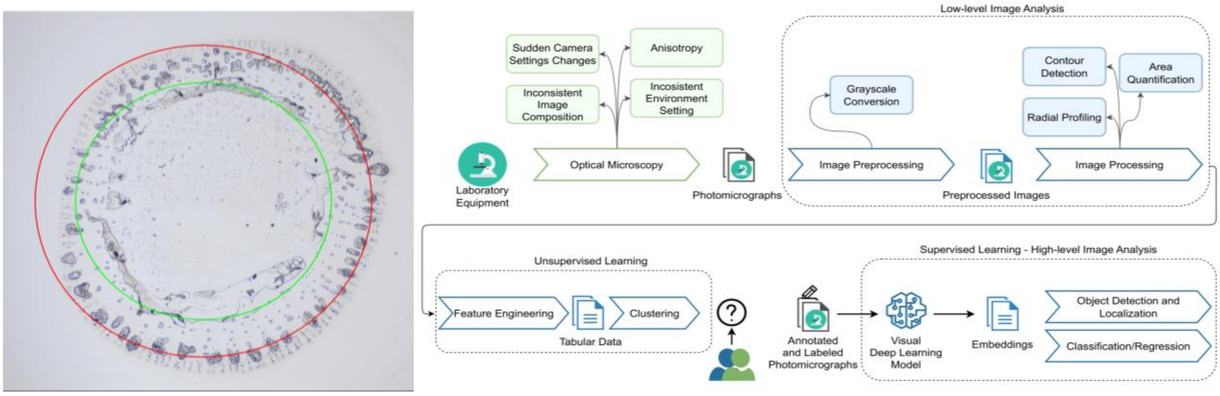

Fig. 1: Representative microscope image overlaid with detected ring boundaries (left) and schematic overview of the analysis process (right).

Acknowledgments:
This paper was funded by the Croatian Science Foundation (IP-2024-05-4339) entitled "Coffee ring effect in 'Lab on a Chip' environments in the development of new drug formulations." Leader prof. Ernest Meštrović.

Preparation, characterization and thermal crosslinking of poly(allylamine hydrochloride)/poly(acrylic acid) multilayers

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Polyelectrolytes are macromolecules with a substantial portion of the constitutional units containing ionic or easily ionizable functional groups. These charged groups enable the formation of polyelectrolyte multilayers through the sequential adsorption of oppositely charged polyelectrolytes onto a solid substrate [1]. The properties of these ultrathin films, for example thickness and roughness, can be precisely controlled by adjusting factors such as pH and ionic strength during fabrication. Additionally, their properties can be further enhanced using post-treatment techniques, for instance thermal annealing [2]. In this study, the surface roughness and morphology of a copper substrate, along with the thickness of its oxide layer, were assessed using atomic force microscopy and ellipsometry. Following this, poly(allylamine hydrochloride) and poly(acrylic acid) multilayers were assembled on the copper surface by layer-by-layer method. The buildup of the multilayers was investigated using ellipsometry. After that, the films were thermally cross-linked. Moreover, the conversion of carboxylate and amine groups into amide bonds was confirmed using attenuated total reflectance IR spectroscopy. Structural and surface characteristics of the multilayers were analyzed by ellipsometry and atomic force microscopy, both before and after thermal cross-linking. It was observed that the film thickness, as well as its root mean square roughness, increased slightly, while the granular structure of the nanofilm surface remained largely unchanged after thermal cross-linking.

Acknowledgments

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Development and Application of Advanced Biofuels in the European Union and Croatia

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The biofuel industry has been experiencing continuous growth in recent years, driven by increasing demands for sustainable energy sources in the transport sector. Currently, biofuels account for approximately 4% of global fuel consumption in transportation [1]. Through the RED III directive, the European Union has set ambitious targets for 2030, a 42.5% share of renewable energy, with an aspirational goal of 45%, and an increase in the share of renewables in transport from 14% to 29%. The directive also requires a minimum of 5.5% share of advanced biofuels [2].

This work presents the analyzes of development and application of biofuels in EU over the past decade, with particular emphasis on the transition from first-generation biofuels to advanced fuels such as HVO and green hydrogen, produced from waste and non-food sources [3]. The situation in Croatia is examined in detail, where the use of biofuels in the transport sector remains very limited or virtually non-existent. Currently available technologies in Croatia, as well as the potential for the development and implementation of advanced biofuels in line with European goals and standards will be presented. Additionally, key challenges in implementation, including technological, economic, and regulatory barriers affecting the wider adoption of biofuels will be presented.

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Steroid Derivatives' Inclusion within Cyclodextrins

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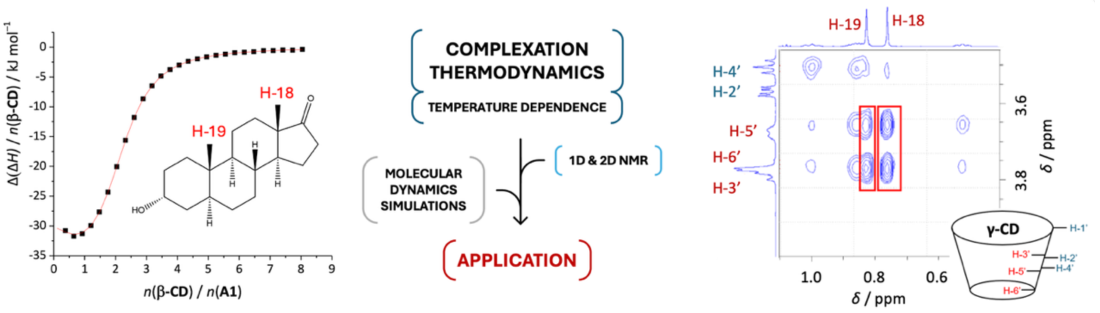
Steroids and their derivatives are involved in numerous physiological processes and have been thoroughly investigated due to their biological, medicinal, and pharmaceutical activity. Unfortunately, application of neutral steroid derivatives is often hindered by scarce solubility in aqueous solutions. This obstacle is (partially) resolved by adding solubilizing excipients such as cyclodextrin derivatives which bind these compounds efficiently, and steroid-cyclodextrin complexation reactions also find their application in *e.g.* cholesterol extraction from fatty foods. [1] However, the comprehensive and detailed investigations of thermodynamic and structural factors governing the steroid complexation reactions by cyclodextrins and their derivatives are often lacking in literature, leaving a gap in understanding of these valuable processes and constraining their further application in numerous fields.

In this work, we have investigated the complexation reactions of several steroids within β- and γ-cyclodextrins and their derivatives in aqueous solutions by means of isothermal titration calorimetry (ITC) and 1D/2D NMR spectroscopy. Stable complexes were formed, with varying complex stoichiometries depending on the structure of the guest molecules and the host size and functionalization. All reactions were enthalpically favorable and, in some cases, predominantly entropy driven. Temperature dependence of standard reaction enthalpy, entropy and Gibbs energy was also addressed, and the negative $\Delta_r C_p^\circ$ values provided an insight into the extent of guest and host cavity dehydration. The observed enthalpy-entropy compensation, a characteristic of such processes, was discussed. [2–4]



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Synthesis and antibacterial evaluation of novel 4-azaindole derivatives

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4-Azaindoles are nitrogen-containing heterocycles structurally analogous to indoles, distinguished by a nitrogen atom replacing the carbon atom at the 4-position of the benzene ring. This structural modification often enhances overall drug-like properties, such as solubility, metabolic stability, and binding affinity, which makes 4-azaindoles a valuable scaffold in medicinal chemistry. 4-Azaindoles and their derivatives have been investigated in the development of kinase inhibitors, as well as antiviral and anticancer agents [1-3].

In this work, we designed and synthesized a series of 6-phenyl-4-azaindole derivatives featuring different substituents on the phenyl ring. The resulting compounds were further modified through alkylation of the pyrrole and pyridine nitrogen atoms using a range of alkyl and benzyl groups. Starting from commercially available 6-bromo-4-azaindole, the designed compounds were prepared by Suzuki coupling, followed by *N*-alkylation at the pyrrole and pyridine nitrogens using alkyl and benzyl groups that differ in stereoelectronic properties. Structures of prepared compounds were determined by 1D and 2D ^{1}H and ^{13}C NMR and high-resolution mass spectrometry. The antibacterial activity of the prepared compounds was evaluated against a panel of Gram-positive and Gram-negative bacterial strains by the broth microdilution method. Most of the synthesized compounds exhibited notable antibacterial activity, with several showing low minimum inhibitory concentrations (MICs), highlighting their potential as promising candidates for antibacterial drug development.

Acknowledgment*: This project is funded by The European Union – NextGenerationEU project ToSiAn (Total synthesis of bioactive metabolites – From deep sea microorganisms to new class of antibiotics and synthetic methodologies, NPOO.C3.2.R2-I1.06.0043).*

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Evaluation of Surfactants for Enhanced Solubilization of Netarsudil Dimesylate and Latanoprost in Ophthalmic Formulations

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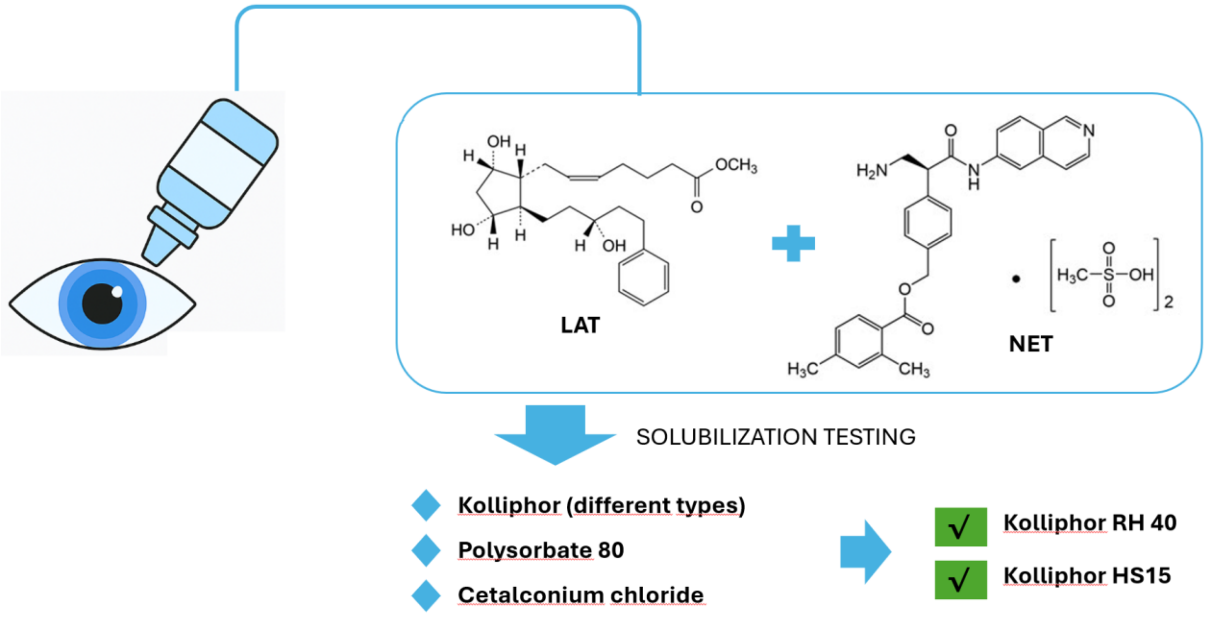
Netarsudil dimesylate (**NET**), a Rho kinase inhibitor, [1] and latanoprost (**LAT**), a prostaglandin F2α analogue, [2], are combined in ophthalmic formulations to lower intraocular pressure in open-angle glaucoma by enhancing aqueous and uveoscleral outflow. This study evaluated the solubilization efficiency of various surfactants for **NET** and **LAT** to identify suitable excipients for ophthalmic formulations. Following surfactants Kolliphor ELP, HS15, RH 40, Polysorbate 80 and cetalkonium chloride were tested at concentrations above their critical micelle concentration as micelle formation is essential for improving the solubility of poorly water-soluble drugs. Parameters such as the assay of **NET** and **LAT**, as well as osmolarity, were evaluated throughout the study. Kolliphor ELP, HS15 and RH40 showed the best solubilization, achieving nearly complete latanoprost content and acceptable **NET** levels. However, high concentrations increased osmolality, necessitating further tests at lower concentrations. At lower concentrations Kolliphor RH40 and HS15 emerged as the most promising candidate in respect to assay and osmolality for developing stable ophthalmic formulations. Polysorbate 80 and cetalkonium chloride were less effective, yielding drug contents similar to surfactant-free solutions. These findings will be further evaluated through long-term stability studies to confirm product's quality, safety and efficacy over time.



SOLUBILIZATION TESTING

- **Kolliphor (different types)**
- **Polysorbate 80**
- **Cetalconium chloride**

✓ **Kolliphor RH 40**
✓ **Kolliphor HS15**

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AUTHOR INDEX

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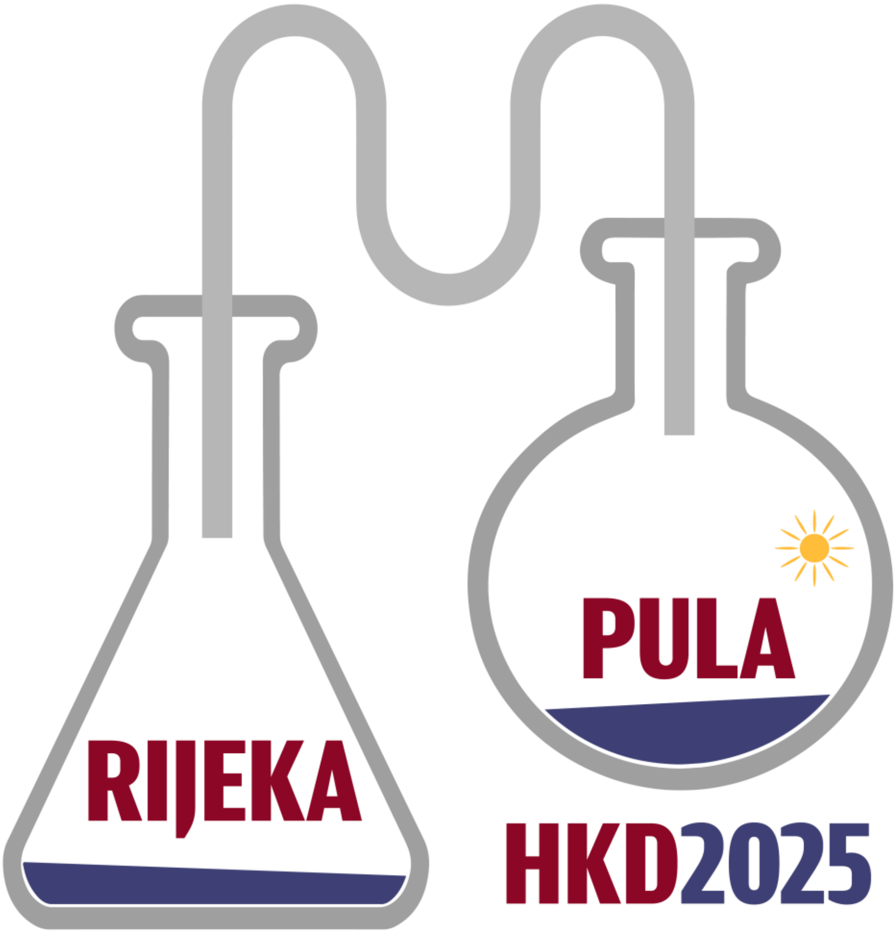
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