ISSN: 2718-2177

International Conference

S+M(L)=KI[16]

19th and 20th February 2026

XVI Meeting of Young Chemical Engineers

www.fkit.unizg.hr/smlki

University of Zagreb Faculty of Chemical Engineering and Technology

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BOOK OF ABSTRACTS

Knjiga sažetaka

19th and 20th February 2026, Zagreb, Croatia

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HRVATSKO DRUŠTVO KEMIJSKIH INŽENJERA I TEHNOLOGA

SVEUČILIŠTE U ZAGREBU

FAKULTET KEMIJSKOG INŽENJERSTVA I TEHNOLOGIJE

XVI. SUSRET MLADIH KEMIJSKIH INŽENJERA

KNJIGA SAŽETAKA

XVI MEETING OF YOUNG CHEMICAL ENGINEERS

BOOK OF ABSTRACTS

Zagreb, 19. i 20. veljače 2026.

Zagreb, 19th and 20th February 2026

Izdavač / *Published by*
Hrvatsko društvo kemijskih inženjera i tehnologa
Croatian Society of Chemical Engineers

Za izdavača / *For the publisher*
Matko Erceg

Urednici / *Editors*
Anita Šalić, Marijan-Pere Marković i Andreja Žužić

Grafički urednik / *Graphical editor*
Zdenko Blažeković

Recenzenti / *Reviewers*
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Svi sažeci objavljeni u ovoj Knjizi sažetaka prošli su recenzijski postupak u organizaciji Znanstvenog odbora skupa.
All abstracts published in this Book of Abstracts were peer-reviewed by the Scientific Committee.

Tekst pripremili / *Text prepared by*
AUTORI, koji su odgovorni za tekst sažetaka
AUTHORS, who are fully responsible for the abstracts

Priprema / *Layout*
Marijan-Pere Marković, Zdenko Blažeković

ISSN 2718-2177

Organizatori / *Organizers*
Hrvatsko društvo kemijskih inženjera i tehnologa / *Croatian Society of Chemical Engineers*
Sveučilište u Zagrebu Fakultet kemijskog inženjerstva i tehnologije / *University of Zagreb Faculty of Chemical Engineering and Technology*

Pokrovitelji / *Under the Auspicies of the*
Ministarstvo znanosti, obrazovanja i mladih / *Ministry of Science, Education and Youth*
Sveučilište u Zagrebu / *University of Zagreb*
Akademija tehničkih znanosti Hrvatske / *Croatian Academy of Engineering*
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UVODNIK

Susret mladih kemijskih inženjera (SMLKI) znanstveno-stručni je skup koji se od 1996. godine tradicionalno održava svake druge godine u organizaciji Hrvatskog društva kemijskih inženjera i tehnologa (HDKI) i Sveučilišta u Zagrebu Fakulteta kemijskog inženjerstva i tehnologije. Od 2022. godine SMLKI prerasta u međunarodni skup, dodatno potvrđujući svoju važnost i prepoznatljivost u znanstvenoj i stručnoj zajednici.

SMLKI 2026 nastavlja ovu dugogodišnju tradiciju kao mjesto susreta studenata, mladih istraživača, kemijskih inženjera i stručnjaka iz srodnih područja, pružajući im priliku za stjecanje prvih iskustava u prezentaciji rezultata vlastitih znanstvenih i stručnih istraživanja. Takva su iskustva iznimno važna za profesionalni razvoj mladih stručnjaka i jačanje struke u cjelini. Glavni cilj skupa jest afirmacija mladih kemijskih inženjera kroz predstavljanje rezultata istraživanja ostvarenih tijekom studija i ranih faza profesionalne karijere. Na ovogodišnjem Susretu sudjeluje 286 sudionika koji su predstavili ukupno 180 znanstvenih i stručnih priopćenja, što svjedoči o kontinuiranom rastu interesa i značaju ovog skupa.

Ovim skupom nastojimo ohrabriti mlade autore na kreiranje i realizaciju novih ideja, potaknuti ih na kritičko promišljanje i otvorenost prema interdisciplinarnom pristupu te omogućiti uspostavu novih profesionalnih i znanstvenih suradnji. Istodobno, SMLKI pruža uvid u suvremene smjerove tehnološkog razvoja, naglašavajući važnost primjene naprednih analitičkih i računalnih metoda, zelenih i održivih tehnologija te prijenosa znanja i tehnologije između akademske zajednice i industrije. Upravo se ti izazovi i potrebe suvremenog kemijskog inženjerstva odražavaju u odabiru plenarnih i pozvanih predavača.

Radovi objedinjeni u ovoj Knjizi sažetaka svjedoče o raznolikosti istraživačkih tema, visokoj razini stručnosti i znanstvene zrelosti mladih autora, ali i o njihovoj motivaciji i entuzijazmu za daljnji razvoj. Posebnu vrijednost skupa čine nagrade za najbolja posterska priopćenja i najbolje usmeno izlaganja, kojima se dodatno potiče izvrsnost i kvaliteta prezentacije znanstvenog rada. Cjeloviti radovi sa skupa bit će objavljeni u posebnom izdanju časopisa Kemija u industriji.

Na kraju, zahvaljujemo svim autorima, sudionicima, predavačima, recenzentima, sponzorima i partnerima na doprinosu uspješnoj realizaciji SMLKI 2026. Vjerujemo da će ovaj Susret, kao i Knjiga sažetaka, biti izvor inspiracije, novih znanja i suradnji te poticaj mladim kemijskim inženjerima da s entuzijazmom prihvate izazove budućnosti i aktivno oblikuju razvoj kemijsko-inženjerske struke u Hrvatskoj i šire.

Svim sudionicima želimo uspješan i ugodan Susret te mnogo uspjeha u daljnjem znanstvenom i profesionalnom radu.

Predsjednica Znanstveno-organizacijskog odbora
Doc. dr. sc. Anita Šalić

FOREWORD

The Meeting of Young Chemical Engineers (SMLKI) is a scientific and professional conference traditionally held every two years since 1996, organised by the Croatian Society of Chemical Engineers and Technologists and the University of Zagreb Faculty of Chemical Engineering and Technology. Since 2022, SMLKI has become an international conference, further confirming its importance and recognition within the scientific and professional community.

SMLKI 2026 continues this long-standing tradition as a meeting place for students, early-career researchers, chemical engineers, and professionals from related fields, providing an opportunity to gain their first experiences in presenting the results of their scientific and professional research. Such experiences are of great importance for the professional development of young experts and for strengthening the profession as a whole.

The main objective of the conference is to promote young chemical engineers by presenting research results achieved during their studies and the early stages of their professional careers. This year's Meeting is attended by 286 participants, who have presented a total of 180 scientific and professional contributions, demonstrating the continuous growth of interest in and significance of this conference.

Through this conference, we aim to encourage young authors to develop and realise new ideas, foster critical thinking and openness to interdisciplinary approaches, and enable the establishment of new professional and scientific collaborations. At the same time, SMLKI provides insight into contemporary directions of technological development, emphasising the importance of advanced analytical and computational methods, green and sustainable technologies, and the transfer of knowledge and technology between academia and industry. These challenges and needs of modern chemical engineering are clearly reflected in the selection of plenary and invited speakers.

The contributions compiled in this Book of Abstracts testify to the diversity of research topics, the high level of expertise and scientific maturity of young authors, as well as their motivation and enthusiasm for further development. A special value of the conference lies in the awards for the best poster and oral presentations, which further promote excellence and the quality of scientific communication. Full papers from the conference will be published in a special issue of the journal Kemija u industriji.

Finally, we would like to express our sincere gratitude to all authors, participants, speakers, reviewers, sponsors, and partners for their contributions to the successful organisation of SMLKI 2026. We believe that this Meeting, as well as the Book of Abstracts, will serve as a source of inspiration, new knowledge, and collaboration, and will encourage young chemical engineers to embrace future challenges with enthusiasm and to contribute actively to the development of the chemical engineering profession in Croatia and beyond.

We wish all participants a successful and enjoyable Meeting and much success in their future scientific and professional work.

Chair of the Scientific and Organizing Committee
Assist. Prof. Anita Šalić, PhD

Prvih 30 godina započelo je ovdje – glasovi onih koji su bili prvi

Dragi studenti, kolegice i kolege,

Dozvolite mi da se prisjetim kako je to bilo prije 30 godina. Tada sam bila predsjednica Upravnog Odbora Hrvatskog društva kemijskih inženjera (HDKI). Pala mi je na pamet ideja, da u ta za Hrvatsku teška, olovna vremena kada je još uvijek bjesnio domovinski rat, mi koji nismo otišli na front damo svoj skromni doprinos izgradnji naše nove države na drugi način, a taj je bio okupiti mlade stručnjake iz industrije i s fakulteta i potaknuti ih na međusobnu razmjenu znanja i motivirati ih da nastave raditi ratu usprkos. Trebamo organizirati Skup tih mladih ljudi. Ideju sam iznijela pok. Akademiku Marinu Hraste i Profesoru Želimiru Kurtanjeku koji su je odmah podržali. Zatim je s prijedlogom upoznat i gospodin Slaven Božić iz PLIVE i gospodin dipl. ing. Marijan Pejčić iz NAFTAPLINA, pa je tako i oformljen prvi Organizacijski odbor, a Upravni odbor HDKI-a je prijedlog prihvatio i podržao. Krenuli smo u organizaciju Skupa. Pliva i INA su Susret podržali financijski pa je prvi Susret organiziran bez kotizacije za sudionike.

Dom Hrvatskog inženjerskog saveza (HIS) u Berislavićevoj ul. 6 je u to doba bio stravično prazan pa je Susret mladih ljudi, ovim prostorima trebao udahnuti život, jer su mnoge ostale aktivnosti tada zamrle. Tako je za mjesto održavanja odabran Dom HIS-a, predavaonica na I katu i veliki lijepi hodnici. Ing. Filip Kljajić iz BELIŠĆA, tada član Upravnog odbora HDKI, odmah je u Belišću dao izraditi drvene nogare i kartonske ploče, pa je organizirana i posterska sekcija, jer nam je Belišće u hodnike u Berislavićevoj 6 dostavilo posterske nogare i kartonske ploče.

Kako je Susret organiziran bez kotizacije u tim teškim vremenima, okupilo se oko 65 sudionika, a u vrijeme trajanja Susreta osjećala se neka posebna atmosfera jer je mladim ljudima pružena mogućnost druženja u tim ratnim vremenima. Na Susretu je održano10 usmenih i 20 posterskih priopćenja, te jedno plenarno predavanje prof. dr. Rolfa Wichmann-a sa Tehničkog Sveučilišta u Dortmundu s naslovom “Kontinuirana sterilizacija”.

Susret je pokazao da postoje mladi ljudi koji su aktivni znanstveno i stručno u području kemijskog inženjerstva. Susretu su se pridružili i stariji nastavnici, te je zaključak bio da to ne može biti jedini Susret nego s njegovom organizacijom treba nastaviti. II Susret je još organiziran u domu HIS-a, zatim je prostor postao premalen te se Susret počeo održavati u prostorima Fakulteta kemijskog inženjerstva i tehnologije i uz potporu Fakulteta.

Ove godine Susret se organizira već šesnaesti (XVI) puta. Pridružili su mu se i mladi iz područja srodnih kemijskom inženjerstvu, a brojka sudionika je iz godine u godinu sve veća.

Kako vidim na ovom, kao i na nekoliko prethodnih Susreta, imamo i goste iz susjednih država, te Susret poprima međunarodni značaj.

Vjerujem da će i ovaj XVI. Susret mladih kemijskih inženjera ponajprije ispuniti očekivanja mladih znanstvenika i stručnjaka koji na njemu sudjeluju, te im pružiti mogućnost međusobnog druženja i razmjene znanja.

Čestitke organizatorima na uspješnoj organizaciji ovogodišnjeg Susreta i hvala svima koji su uložili trud i svoje vrijeme kako bi ovaj skup preživio i doživio svoju 30. Obljetnicu.

Hvala svima koji su pomogli i poduprli financijski organizaciju ovog Susreta i ostalih kroz vrijeme.

Prof. emerita Đurđa Vasić-Rački

Dragi kolege i studenti,

Kada su mi profesori Đurđa Vasić-Rački i akademik Marin Hraste predložili da im se u organizaciji Hrvatskog društva kemijskih inženjera (HDKI) pridružim u osnivanju skupa studenata kemijskog inženjerstva to sam prihvatio s velikim zadovoljstvom i vidio kao priliku da prenesem neka svoja iskustva iz rada studenata u organizaciji Američkog društva kemijskih inženjera (AIChE). Temeljna zamisao skupa američkih studenata, budućih diplomiranih kemijskih inženjera, je pružiti šanse studentima da se istaknu svojim originalnim znanstvenim idejama i da ostvare što više kontakata s kompanijama koje zapošljavaju kemijske inženjere. Skupovi su u organizaciji studenata, uz nužnu pomoć profesora, predsjednici sekcija su studenti, sekcijska predavanja su praćena brojnim studentskim pitanjima oslobođenih profesorskih kritika, i često su popraćena veselim dosjetkama i šalama. Uz studentska izlaganja organiziraju se i demonstracije laboratorijskih uređaja i natjecanja, kao na primjer nove baterije za električne automobile. Cjelokupna aktivnost studenata praćena je pozornim interesom predstavnika kompanija koje zapošljavaju.
Prijedlog održavanja susreta mladih kemijskih inženjera (SMLKI, Susret mladih kemijskih inženjera) u Hrvatskoj je izvrsno prihvaćen, organizira se od 1996. svake druge godine, a do danas je postao tradicionalni znanstveno-stručni skup koji će 2026. biti 16.-ti po redu. Skupovi su u organizaciji HDKI-a i FKIT-a i omogućuju mladim kemijskim inženjerima i studentima da održe izlaganja iz svojih znanstvenih istraživanja na dodiplomskim i doktorskim projektima. Od početnog skupa 1996., broj sudionika 45 i radova 31, stalno se povećava i 2024. bilo je 237 sudionika s 193 radova. Nažalost broj sudionika iz industrijskih firmi nije pratio stalni porast znanstvenih radova. Tijekom zadnjih skupova sudjelovali su autori iz Njemačke, Mađarske, Slovenije, Bosne i Hercegovine, Srbije i Ujedinjenog Kraljevstva, tako da SMILKI ima Europski značaj koji je potvrđen podrškom Europskog društva kemije (EuChemS, European Chemical Society). Nadolazeći XVI SMLKI skup održava se u tradicionalnim inženjerskim sekcijama: kemijsko, biokemijsko, okolišno, materijali, primijenjena kemija. Iako su sekcije tradicionalne, uvjeren sam da će se utjecaj umjetne inteligencije prepoznati u svakom projektu i da će se na idućem skupu održati i nova sekcija pod nazivom Umjetna inteligencija u kemijskom inženjerstvu.

Prof. dr. sc. Želimir Kurtanjek (u mirovini)

Dragi kolege i studenti,

Tehnološki razvoj, kao nužan pokretač gospodarstva i društva u cjelini, težnja je svake moderne države. Tih su godina nositelji razvoja bile domaće kompanije poput Plive, INE, DINE, Naftaplina, Chromosa, Podravke i mnogih drugih. Svoja iskustva stečena u radu s domaćim i svjetskim kompanijama prenio sam u Plivu, od proizvodnje do rada u istraživanju i razvoju, što je bilo u skladu s opredjeljenjem da razvoj novih proizvoda i procesa, koji se uklapaju u okoliš i zadovoljavaju svjetske standarde, bude naš cilj. Kao tadašnji izvršni potpredsjednik uprave Plive smatrao sam da za istraživanje i razvoj moraju postojati sredstva, ali i ključan mladi kadar koji će svojim pogledima i rješenjima doprinositi tehnološkom i društvenom razvoju.
SMLKI je mogao donijeti tim potrebnim mladim kadrovima nove kontakte, poglede na druge modele i metodologije rada, kao i nova poznanstva, te sam to podržavao i vjerovao u uspjeh. SMLKI je bio aktivni pokretač uključivanja mladih inženjera i studenata završnih godina kao nositelja budućeg razvoja i izvora novih ideja, koje bi oni na zajedničkim okupljanjima i druženjima prezentirali i bili u prvom planu. Važnost usvajanja načela održivosti i integriranja zaštite okoliša u sve aspekte razvoja društva prepoznata je kroz ekoinženjerstvo kao važan i ispravan put. Kao glavni govornici, prezentirajući svoje radove kolegama, govoreći o poteškoćama, problemima i uspjesima, razmjenjivali bi iskustva i stvarali prijateljstva u poslovnom i osobnom životu, što je ključ uspjeha.
Iako me posao odveo na drugi kraj svijeta, sretan sam što sam dao podršku ovom projektu i zadovoljan što je SMLKI već 30 godina zadržao fokus na mladim ljudima i postao međunarodno poznat.

Slaven Božić, dipl. ing. kem. tehn. (u mirovini)

The first 30 years began here – the voices of those who were first

Dear students, colleagues,

Allow me to recall how it was thirty years ago. At that time, I was the President of the Executive Board of the Croatian Society of Chemical Engineers (HDKI). An idea occurred to me that, in those difficult and oppressive times for Croatia, when the Homeland War was still raging, those of us who had not gone to the front could make a modest contribution to building our new state in another way. That contribution was to bring together young professionals from industry and academia, encourage the exchange of knowledge among them, and motivate them to continue their work despite the war. We needed to organize a meeting of these young professionals.

I presented this idea to the late Academician Marin Hraste and Professor Želimir Kurtanjek, who immediately supported it. Subsequently, Mr. Slaven Božić from PLIVA and dipl. ing. Marijan Pejčić, from NAFTAPLIN were informed of the proposal, and thus the first Organizing Committee was formed. The Executive Board of the HDKI accepted and supported the proposal, and we began organizing the Meeting. PLIVA and INA provided financial support, enabling the first Meeting to be organized without a registration fee for participants.

At that time, the premises of the Croatian Engineering Association (HIS) at Berislavićeva 6 were remarkably empty, and the Meeting of young professionals was intended to bring life back into these spaces, as many other activities had ceased. Therefore, the HIS building was chosen as the venue, including the lecture hall on the first floor and the large, elegant corridors. Engineer Filip Kljajić from BELIŠĆE, then a member of the HDKI Executive Board, promptly arranged for the production of wooden poster stands and cardboard panels in Belišće, which enabled the organization of a poster session. These poster stands and panels were delivered to the HIS building at Berislavićeva 6. As the Meeting was organized without a registration fee during those difficult times, approximately 65 participants attended. Throughout the Meeting, a special atmosphere could be felt, as young people were given the opportunity to meet and socialize during wartime. The program included 10 oral presentations, 20 poster presentations, and one plenary lecture by Prof. Dr. Rolf Wichmann from the Technical University of Dortmund entitled “Continuous Sterilization”.

The Meeting demonstrated that there were young individuals who were scientifically and professionally active in the field of chemical engineering. Senior faculty members also joined the Meeting, and the conclusion was that this should not be a one-time event, but that its organization should continue. The second Meeting was also held at the HIS building; however, as the venue soon became too small, the Meeting was subsequently held at the Faculty of Chemical Engineering and Technology, with the Faculty’s support.This year, the Meeting is being organized for the sixteenth (XVI) time. Young professionals from fields related to chemical engineering have also joined, and the number of participants has been steadily increasing each year. As I observe at this and several previous Meetings, we also welcome guests from neighboring countries, giving the Meeting an increasingly international character.

I believe that this XVI Meeting of Young Chemical Engineers will primarily meet the expectations of the young scientists and professionals participating in it, while providing them with opportunities for networking and the exchange of knowledge.

I extend my congratulations to the organizers for the successful organization of this year’s Meeting and thank all those who have invested their effort and time to ensure that this event has endured and reached its 30th anniversary. I also thank everyone who has supported the organization of this Meeting and previous ones financially over the years.

Prof. Emerita Đurđa Vasić-Rački, PhD

Dear colleagues and students,

When Professor Đurđa Vasić-Rački and Academician Marin Hraste invited me to join them, within the framework of the Croatian Society of Chemical Engineers (HDKI), in establishing a meeting for students of chemical engineering, I accepted with great pleasure and saw it as an opportunity to share some of my experiences gained through working with students within the American Institute of Chemical Engineers (AIChE).

The fundamental idea of meetings organized by American students, future graduate chemical engineers, is to provide students with opportunities to distinguish themselves through original scientific ideas and to establish as many contacts as possible with companies that employ chemical engineers. These meetings are organized by students, with the necessary support of professors; session chairs are students; and session presentations are followed by numerous student questions, free from professorial criticism, and often accompanied by witty remarks and humor. In addition to student presentations, demonstrations of laboratory equipment and competitions are organized, such as those focused on new batteries for electric vehicles. All student activities are closely followed by representatives of companies seeking to employ chemical engineers.

The proposal to organize the Meeting of Young Chemical Engineers (SMLKI) in Croatia was very well received. It has been organized biennially since 1996 and has grown into a traditional scientific and professional meeting, which will be held for the sixteenth (XVI) time in 2026. The meetings are organized jointly by the HDKI and the Faculty of Chemical Engineering and Technology (FCET), providing young chemical engineers and students with the opportunity to present the results of their scientific research conducted within undergraduate and doctoral projects. Since the inaugural meeting in 1996, which hosted 45 participants and 31 papers, the numbers have steadily increased, reaching 237 participants and 193 papers in 2024. Unfortunately, the number of participants from industrial companies has not followed the continuous growth in scientific contributions.

In recent meetings, authors from Germany, Hungary, Slovenia, Bosnia and Herzegovina, Serbia, and the United Kingdom have participated, giving SMLKI a European dimension, further confirmed by the support of the European Chemical Society (EuChemS). The upcoming XVI SMLKI meeting will be organized within the traditional engineering sections: chemical, biochemical, environmental, materials, and applied chemistry. Although these sections are traditional, I am confident that the influence of artificial intelligence will be evident in every project, and that the next meeting will also include a new section entitled Artificial Intelligence in Chemical Engineering.

Prof. Želimir Kurtanjek, PhD (Retired)

Dear colleagues and students,

Technological development, as a necessary driver of the economy and society as a whole, is an aspiration of every modern state. In those years, the key drivers of development were domestic companies such as Pliva, INA, DINA, Naftaplin, Chromos, Podravka, and many others. The experience I gained through collaboration with both domestic and international companies, spanning production as well as research and development activities, I brought to Pliva. This aligned with our commitment to making the development of new products and processes, compatible with environmental requirements and compliant with global standards, our primary objective. As the then Executive Vice President of Pliva, I believed that research and development required not only financial resources but also a strong base of young professionals whose perspectives and solutions could contribute to technological and societal progress.

SMLKI was able to provide these much-needed young professionals with new contacts, insights into alternative models and methodologies of work, and valuable professional connections. For this reason, I strongly supported the initiative and believed in its success. SMLKI actively fostered the involvement of young engineers and final-year students as key contributors to future development and as sources of new ideas. Through joint meetings and networking opportunities, they were encouraged to present their work, take center stage, and actively participate. The importance of adopting sustainability principles and integrating environmental protection into all aspects of societal development was recognized through eco-engineering as a meaningful and appropriate path forward. As keynote speakers, participants presented their work to peers, discussed challenges, problems, and successes, exchanged experiences, and formed professional and personal friendships, elements that are essential to long-term success.

Although my professional career eventually took me to the other side of the world, I am pleased to have supported this initiative and gratified that SMLKI has maintained its focus on young people for over 30 years and has grown into an internationally recognized meeting.

Slaven Božić, BSc in Chemical Engineering (Retired)

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PLENARNA PREDAVANJA
PLENARY LECTURE

ULOGA KEMIJSKIH INŽENJERA U ENERGETSKOJ TRANZICIJI

THE ROLE OF CHEMICAL ENGINEERS IN THE ENERGY TRANSITION

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Transition to decarbonized energy systems is becoming more attractive with fall of investment costs of renewables and volatile prices and insecurity of fossil fuel supply. The renewable energy resources are bountiful, especially wind and solar, while integrating them into current energy systems is a challenge. While in regions with lower seasonal variability of solar energy, like most of tropical and subtropical areas, solar with batteries will be able to cover most of demand, further from Equator batteries will not be enough and wind will be needed in wintertime. The limit of cheap and easy integration for wind is around 20% of yearly electricity generation, while a combined wind and solar may reach 30%, pending on necessary improving of transmission capacities and flexibilization of conventional power plants. Going any further requires implementation of energy markets, demand response, coupling of wholesale and retail energy prices, and integration of electricity, heating/cooling, water and transportation systems, as well as industrial systems. The cheapest and simplest way is integrating power and heating/cooling systems through the use of district heating and cooling (which may be centrally controlled and may have significant heat storage capacity), since power to heat technologies are excellent for demand response. Electrification of residential heating with heat pumps is obvious solution for individual houses but would require smart grid implementation to make it participate in demand response. Electrification of low energy density transportation (personal cars, local delivery and local buses) allows not only for significant increase of energy efficiency, but also, the electric cars, due to low daily use, may be excellent for demand response and even for storage. This will necessarily bring smart grids development and digitalization of power systems, allowing also for demand response from buildings, appliances etc. Smart electrification of heating/cooling, transport, and industry can raise renewable penetration above 80%. The remaining 20% - long-distance transport, hard-to-electrify industrial processes, feedstocks, and backup generation - will require breakthroughs. Waste biomass could cover roughly half of these needs, while hydrogen from surplus renewables can serve high-temperature processes or feedstock for e-ammonia. Captured CO_2 from biomass can enable production of e-fuels such as e-methane and e-methanol. Chemical engineers play a critical role in this transition through electrochemistry (batteries, electrolysis), catalysis (Haber–Bosch, hydrogenation), and synthesis pathways underpinning the methanol economy.

SYNERGISTIC DESIGN OF RESVERATROL-BASED SMALL-MOLECULE FOR NEUROPROTECTION

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The development of small-molecule ligands targeting cholinesterase enzymes remains a central focus in neuropharmacology, particularly for the treatment of neurodegenerative disorders and organophosphate (OP) poisoning. Acetylcholinesterase (AChE) and butyrylcholinesterase (BChE) are two related enzymes that represent pharmacologically suitable targets in neurodegenerative disorders, given their physiological roles in the body [1]. The treatment of neurodegenerative disorders currently includes common reversible or irreversible inhibitors of cholinesterases such as galantamine or rivastigmine [2]. Treating patients with acute OP poisoning is still a challenge despite the development of a large number of oxime compounds that should have the capacity to reactivate AChE and BChE. This lecture highlights the rational design, synthesis, and biological profiling of resveratrol-based small-molecules, variously functionalized heterostilbenes, as inhibitors and reactivators of AChE and BChE. Oxazolostilbenes and their photoproducts exhibited selective BChE inhibition, while naphthoxazole and charged triazole-containing scaffolds demonstrated promising dual-target or BChE-selective profiles. Several uncharged oximes, such as thienostilbene oximes, showed potential for reactivating cyclosarin-inhibited BChE, supporting their further development as CNS-permeable antidotes. Additionally, resveratrol-based triazoles and carbamates revealed enhanced BChE inhibition, antioxidant activity, and favorable selectivity [3, 4]. All the experimental results are interpreted by molecular modeling and for the most bioactive compounds citotoxicity and genotoxicity are also tested. In parallel, the photosensitivity of the best resveratrol-based carbamates is also being examined. In order to increase the efficiency of the Wittig and Vilsmeier reactions, the replacement of batch reactors with flow millireactors is also being tested. Millireactors enabled better conversion and isomers ratio and reduced time required for the synthesis of key heterostilbenes [5]. Additionally, custom-designed 3D printed flow reactors were fabricated using digital light processing technology and evaluated for the photocyclization of triazolostilbenes enabling rapid, low-cost photochemical synthesis of targeted compounds for neuroprotection.

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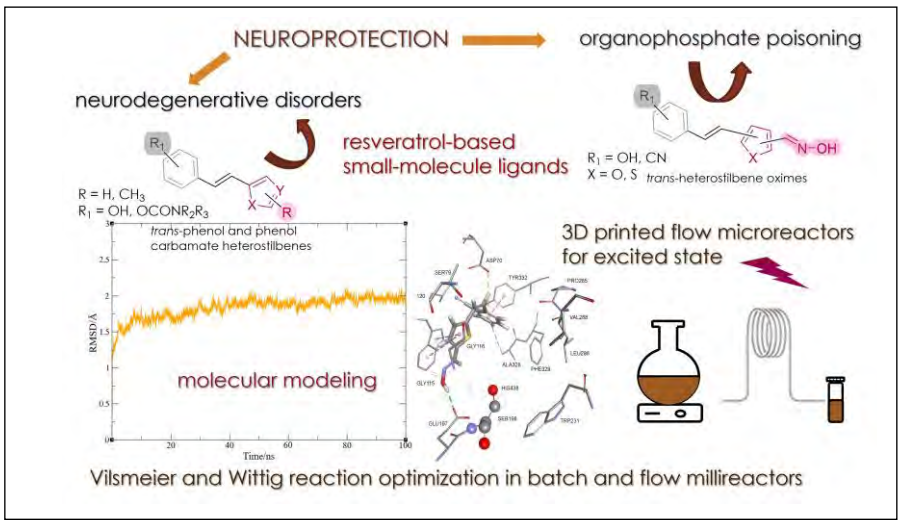

POZVANA PREDAVANJA
INVITED LECTURES

THE IMPORTANCE OF THERMAL ADAPTATIONS IN A WARMING WORLD

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Global warming poses a significant threat to insects, which play indispensable roles in terrestrial ecosystems and whose body temperatures closely track habitat temperatures. As small ectotherms, insects may be especially vulnerable to warming, making it essential to identify the taxa and traits that determine survival. To address this challenge, we use ants as model insects, given their global distribution and ecological importance. Ant activity is directly governed by their thermal limits, so we test how habitat temperature shapes these thermal adaptations across spatial scales, from macrophysiological patterns to local responses. We found greater variability in ants' cold tolerance than in their heat tolerance. Although less variable, heat tolerance can be plastic. Specifically, we show that ant heat tolerance can be altered by habitat temperature, seasonal temperature fluctuations, and nutrition. Such plasticity may be crucial for withstanding global warming as it allows insects to adjust their physiology to rising temperatures. However, an insect's first line of defense against overheating is behavior. An ant can escape to a cooler microclimate if such microclimate is available. We use novel approaches including drone-based thermal imaging, to quantify that microclimatic availability. Integrating physiological and behavioral responses with relevant climatic data improves our understanding of insect resilience to thermal stress and their responses to climate change.

PRECLINICAL DEVELOPMENT OF OSTEOGROW-C: A NOVEL OSTEOINDUCTIVE DEVICE FOR BONE REGENERATION

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PURPOSE/OBJECTIVE: Degenerative spine diseases and segmental long-bone defects represent some of the most challenging conditions in clinical practice. Osteogrow is a novel osteoinductive device based on recombinant human bone morphogenetic protein 6 (rhBMP6) delivered within an autologous blood coagulum. For clinical indications exposed to significant compressive forces - such as large segmental bone defects and posterolateral spinal fusion (PLF) - Osteogrow requires supplementation with a compression-resistant matrix (CRM). Synthetic calcium phosphate (CaP) ceramics, known for their osteoconductivity and clinical versatility, are promising CRM candidates. This series of preclinical studies aimed to evaluate the safety and efficacy of Osteogrow combined with CaP ceramics (Osteogrow-C) and to investigate how ceramic chemical composition and particle size influence the properties of the newly formed bone.

METHODOLOGY: The preclinical development of Osteogrow-C involved extensive animal studies, including a rat subcutaneous ectopic bone formation assay, rabbit and sheep PLF models, and a rabbit ulnar segmental defect model. We tested various CaP ceramics differing in particle size (ranging from 74 to 4000 μm) and chemical composition - hydroxyapatite (HA), tricalcium phosphate (TCP), and biphasic calcium phosphate (BCP, containing both HA and TCP). Additionally, we characterized the timeline of BMP-mediated ectopic osteogenesis across species and assessed the long-term stability of the induced bone with up to one year of follow-up. All animal studies were approved by the National Ethics Committee.

RESULTS: At the rat ectopic site, the volume of bone induced by Osteogrow-C implants was dependent on ceramic particle size, with smaller particles producing significantly higher bone volumes. In rabbit and sheep PLF models, as well as in the rabbit ulnar defect model, Osteogrow-C implants supported rapid and robust bone formation, achieving spinal fusion and complete defect rebridgment without adverse effects. MicroCT and histological analyses confirmed integration of the newly formed bone with native transverse processes, while biomechanical (three-point bending) testing demonstrated mechanically competent fusion. The chemical composition of the ceramics affected their resorption; TCP particles were resorbed significantly faster than HA, with resorption occurring more rapidly in rabbit models than in rat ectopic sites. The sequence of BMP-mediated osteogenesis was conserved across species, but the overall rate of bone formation decreased with increasing animal size.

CONCLUSION/SIGNIFICANCE: Preclinical studies demonstrated that Osteogrow-C is both safe and effective, supporting its translational potential as a therapeutic option for patients with degenerative spine disease and large bone defects. The size and chemical composition of CaP ceramics were identified as key factors governing the extent of bone formation, residual ceramic presence, and structural characteristics of the newly regenerated bone.

MODELIRANJE TEMELJENO NA PODACIMA U BIOKEMIJSKOM INŽENJERSTVU: OD VELIKIH PODATAKA DO PREDIKTIVNOG DIZAJNA

DATA-DRIVEN MODELING IN BIOCHEMICAL ENGINEERING: FROM BIG DATA TO PREDICTIVE DESIGN

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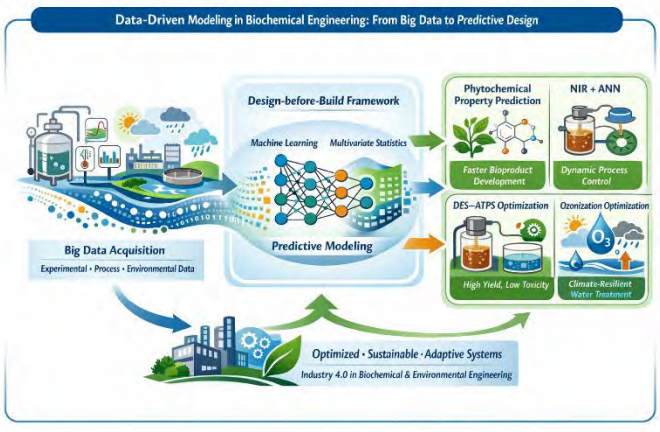
Modern biochemical engineering is undergoing a profound paradigm shift, moving away from predominantly empirical, trial-and-error methodologies toward a predictive design framework powered by big data and artificial intelligence. As biological and environmental systems are inherently non-linear, multiscale, and stochastic, traditional mechanistic models often struggle to fully capture process complexity, variability, and uncertainty. This lecture explores the evolution from raw data acquisition to the development of robust, data-driven models that enable a true "design-before-build" approach in biotechnology and environmental engineering. By leveraging advanced machine learning architectures, multivariate statistics, and big data analytics, high-dimensional experimental and process datasets can be transformed into actionable knowledge for system optimization and control.

To demonstrate the efficacy and versatility of predictive modelling, several representative applications are discussed. First, phytochemical property prediction is presented, where intelligent algorithms are employed to accurately forecast the physicochemical and bioactive properties of medicinal herb extracts, significantly accelerating the development of high-value bioproducts. Second, real-time bioprocess monitoring is illustrated through the integration of near-infrared (NIR) spectroscopy with artificial neural networks (ANN) for dynamic control of grape skin composting, highlighting how data-driven models effectively manage biological variability in circular waste-to-energy systems. Third, advanced extraction optimization is showcased via predictive modelling for lipase extraction using low-toxicity deep eutectic solvent (DES)-based aqueous two-phase systems (ATPS), demonstrating how model-guided design can simultaneously maximize yield and minimize environmental impact. The lecture also introduces an example from drinking water treatment, focusing on the optimization of ozonization processes as an adaptive response to climate change. All mentioned case studies underscore the critical role of data-driven modelling as a cornerstone of the Industry 4.0 transformation in biochemical and environmental engineering. By enabling predictive design, real-time control, and sustainability-oriented optimization, these approaches facilitate the development of efficient, adaptive, and environmentally responsible bioprocesses and treatment systems.



PROCJENA ŽIVOTNOG CIKLUSA *EX CATHEDRA* – KAKO IZBJEĆI ZAMKE I ZABLUDE

LIFE CYCLE ASSESSMENT *EX CATHEDRA* – AVOIDING PITFALLS AND MISCONCEPTIONS

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Life cycle assessment (LCA) is a cornerstone tool in environmental management and sustainability decision-making. LCA provides a structured, systems-based view of the potential environmental impacts associated with the products and services across their lifecycle. Considering that LCA may be applied to a vast spectrum of product systems, which vary widely in complexity on their own, some modelling choices are more critical than others. Furthermore, these choices are often made by junior engineers or less experienced LCA practitioners. These errors made early on in the study can result in unnecessary overhead and lead to time and budget overruns. Even worse, due to oversimplification, poor justification or even inadvertent erroneous application of the LCA framework, the outcomes of the analysis may be greatly skewed and biased. Herein, through practical examples, based on deceptively simple everyday product systems, the common pitfalls which may occur during (i) the defining of the functional unit, (ii) selecting and document cut-off rules and boundaries, (iii) life-cycle inventory analysis, (iv) and environmental impact allocation to secondary products will be showcased. Beyond diagnosing early mistakes, a concise mitigation strategy and quality checklist will be presented, that may help inexperienced practitioners. The overall aim is to strengthen the vantage point of LCA as an analytical tool, instead of a rhetorical one.

FROM RESEARCH TO STARTUP: BUILDING NADES DESIGN FOR A GREENER INDUSTRY

OD ZNANOSTI DO PODUZETNIŠTVA: IZGRADNJA NADES DESIGN-a ZA ZELENIJU INDUSTRIJU

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Industrijska primjena otapala na bazi nafte predstavlja ozbiljan ekološki i sigurnosni problem zbog njihove toksičnosti, hlapljivosti i zapaljivosti. Ovo predavanje prikazuje put od znanstvenog istraživanja do osnivanja startupa NADES Design, s ciljem razvoja održivih otapala koja bi mogla zamijeniti trenutno korištena otapala u industriji. U fokusu su prirodna niskotemperaturna eutektička otapala (tzv. NADES otapala) – 100 % prirodna, biorazgradiva, nehlapljiva i ekološki prihvatljivija alternativa konvencionalnim otapalima.
Istraživanje obuhvaća razvoj i primjenu NADES otapala u ekstrakciji biljnih spojeva te njihovu komercijalnu valorizaciju kroz liniju tekućih dodataka prehrani NADES Drops+ kao i sirovine za industrijsku primjenu. Primjena NADES-a omogućuje povećanu topljivost, stabilnost i dokazani biološki učinak biljnih ekstrakata *in vitro* i *in vivo*, uz poboljšanu sigurnost i produljeni rok trajanja proizvoda. Poseban naglasak stavljen je na *in silico* dizajn otapala, optimizaciju procesa i usklađenost s regulatornim zahtjevima, ilustrirajući kako temeljna istraživanja mogu rezultirati tržišno relevantnim, održivim inovacijama.

The work is co-financed by EU funds (Grant No. NPOO.C3.2.R2-I1.04.0047).

OD KEMIJSKOG SASTAVA DO ELEKTRIČKIH SVOJSTAVA: INTERDISCIPLINARNI PRISTUP MATERIJALIMA ELEKTROINDUSTRIJE

FROM CHEMICAL COMPOSITION TO ELECTRICAL PROPERTIES: AN INTERDISCIPLINARY APPROACH TO MATERIALS IN THE ELECTRICAL INDUSTRY

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Kemijska tehnologija i elektroindustrija, iako naizgled udaljena područja, dijele snažnu poveznicu kroz materijale i procese koji čine temelj suvremene tehnike. Razumijevanje kemijskog sastava, reakcija i strukture materijala ključno je za razvoj pouzdanih električnih uređaja i komponenti, izolacijskih sustava i tehnoloških rješenja u elektroindustriji. Upravo se na spoju tih dviju disciplina otvara prostor za inovacije – od formulacije novih materijala do poboljšanja njihove učinkovitosti i trajnosti u zahtjevnim radnim uvjetima.

Predavanje donosi pregled prijenosa znanja i vještina iz područja kemijskog inženjerstva u elektroindustriju, s naglaskom na primjenu kemijsko-tehnoloških principa u ispitivanju, karakterizaciji i razumijevanju materijala. Posebna pozornost posvećena je povezanosti kemijskog sastava s fizikalnim, električkim i mehaničkim svojstvima te njihovom utjecaju na pouzdanost i trajnost materijala u elektroenergetskim sustavima. Kroz prikaz razvoja laboratorijskih ispitivanja i tehnoloških rješenja naglašava se važnost interdisciplinarnosti, suradnje kemijskog inženjerstva, elektrotehnike i strojarstva te uloga cjeloživotnog učenja i prilagodljivosti u tehničkim strukama.

FROM INNOVATION TO MARKET: OUR JOURNEY TO TECHNOLOGY COMMERCIALIZATION

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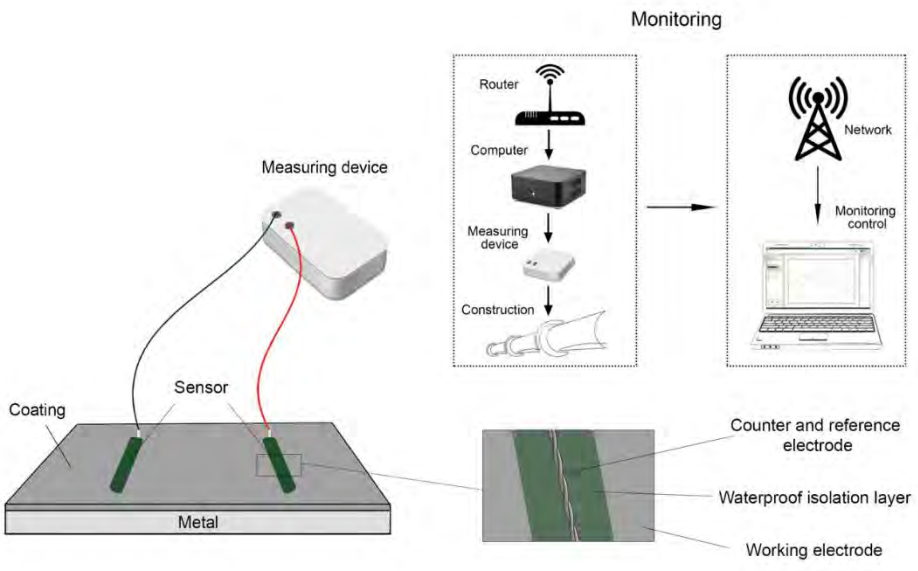
Many scientific ideas with strong experimental foundations never reach real-world application. One of the main reasons is the gap between laboratory-oriented research and the practical needs of industry. Electrochemical impedance spectroscopy (EIS) is a good example: although it is a powerful and sensitive method for assessing coating performance and material degradation, its routine use outside the laboratory has long been limited by complex measurement procedures and demanding data interpretation.

This lecture presents the journey of transforming an academic research concept into a market-ready technology through the development of the ReCorrQCQ method and the establishment of the spin-off company ReCorrTech. The original scientific goal was to understand how impedance loss reflects coating degradation. The technological challenge was to redesign this knowledge into a fast, robust, and repeatable method suitable for laboratory testing, field inspections, and long-term monitoring.

The presentation highlights key steps in technology commercialization: identifying a real industrial problem, simplifying a sophisticated electrochemical method without losing its physical meaning, validating the technology under realistic environmental conditions, and translating complex impedance spectra into clear, quantitative indicators such as coating impedance and water uptake.

By sharing both successes and obstacles encountered along the way, this presentation demonstrates how fundamental chemical and electrochemical knowledge can evolve into an applied technology with real economic and societal impact. The presented work shows that successful innovation requires strong scientific foundations, combined with an understanding of practical limitations and the translation of experimental data into reliable engineering outcomes.



USMENA IZLAGANJA
ORAL PRESENTATIONS

COMPUTATIONAL PROFILING OF QUINOLINE-THIAZOLE HYBRID BINDING TO HUMAN SERUM ALBUMIN

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Human Serum Albumin (HSA) serves as the primary carrier protein for diverse endogenous and exogenous compounds, making the characterization of ligand–HSA interactions essential for drug development. This study presents an atomistic characterization of the binding landscape for three novel quinoline-thiazole hybrids (1c, 2b, 3c) within HSA. A multi-scale computational workflow - combining molecular docking, 200 ns molecular dynamics (MD) simulations, and MM-GBSA free-energy calculations - was employed to assess ligand behavior across the three major HSA subdomains (IB, IIA, IIIA). Comparative MD analysis revealed that interactions within Subdomain IB were transient and destabilizing, marked by elevated backbone fluctuations (RMSF) in residues 110–120 and poor structural convergence of the 2b–IB complex. Similarly, Subdomain IIIA (Sudlow Site II) exhibited only moderate structural adaptation and lacked the conformational stabilization characteristic of strong, persistent binding. In contrast, Subdomain IIA (Sudlow Site I) emerged as the primary high-affinity binding site. Ligands 1c and 2b displayed pronounced structural convergence and reduced flexibility of the binding pocket, while 3c remained comparatively more dynamic. MM-GBSA analysis confirmed the enhanced stability of the 1c– and 2b–IIA complexes, driven by dominant van der Waals contributions (≈ –50 kcal/mol) and sidechain-mediated anchoring by Arg205. Collectively, these results identify ligands 1c and 2b as promising scaffolds for site-specific albumin binding and transport, and provide a structure-guided framework for the rational design of HSA-targeted delivery systems.

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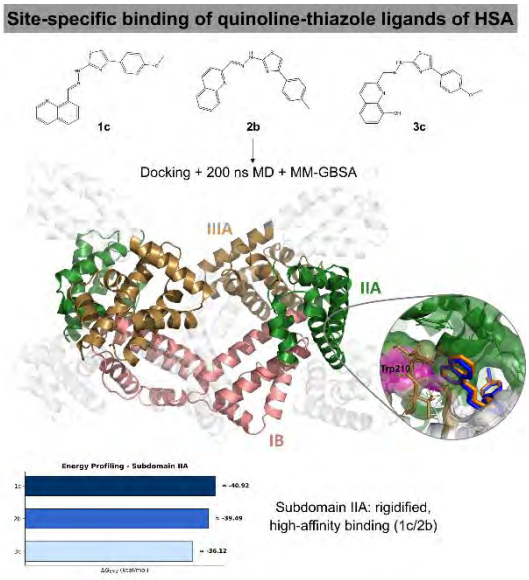

KVALITETA ZRAKA: ZNAČAJ ANALIZE ONEČIŠĆUJUĆIH TVARI I PROGNOZE KVALITETE ZRAKA

AIR QUALITY: THE IMPORTANCE OF POLLUTANT ANALYSIS AND AIR QUALITY FORECASTING

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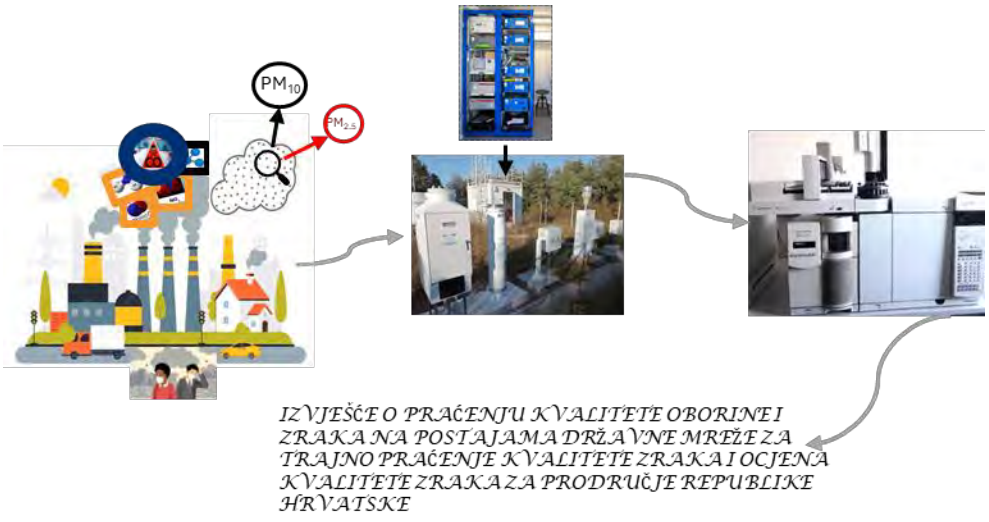
Onečišćenje zraka predstavlja i lokalni i globalni problem jer nastaje kada je njegov prirodni sastav narušen prisutnošću onečišćujućih tvari. Do takvih onečišćenja dolazi kada su te tvari prisutne u koncentracijama koje tijekom određenog vremena mogu uzrokovati štetu za zdravlje ljudi i okoliš. Uredbom o razinama onečišćujućih tvari u zraku, NN 77/2020 kao onečišćujuće tvari u zraku navedene su plinovite tvari (SO_2, NO_x, CO, H_2S, NH_3, formaldehid, benzen, merkaptani, prizemni O_3), lebdeće čestice (PM_{10}, $PM_{2,5}$), teški metali (Pb, Cd, As, Ni), ukupna plinovita Hg te kancerogeni i toksični spojevi u česticama i ukupnoj taložnoj tvari. [2] Rezultati znanstvenih istraživanja pokazuju da navedene onečišćujuće tvari u zraku imaju direktan negativan učinak na zdravlje ljudi te da su povezani s nekoliko nezaraznih bolesti, nepovoljnih zdravstvenih stanja i povećanom smrtnošću. [3]

S ciljem zaštite zdravlja i dobrobiti građana te očuvanja okoliša, Sektor za kvalitetu zraka Državnog hidrometeorološkog zavoda provodi sustavne analize oborine, zraka i lebdećih čestica, mjeri koncentracije plinova i čestica u realnom vremenu te izrađuje prognozu kvalitete zraka za cijelo područje Republike Hrvatske.

Redovitim praćenjem navedenih parametara omogućuje se precizna procjena izloženosti stanovništva onečišćujućim tvarima, što predstavlja ključnu osnovu za donošenje učinkovitih mjera zaštite okoliša i jačanje javnozdravstvenih politika. Na temelju tako prikupljenih podataka moguće je izraditi vrlo precizne prognoze kvalitete zraka te procijeniti rizike kojima su građani izloženi, osobito u urbanim sredinama i područjima pod povećanim utjecajem emisija iz malih kućnih ložišta, prometa i industrije.

[1] NN 127/19, NN 57/22, NN 136/24 Zakon o zaštiti zraka.
[2] NN 77/20, Uredba o razinama onečišćujućih tvari u zraku.
[3] Direktiva (EU) 2024/2881 EU Parlamenta i Vijeća od 23.10.2024. o kvaliteti zraka i čišćem zraku za Europu (preinaka)



POJAVA HIPOKSIJE U VODENOM STUPCU ROGOZNIČKOG JEZERA-ZMAJEVOG OKA U JESEN 2025. GODINE

THE OCCASION OF HYPOXIA IN THE WATER COLUMN OF ROGOZNICA LAKE-DRAGON'S EYE IN THE AUTUMN OF 2025

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Rogozničko jezero (RJ), Zmajevo oko je jedinstveno krško prirodno i euksinično (slobodan sumporovodik u vodenom stupcu) morsko jezero smješteno na poluotoku Gradina u Rogoznici. RJ je pod stalnim utjecajem meteoroloških (ravnoteža između oborina i isparavanja, izmjena topline, učestalost ekstremnih vremenskih događaja) i oceanografskih prilika Jadrana koje mijenjaju kemijsku, biološku i mikrobiološku raznolikost unutar vodenog stupca jezera. Vertikalna stabilna stratifikacija slojeva morske vode koji se ne miješaju glavna je karakteristika RJ te je najizraženija tijekom proljetnih mjeseci [1, 2]. Stratifikacija s obzirom na temperaturu (T; termoklina), salinitet (S; haloklina), koncentraciju kisika (O_2) i toksičnog sumporovodika (H_2S; kemoklina) razdvaja površinski oksični sloj (miksolimnion, obično 0-8 m) i pridneni anoksični sloj (monimolimnion, ispod 8 m). Između miksolimniona i pridnenog monimolimniona se obično nalazi gusti, ljubičasto obojen, sloj obogaćen anaerobnim fotoautotrofnim sumpornim bakterijama tzv. kemoklina, koja je zbog relativne plitkoće, izložena brojnim promjenama fizikalno-kemijskih (T, S, O_2, intenzitet svjetlosti), ali i bioloških parametara. RJ se zbog svojih specifičnih karakteristika može smatrati i prirodnim bioreaktorom [1, 3]. Krajem ljeta i početkom jeseni, kao direktna posljedica pojačane evaporacije (krajem ljeta) i hlađenja površinskog sloja (početkom jeseni), dolazi do razbijanja stratifikacije, odnosno halokline i termokline, što dovodi do izmješavanja slojeva morske vode. Uslijed izmješavanja i oksidacije sulfida iz monimolimniona, O_2 u površinskom sloju se uvelike smanjuje, te posljedično cijeli vodeni stupac RJ postaje hipoksičan ($O_2 < 4$ mg/L) ili anoksičan ($O_2 = 0$), što je pogubno za sav živi svijet u RJ [1, 3].

U ovom radu in-situ praćenjem fizikalno-kemijskih parametara CTD sondom (termohalina gustoća, T, S, O_2, klorofil-*a* i turbiditet) vodenog stupca RJ tijekom dvije različite sezone u 2025. godini, uočeno je: 1) raslojavanje vodenog stupca u zimi (14.01.2025.) s oksičnim slojem u prvih 4 m dubine, gdje je T varirala od 9 do 14 °C, S od 33 do 35 i O_2 od 10 do 6 mg/L od 0,5 do 4 m dubine te 2) izmješavanje vodenog stupca u jesen (14.10.2025.) s uniformnim vrijednostima fizičko-kemijskih parametara ispod 0,5 m dubine (T = 19,6 °C, S = 36,6, O_2 ~ 0,5 mg/L; grafički abstrakt) kada se cijeli vodeni stupac može okarakterizirati kao hipoksičan ($O_2 < 2$ mg/L) .

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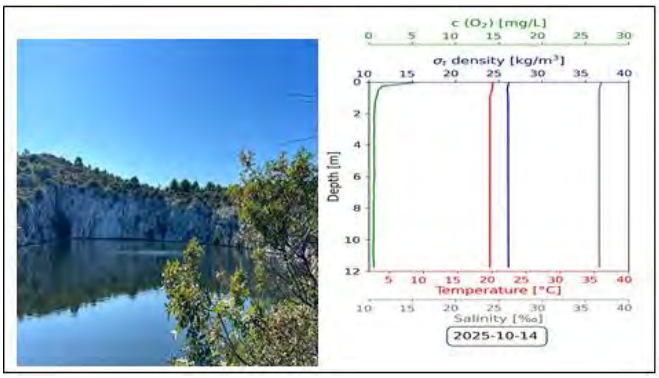
Istraživanje je omogućeno potporom Hrvatske zaklade za znanost IP-2024-05-2377- ISO-ZOKO i dijelom IP-2022-10-3064-GLOMETS.



EVALUATION OF QUINALPHOS BIOAVAILABILITY IN SOILS

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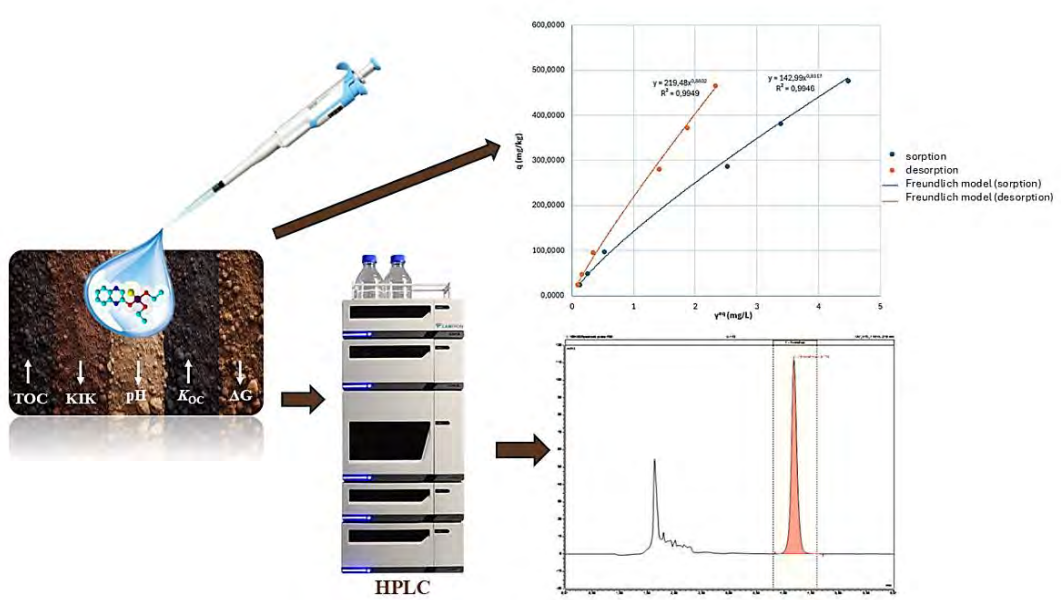
Quinalphos is an organophosphorus insecticide whose use has been banned in Croatia due to its toxicity, bioaccumulative potential and negative impact on the environment. However, due to its chemical stability and its former widespread use, this compound may still be present in agricultural soils and pose a risk to groundwater and ecosystems. Understanding the behaviour of quinalphos in soil, especially sorption and desorption processes, is crucial for assessing its environmental impact and managing contaminated areas.

In this study, the sorption-desorption behaviour of quinalphos was investigated in seven soil samples with different physicochemical properties from different regions of Croatia. Laboratory experiments were carried out to determine the sorption and desorption isotherms and to calculate the relevant sorption and desorption coefficients. In addition, multivariate statistical analyses (PCA, HCA, regression) were performed to identify dominant factors influencing the retention of quinalphos in soil.

The results showed that quinalphos exhibited selective behaviour in different soils—its sorption was most pronounced in soils with high organic matter and clay fraction content. In contrast, soils with a higher cation exchange capacity, especially those rich in calcium and magnesium, showed a lower affinity for sorption, which is due to competition between cations for sorption sites. Soil pH had a significant effect on sorption, with more acidic soils having a higher binding capacity for quinalphos. Desorption experiments indicated partial irreversibility of the process, suggesting the persistent presence of quinalphos in the surface soil layer. Multivariate analyses confirmed that the organic matter content (TOC), clay, K_{OC} and free sorption energy (ΔG) are the most important predictors for the behaviour of quinalphos in soil. The results underline the importance of site specific soil analyses in assessing the ecotoxicological risk of quinalphos.

In summary, the results of this research contribute to a better understanding of the behaviour of quinalphos in the environment and underline the need for an integrated approach to agricultural soil management that includes scientific soil analysis, the banning of high-risk compounds and the development of predictive models for pesticide behaviour under real agroecological conditions.



STUDY OF CATALYTIC POTENTIAL OF 3D-PRINTED CERAMIC MONOLITHIC CATALYSTS FOR THE OXIDATION OF VOLATILE ORGANIC COMPOUNDS

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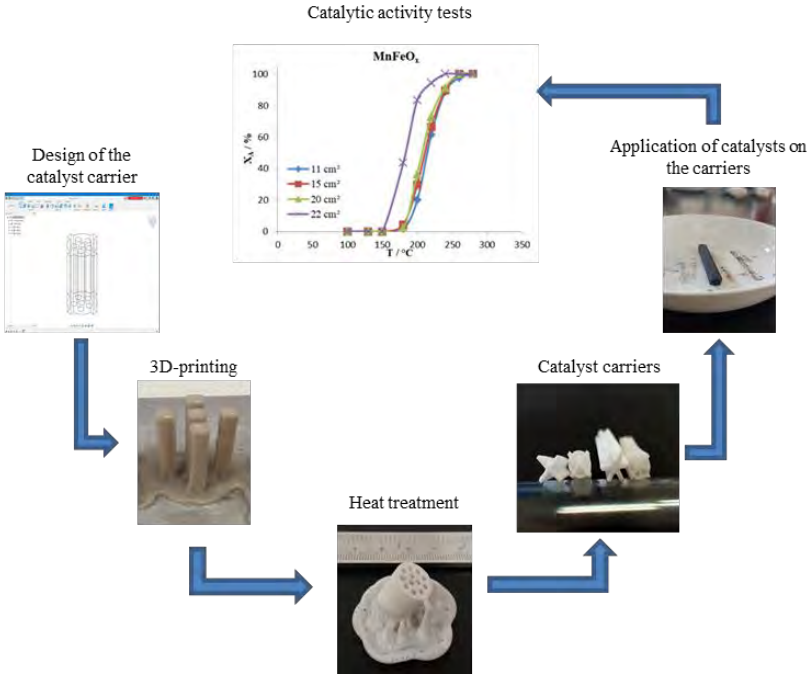
The aim of this work was to develop 3D-printed monolithic catalysts for the catalytic oxidation of aromatic volatile organic compounds. Stereolithography (SLA) and fused filament fabrication (FFF) were used to 3D-print ceramic monoliths for the catalytic oxidation of a gaseous mixture of benzene, toluene, ethylbenzene, and xylene (BTEX). This approach involves 3D-printing inert catalyst carriers and depositing the catalytically active components (mixed manganese oxides of iron, copper, nickel, cobalt and chromium) onto them using the wet impregnation technique. The prepared monolithic catalysts differed in the geometry of their channels, resulting in different geometric surface areas. Reactions were carried out in a monolithic reactor at various temperatures, with a constant initial concentration of reactants and a constant reactant-to-oxidant (synthetic air) ratio. Gaseous mixtures were analysed on-line before and after every reaction using gas chromatography. The work involved determining the optimal geometry of the monolithic catalyst carrier, optimal chemical composition of the catalytic layer on the 3D-printed ceramic monolithic catalyst carriers, and comparison of the results obtained using SLA and FFF technology with commercial cordierite monolithic catalyst. The prepared monolithic catalysts exhibited excellent mechanical stability and high performance, achieving high conversion values (>99 %) for all BTEX components at temperatures below 250 °C.



PYROPHYLITE COMPOSITE OBTAINED BY DISPOSING RED MUD AS A RAW MATERIAL FOR THE PRODUCTION OF BUILDING MATERIALS

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Although red mud is a toxic waste stream produced by the processing of bauxite ore to alumina, using the Bayer process, it contains valuable materials such as rare earth elements, silicon, titanium, iron, aluminum, sodium and calcium that are not exploited just by dumping them in a landfill. Since large amounts of red mud are produced annually, about 150 million tons, the methods of recycling those elements are not very practical and cost-effective for such amounts of red mud, so it is increasingly used for the production of construction materials, wastewater treatment, etc.
The aim of this work was to examine the possibility of stabilizing red mud with a natural mineral, i.e. pyrophyllite slate, to the extent that it is not harmful to the environment, as well as the use of such a stabilized composite for the production of building materials such as bricks, in order to eventually achieve a complete circle of cir cular economy, where on the one hand there would be the use of waste material, preservation of the environment and natural resources, and on the other hand obtaining products of the same quality.
Based on the set goal, the paper presents the results for the composition of red mud and pyrophyllite schist as well as the stabilized composite before and after heat treatment at 900 °C, and they show that there is a reduction in the proportion of all oxides present in the mixture except for silicon, because it has over 63 % in pyrophyllite schist. Based on the stabilized composite, clay building block samples were formed with composite proportions of 0 %, 20 %, 40 % and 60 %, and based on all the tested properties, it was concluded that sample 1 with 20 % composite proportion had the best results, both in terms of compressive strength and water absorption properties, and that it represents an economically, environmentally and technologically acceptable method of red mud disposal through the formation of a building block.

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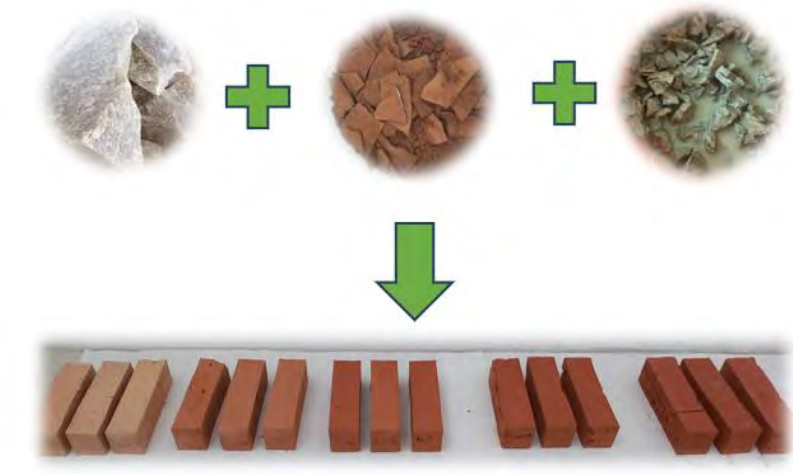

MATHEMATICAL MODELING AND OPTIMIZATION OF VILSMEIER FORMYLATION FOR EFFICIENT FLOW PROCESSING

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In recent years, considerable attention has been directed toward developing compounds to treat neurological disorders such as Alzheimer's and Parkinson's disease, as well as to counteract organophosphate poisoning from pesticides and nerve agents. Oximes are of particular interest for their ability to reactivate acetylcholinesterase and butyrylcholinesterase, enzymes inhibited in these conditions. Stilbene derivatives, including resveratrol analogues, are also recognized for their therapeutic potential. Introducing oxime functionality into stilbenes offers a way to enhance or diversify bioactivity. Such oximes can be prepared from stilbenes *via* a two-step route starting with formylation, commonly achieved through the Vilsmeier reaction using dimethylformamide (DMF) and phosphoryl chloride ($POCl_3$) [1]. This highly exothermic process poses safety risks in batch mode, whereas continuous millireactor systems provide superior heat control and improved process safety [2].
In this study, the Vilsmeier formylation of a stilbene compound was investigated and optimized using a mathematical modeling approach. The resulting product serves as a key intermediate in the synthesis of a bioactive oxime, and the optimization aimed to facilitate transfer to a continuous-flow reactor [3]. The model was developed based on batch experiments and successfully validated in both a batch reactor and a continuous millireactor. Under optimized conditions, the process exhibited significant improvements in efficiency, while the continuous-flow process enhanced safety compared to batch operation due to improved thermal control, which minimized the risk of localized overheating. These results demonstrate the potential of continuous-flow technology for safer and more sustainable processing of highly exothermic reactions such as Vilsmeier formylation.

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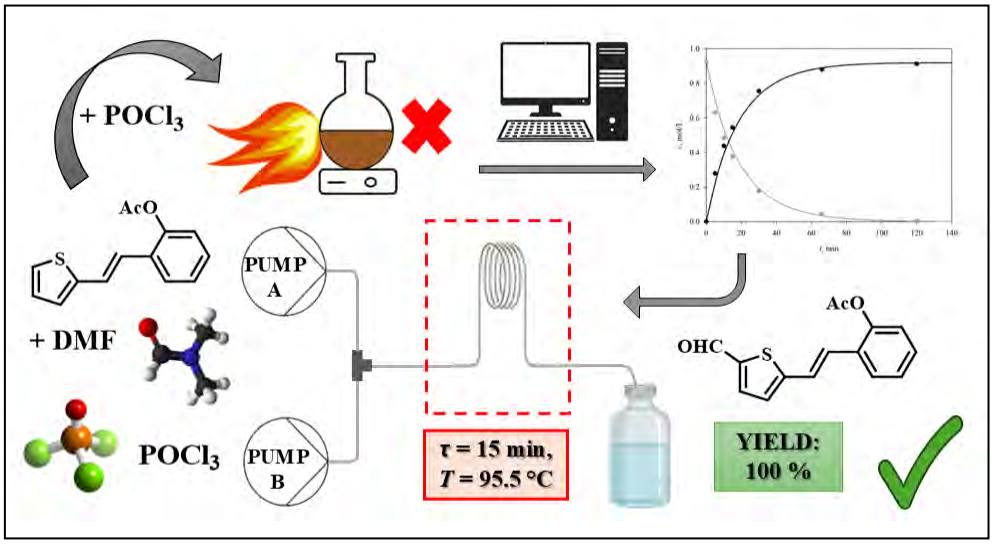

IRON-CATALYZED OXYGEN MIGRATION IN P–O–C CROSSLINKED CARBON: TRANSFORMING HAZELNUT SHELL–DERIVED ACTIVATED CARBON INTO HIERARCHICAL TURBOSTRATIC CARBON NANOSHEETS

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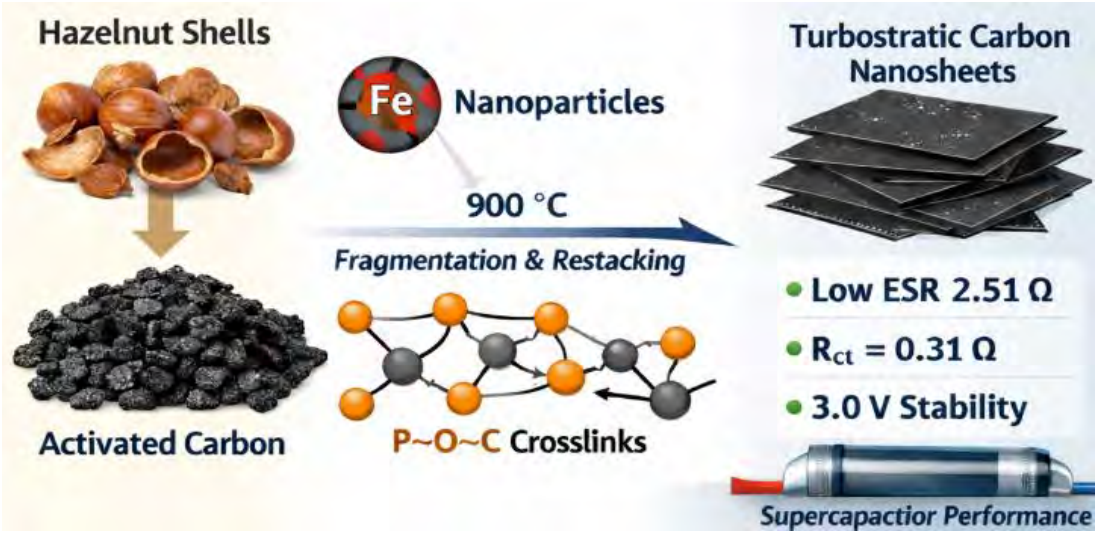
Phosphoric acid–activated biomass carbons possess high surface area but are structurally constrained by rigid phosphorus–oxygen–carbon (P–O–C) crosslinks that suppress graphitic ordering and limit electrical conductivity [1]. In this work, hazelnut shell–derived activated carbon is transformed into hierarchical turbostratic carbon nanosheets via a transient catalytic strategy using ferrocene-derived iron nanoparticles. During high-temperature treatment, short-lived Fe nanoparticles selectively reorganize P–O–C crosslinks, inducing an amorphous-to-turbostratic fragmentation–restacking transition. This restructuring converts bulk crosslinked carbon into thin, restacked turbostratic nanosheets, increases coherent stacking height (Lc: 1.15 → 1.70 nm), and enhances micropore volume by 71 % through the formation of slit-shaped pores between nanosheets. Simultaneously, phosphorus migrates from the bulk to nanosheet edges, passivating high-energy sites generated during fragmentation. As a result, symmetric supercapacitors based on turbostratic nanosheets exhibit a 42 % reduction in equivalent series resistance (to 2.51 Ω), the emergence of discrete charge-transfer resistance (Rct = 0.31 Ω), and stable operation up to 3.0 V with 95.3 % capacitance retention. These results demonstrate that transient catalytic crosslink transformation enables the rational design of turbostratic carbon nanosheets that reconcile high porosity with robust electronic transport in sustainable biomass-derived carbons.

[1] I. Neme et al., Heliyon 8 (2022) 1–12



ENGINEERING AND APPLICATION OF A CORE-SHELL MAGNETIC NANOCATALYST FOR BIO-BASED COMPOUND HYDROGENATION

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As the world faces a necessary transition from traditional fossil-fuel energy sources to new, greener ones, scientists and engineers put tremendous effort in the research, development, and application of new materials which could facilitate this process. One such renewable energy source is biomass. Woody biomass is rich in natural C5 and C6 sugar polymers. For example, acid hydrolysis decomposes these polymers to useful platform chemicals, such as furfural, 5-hydroxymethylfurfural (HMF), sometimes referred to as the „sleeping giant of sustainable chemistry“, and levulinic acid [1–3]. The processing of these platform chemical leads to value-added compounds which find their application in various industrial branches, such as pharmaceutics, fuel industry, cosmetics, to mention a few [4]. Furfural is one of the most important biomass platform chemicals due to its reactive groups (aldehyde group and unsaturated furan ring), which enables the yield of different value-added chemicals through furfural hydrotreatment. Some important products of furfural hydrogenation are: furfuryl alcohol (FA), tetrahydrofurfuryl alcohol (THFA), 1,2-pentanediol and 1,5-pentanediol [5].

Due to the thermal instability of bio-based compounds, the idea of this work is to propose electrified furfural hydrogenation by using magnetic heating of the catalyst. This enables contactless heating of the catalyst slurry within the batch reactor while bulk of the medium remains at substantially lower temperature The prepared catalyst is a nanocomposite composed of iron oxide nanoparticles, which serve as a heat source, nanolamellar γ-Al_2O_3 as a catalyst support, and Ru as a catalytic material [2,6]. A comparison between magnetically- and conventionally-heated batch reactor system is performed and compared in order to gain an insight into the pathway of furfural-to-value-added products reaction.

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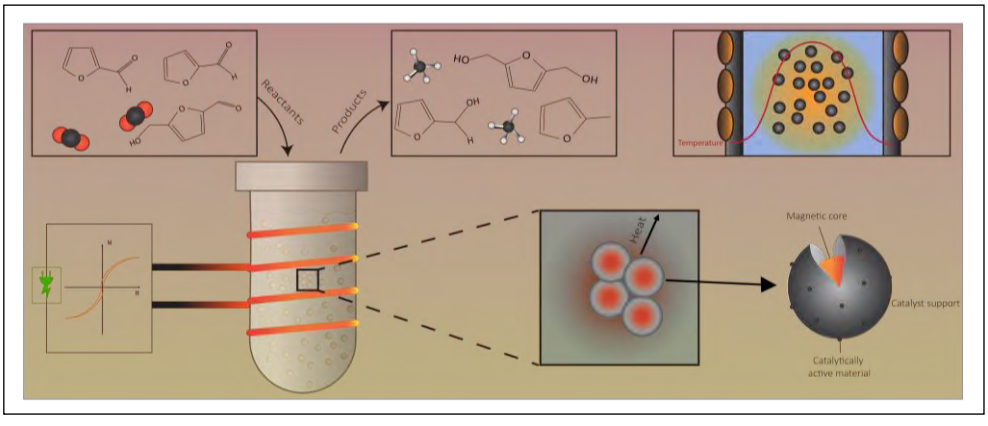

UTVRĐIVANJE UTJECAJA POJEDINIH SASTOJAKA NA REOLOŠKA SVOJSTVA SUSPENZIJA ZA IZRADU POZITIVNIH ELEKTRODA ZA LITIJ IONSKE GALVANSKE ČLANKE

DETERMINATION OF THE INFLUENCE OF INDIVIDUAL INGREDIENTS ON THE RHEOLOGICAL PROPERTIES OF SLURRIES FOR THE PRODUCTION OF POSITIVE ELECTRODES FOR LITHIUM ION BATTERIES

Hrvoje Tašner, Grgur Mihalinec, Zoran Mandić

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Proizvodnja litij-ionske baterije uključuje nekoliko ključnih koraka: pripremu paste (miješanje aktivnih materijala, veziva i otapala za katodu i anodu), premazivanje i sušenje na metalnim folijama (aluminij za katodu, bakar za anodu), rezanje elektroda, namatanje elektroda, ubrizgavanje elektrolita, zatvaranje članka i formiranje (inicijalno punjenje/pražnjenje za stabilizaciju).

Priprema paste jedan je od ključnih koraka u procesu proizvodnje elektroda za litij ionske galvanske članke. Svojstva paste, poput udjela suhe tvari, omjera sastojaka, viskoznosti, disperziranosti krutih čestica i drugih, direktno utječu na mikrostrukturu gotove elektrode. Mikrostrukturne karakteristike elektroda određuju dugovječnost, kapacitet i snagu te retenciju kapaciteta litij-ionskih galvanskih članaka. Stoga je postizanje optimalne mikrostrukture ključno za unaprjeđenje litij ionskih galvanskih članaka.

U ovom radu istraženo je reološko ponašanje paste i smjesa sastojaka za izradu pozitivnih elektroda. Cilj rada je određivanje doprinosa pojedinih sastojaka na reološka svojstva konačne smjese. Razumijevanjem reologije omogućava se optimizacija i unaprjeđenje procesa miješanja elektrodne paste te njenog nanošenja na strujni kolektor.

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Ovaj rad poduprt je kroz projekt NPOO.C3.2.R3-I1.04.0187: Razvoj novih materijala te naprednih inovativnih tehnologija za proizvodnju litij-ionskih baterija.

IN VITRO CELL VIABILITY ASSESSMENT OF FATTY ACID-BASED COATINGS ON STAINLESS STEEL FOR BIOMEDICAL APPLICATIONS

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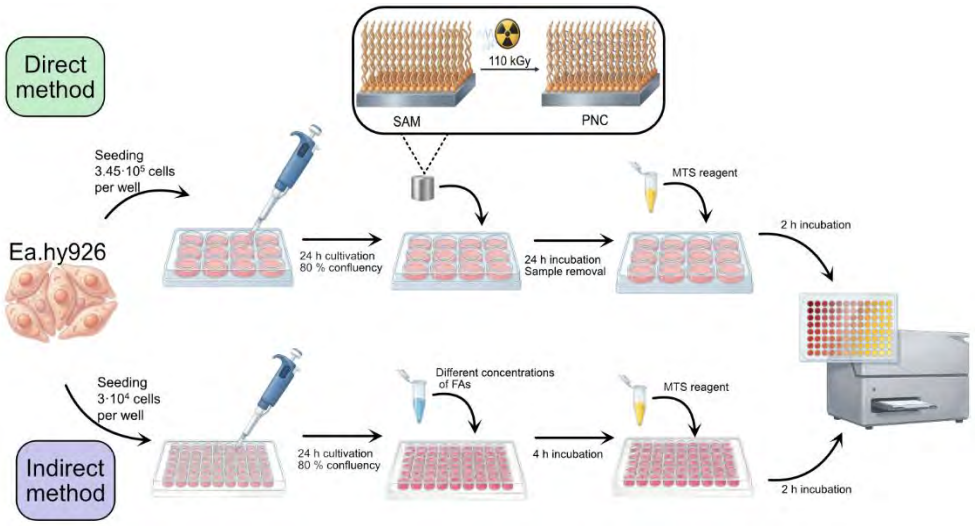
Biomedical stainless steel, often used as a metallic implant material, can be functionalised with fatty acids (FAs) to ensure long-term stability in the human body. FA chain length and degree of saturation determine their physicochemical properties and biological responses. Saturated, monounsaturated, and polyunsaturated FAs have distinct roles in cellular signalling, metabolism, inflammatory processes, and tissue regeneration. Due to these differences, it is important to identify which classes of FAs are most suitable for specific biomedical applications. FAs have the ability to form densely packed self-assembled monolayers (SAMs) on metal surfaces. To further enhance FA properties, they can be radiation-crosslinked on the metal surface to form a polymer nanocoating (PNC). Although FAs are naturally present in the human body and are degraded into non-toxic byproducts, their crosslinking on metallic implant surfaces may alter their chemical structure and consequently affect the biological properties of the surface. This study investigates the cell viability of selected saturated (octanoic, stearic, behenic), unsaturated (elaidic, oleic) and polyunsaturated (linoleic) FAs using the human endothelial cell line Ea.hy926 in accordance with ISO 10993-5. The indirect method was used to obtain cell viability data from FA extracts. In the direct method, cells were exposed to the functionalised metal surfaces (SAM and PNC) through direct contact for 24 hours and cell viability was measured. A correlation between molecular structure and cellular response was identified, offering insight into the mechanisms underlying cellular interactions with fatty acids.

This work was supported by the Croatian Science Foundation (HRZZ MOBDOK-2023-7329).



MORIN-CYCLODEXTRIN/PCL NANOFIBER SCAFFOLDS FOR SUSTAINED BONE REGENERATION

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Bone tissue engineering necessitates sophisticated biomaterials capable of delivering bioactive agents, such as the osteogenic flavonoid morin, whose clinical utility is often hampered by low solubility and poor bioavailability [1]. This study introduces a novel phytopharmaceutical delivery system by synergistically combining supramolecular inclusion complexation with electrospinning technology to create functional scaffolds for sustained osteoinduction.
The complexation of morin with three distinct hydroxypropyl-cyclodextrin (HP-CD) derivatives, HP-α-CD, HP-β-CD, and HP-γ-CD, was systematically investigated to identify the optimal host-guest interaction for enhancing morin's physicochemical properties. Computational modeling, including molecular dynamics and docking simulations, was employed to accurately predict the geometric fit and stability of morin within the varying hydrophobic cyclodextrin cavities. Subsequently, the optimized inclusion complexes were successfully integrated into a poly(ε-caprolactone) (PCL) matrix via electrospinning [2]. Morphological analysis using Optical Microscopy and Scanning Electron Microscopy (SEM) revealed that the incorporation of the cyclodextrin complexes induced a beneficial transition from a typical smooth fiber morphology to a characteristic "beads-on-string" architecture . These "beads" function as micro-reservoirs, effectively encapsulating the drug payload and mitigating the undesirable "burst release" phenomenon prevalent in conventional nanofiber systems.
Furthermore, *in vitro* release profiling demonstrated that the cyclodextrin-modified fibers significantly modulate the release kinetics. The nanofiber-encapsulated complexes provide a protective microenvironment that significantly slows degradation, thereby ensuring the sustained and controlled release of the bioactive morin. This work confirms that the synergistic combination of cyclodextrin complexation and electrospun PCL nanofibers yields a superior, bioactive scaffold with high translational potential for orthopedic regenerative applications.

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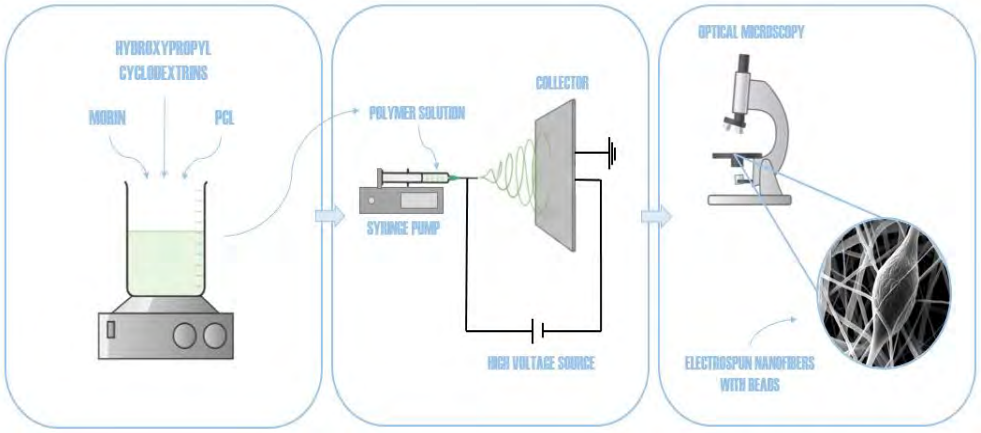
This research was funded by the Croatian Science Foundation through the project IP-2024-05-4339 entitled "Coffee ring' effect in 'Lab on a Chip' environments in the development of new drug formulations.", leader prof. Ernest Meštrović.



FROM DEWETTING-INDUCED MORPHOLOGY TO CELL ADHESION: POLYMER SUBSTRATES FOR *IN VITRO* STUDIES

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An important aspect of tissue engineering is the appropriate selection of substrates that enable control over cell distribution on their surface. Substrates used for cell culture can significantly influence cell adhesion, proliferation, and directed cell growth.
The aim of this study was to obtain substrates with controlled surface morphology using the dewetting phenomenon of polymer films on glass microscope slides, followed by the evaluation of their physicochemical and biological properties in the context of potential applications in cell culture.
Substrates with controlled morphology were obtained via the dewetting process, which involves the disintegration of an unstable polymer film under the influence of external factors. One of the key factors is the application of a polar solvent, in which the polymer layer is melted. As a result of this process, polymer droplets are formed on the substrate and subsequently solidify, creating an array of hemispherical particles [1].
In this study, polycaprolactone (PCL) was used as a surface-modifying material for cell culture substrates. The morphology of polymer films and particles was characterized using optical microscopy, atomic force microscopy (AFM), scanning electron microscopy (SEM), and contact angle measurements.
The application of the dewetting process enabled the fabrication of substrates with controlled morphology. A correlation between the thickness of the polymer film on the glass substrate and the size of the resulting particles was observed, with thicker films leading to the formation of larger particles. The obtained structures exhibited varied hydrophobicity depending on the degree of substrate modification. In vitro studies showed that the modified substrates did not induce cytotoxic effects and revealed differences in cell growth compared to unmodified glass substrates.

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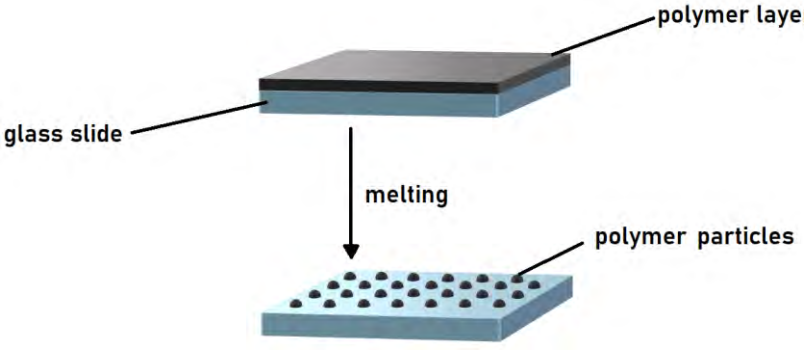

Preparation of surface-supported polymer particles by melting polymer layer in contact with polar solvent.

MECHANOCHEMISTRY FOR SUSTAINABLE GUANIDINE SYNTHESIS

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Mechanochemical synthesis offers several significant advantages over traditional solution methods. Firstly, it substantially reduces or even eliminates the need for solvents, making reactions greener, more environmentally benign, avoiding the waste and toxicity associated with solvent use [1-4]. Secondly, mechanochemistry can enable reactions that are challenging or impossible in solution, such as those involving insoluble solids or reagents that interfere with solvents. This approach can also lead to increased reaction efficiency, shorter reaction times, and higher yields [5-6]. Our investigation focuses on the mechanochemical synthesis of novel trisubstituted guanidine derivatives, a vital class of organic compounds found in both natural sources and pharmaceutical applications [7]. This synthesis proceeds from isothiocyanates, which react with amines to form thioureas through mechanochemical processes, followed by the conversion of these thioureas into guanidines. A key objective is to demonstrate these reactions employing diverse desulfurization reagents, with the intent of replacing hazardous substances like mercury-based reagents, traditionally used in such syntheses, with greener alternatives such as silver, iron, or bismuth-based reagents [8,9]. To quantify the environmental benefits, this study will also include the calculation of green metrics such as Process Mass Intensity (PMI), Atom Economy (AE), Reaction Mass Efficiency (RME), and E-factor, illustrating how mechanochemical approaches often lead to improved sustainability compared to conventional solution methods [2,6]. This study, incorporating traditional methods for transforming thioureas into guanidines, aims to develop more sustainable and environmentally conscious synthetic routes for guanidines.

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This work is financially supported by the Croatian Science Foundation (grant No IP-2022-10-4385, Space-G).

COLOURIMETRIC DETECTION OF PHYSIOLOGICALLY RELEVANT BIOMARKERS FOR WEARABLE APPLICATIONS USING COVALENTLY IMMOBILISED AZO DYES ON CELLULOSE

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Azo dyes represent a versatile class of organic chromophores widely used in optical sensing due to their strong visible-light absorption, structural tunability, and chemical robustness. Of particular interest are vinylsulfonyl functionalized azo dyes, which enable efficient covalent immobilization via Michael addition onto hydroxyl-rich substrates, such as cellulose [1, 2]. Various cellulose-based materials including paper, textile, thin transparent cellulose films, cellophane, and cellulose microparticles offer biocompatibility and diversity in terms of optical and application properties, making them attractive platforms for the development of optical sensors for wearable applications [3]. By tailoring substituents on the benzene and naphthalene rings, the sensing properties of azo dyes can be systematically tuned, enabling the detection of different target analytes. In this work, we developed optical sensors for Mg^{2+} ions based on covalently immobilized pH-sensitive azo dye Hyphan I on both thin transparent cellulose film and paper. The sensing system was optimized at pH 8 and exhibited a wide dynamic range (0.625-100 mM), excellent reversibility, high stability, biocompatibility and negligible influence of common physiological interferents such as Na^+, K^+ and Ca^{2+}. The observed pK_a values, 5.84 for film and 5.63 for paper, demonstrate matrix-dependent behavior while remaining suitable for applications such as sweat pH analysis. Furthermore, a printed biosensing platform for urea detection is currently under development. Cellulose microparticles with covalently immobilized pH-sensitive azo dye were dispersed within a hydrogel together with enzyme urease. Urease driven hydrolysis of urea leads to a local increase in pH, which induces a measurable colour change of the immobilised dye and provides a straightforward way of quantifying urea. This approach highlights the potential of cost-efficient, biocompatible, and easily fabricated cellulose-based optical biosensors for monitoring physiologically relevant analytes.

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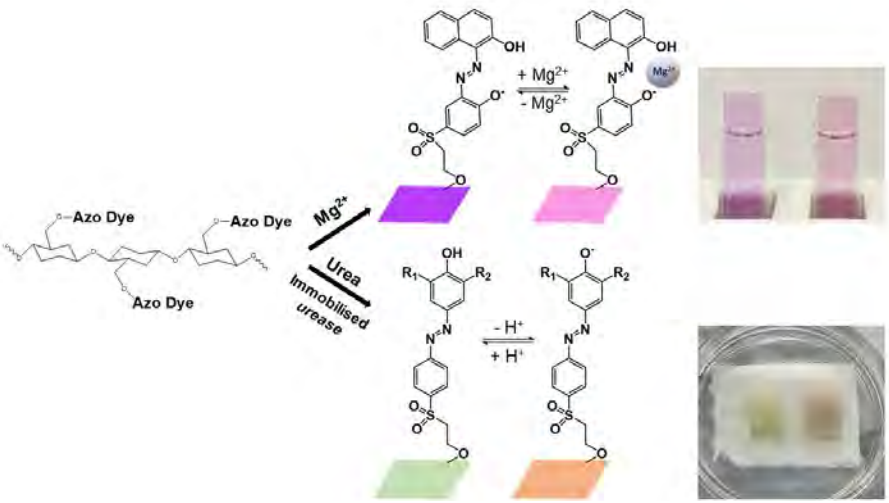

RAČUNALNI DIZAJN KIRALNIH CIKLOPENTADIENILNIH KATALIZATORA SA PODESIVIM STERIČKIM ELEMENTIMA

COMPUTATIONAL DESIGN OF CHIRAL CYCLOPENTADIENYL CATALYSTS WITH TUNABLE STERIC ELEMENTS

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Kiralni ciklopentadienilni (Cp) ligandi uvelike se koriste u reakcijama kataliziranim prijelaznim metalima za postizanje stereoselektivnih transformacija. Kiralni Cp-ligand koordinira atom prijelaznog metala, a sami Cp-prsten moguće je modificirati dodatnim supstituentima koji utječu na različita sterička i elektronska svojstva [1, 2]. Do sada istraženi kiralni Cp-ligandi s 3,3'-metoksi binaftilnom okosnicom te trisupstituiranim Cp-prstenom pokazali su se vrlo efikasnim, naročito kada sadrže voluminozne skupine poput *tert*-butilne. Dva su se glavna molekulska deskriptora pokazala važnima za dizajniranje kiralnih Cp-liganada, a to su postotak ukopanog volumena te stereotopografske mape [3].
U ovom radu je prikazan dizajn novog Co(III) Cp-katalizatora s binaftilnom okosnicom i dvije fenilne skupine na Cp-jezgri. Dizajnirani katalizator ima vrlo sličan ukopani volumen (50.4 %) prethodno poznatim katalizatorima (50.3 %) [3], ali različita stereoelektronska svojstva, što omogućava detaljno istraživanje utjecaja molekulskih deskriptora te ugađanja katalitičkih svojstava u asimetričnoj sintezi. DFT računalna istraživanja reakcijskih mehanizama i enantioselektivnosti u Co(III)-kataliziranoj anulaciji *N*-klorbenzamida sa stirenom pokazala su da je prilaz stirena ligandu stereodeterminirajući korak reakcije. Pritom je povoljnija reakcija sa strane Cp-fenila, radi stabilizirajućih π-π aromatskih interakcija. Aktivacijske barijere pokazuju da supstitucija liganda s metoksi skupinama na položajima 3,3' ne utječe značajno na katalitičku efikasnost, a posljedično i regio- te enantioselektivnost. Takvi pristupi otvaraju nove mogućnosti prema što učinkovitijoj pripravi i upotrebi kiralnih Cp- katalizatora.

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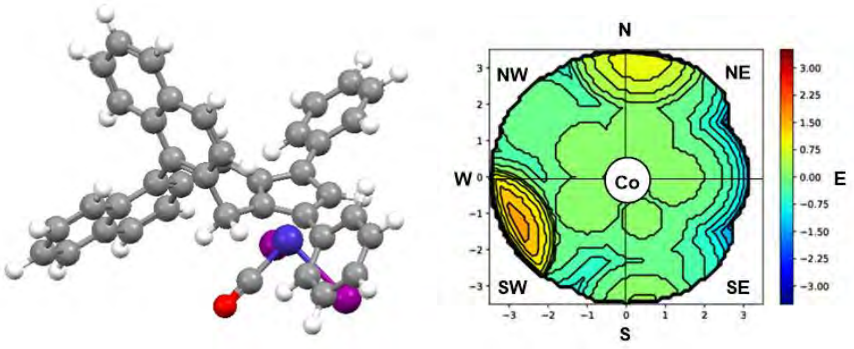

SYNTHESIS, INTERACTION WITH CT-DNA AND UV/VIS pH TITRATION OF NEW PYRIDINE DERIVATIVES

Antonija Mamić[1], Ena Kraljić[1], Iva Kulušić[1], Paula Šimunić[1], Kristina Butković[2], Leentje Persoons[3], Dirk Daelemans[3], Marijana Radić Stojković[4], Marijana Hranjec[1]

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Nitrogen containing heterocycles play a significant role in medicinal chemistry and pharmacology due to their wide range of biological activities. Among them, pyridine and its derivatives possess many properties including polarity, basicity, and hydrogen bond-forming capacity which are important for interactions with biological targets [1]. In this work, we prepared new pyridine benzamides and acrylonitriles in order to investigate the pH-sensing potential of hydroxy substituted benzamides and the interaction of acrylonitriles with ct-DNA, as well as the antiproliferative activity *in vitro* of all synthesized derivatives against several human cancer cell lines. Starting from methoxy substituted benzoyl-chlorides and 2-aminopyridines, methoxy substituted benzamides were synthesized, followed by demethylation with BBr_3 to obtain the corresponding hydroxy derivatives [2]. On the other hand, acrylonitriles were prepared via an addition reaction between differently substituted benzaldehydes and acenonitriles in methanol, using $NaOCH_3$ as a base [3]. The structures of the newly prepared compounds were confirmed by means of ^1H and ^{13}C NMR spectroscopy and mass spectrometry. pH spectroscopic titrations in buffered aqueous solutions were performed to evaluate their potential application as pH sensors.

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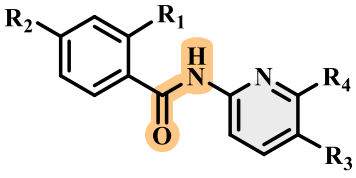
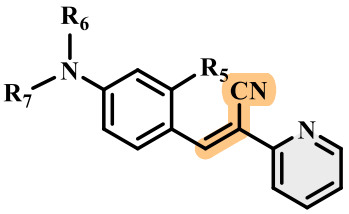


R_1 - R_4 = H, OH



R_5 - R_7 = H, CH_3, CH_2CH_2CN, CH_2CH_2Cl

STRUCTURALLY EXPANDED MOF-74 DERIVATIVES DERIVED BY THERMO-MECHANOCHEMISTRY

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MOF-74 materials are metal-organic frameworks (MOFs) composed of divalent metal ions and 2,5-dihydroxyterephthalic acid (dhta) or 4,6-dihydroxyisophthalic acid (dhia) linkers in a 2:1 ratio [1,2]. They represent one of the most thoroughly investigated families of metal-organic frameworks because of their high stability and unique properties [3]. They are characterized by a hexagonal honeycomb structure with one-dimensional channels and exhibit exceptional properties, including high surface area, tunable porosity, thermal stability, and magnetic behavior, making them attractive for a wide range of applications [4]. The MOF-74 materials can be precisely tailored by varying the metal center and/or organic ligand [5]. This enables fine-tuning of structural features and properties, which expands their application potential. Although solvothermal synthesis is still the conventional method for MOF preparation, these materials can be synthesized significantly faster and more efficiently via mechanochemical methods. A mechanochemical reaction is defined as a chemical transformation induced by the direct absorption of mechanical energy [6]. It allows reduced reagent consumption, higher yields, minimal use of solvents, and substantial savings in energy and time.
In this work, we developed a thermo-mechanochemical approach [5] for a rapid, controllable, and efficient synthesis of expanded MOF-74 employing zinc(II) ions as metal centers and 4,4′-dihydroxy-[1,1′-biphenyl]-3,3′-dicarboxylic acid (bidhia). Furthermore, two-step thermo-mechanochemical synthesis enabled the preparation of a coordination polymer intermediate with 1:1 metal to ligand stoichiometric composition [7], enabling synthesis of a unique, bimetallic bidhia-MOF-74 analogue incorporating both zinc(II) and magnesium(II) cations.

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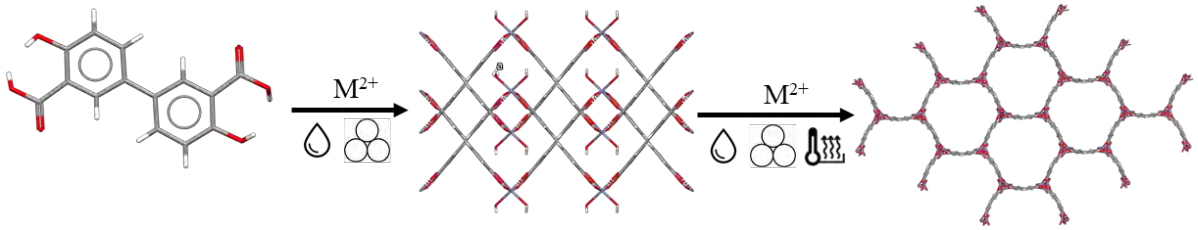

VANADIUM COMPLEXES FOR SELECTIVE OXIDATION OF SUBSTITUTED BENZYL ALCOHOLS

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Selective oxidation of alcohols is a key transformation in organic synthesis, with broad applications in fine chemicals, pharmaceuticals and food industries [1–3]. Substituted benzyl alcohols can be oxidized to the corresponding benzaldehydes or further to benzoic acids depending on reaction conditions, catalyst structure and the oxidant employed [4,5]. Achieving high selectivity towards the aldehyde products while minimizing overoxidation or competing side reactions remains a persistent challenge.

A series of vanadium complexes were synthesized using hydrazide-based ligand derived from 4-methoxysalicylaldehyde and iso-nicotinoylhydrazide, employing different alcohols as reaction media. The incorporation of solvent molecules led to a series of vanadium catalysts featuring different alcohols coordinated at the vanadium centre. The catalytic performance of these complexes was evaluated in the selective oxidation of *p*-substituted benzyl alcohols to the corresponding aldehydes using *tert*-butyl hydroperoxide in aqueous medium. Also influence of various co-solvents on activity and selectivity was systematically investigated. Catalytic performance was assessed relative to the reference vanadium system.

Our investigation of the catalytic activity of selected vanadium complexes in the oxidation of *p*-substituted benzyl alcohols revealed that both the coordination environment around the V(V) centres and the choice of co-solvent have a significant impact on catalytic performance. These results underscore the critical influence of reaction conditions on reaction pathways and provide valuable insights for the rational design of efficient and tunable vanadium catalysts for selective oxidation of substituted benzyl alcohols.

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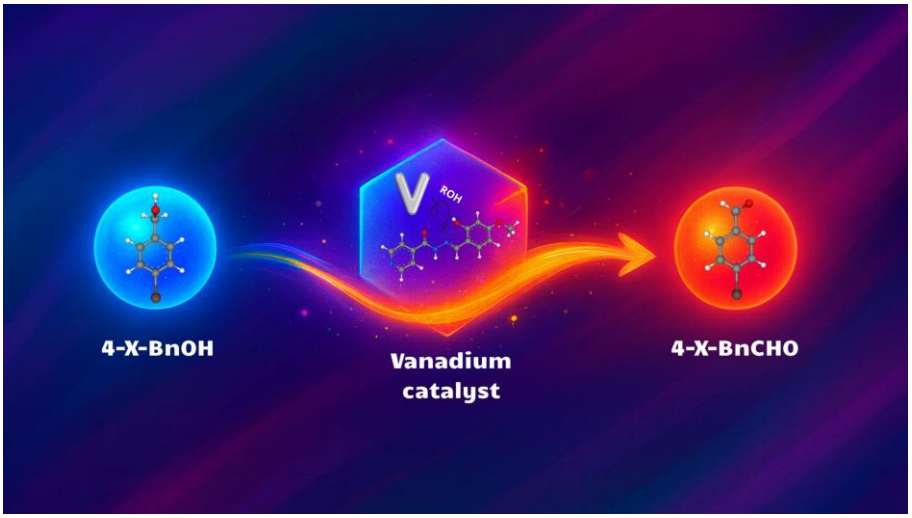

ALDO-KETO REDUCTASE INHIBITORY AND STEROID RECEPTOR-BINDING ACTIVITIES OF POLYPHENOLICS FROM *FISTULINA HEPATICA* EXTRACTS

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Edible macrofungi are increasingly valued, not only as nutrient-rich foods but also as sources of bioactive metabolites with health-promoting potential [1]. To evaluate the bioactivity of *Fistulina hepatica*, 70% EtOH and H_2O extracts were examined for interactions with steroid-regulated pathways relevant to metabolic and hormone-dependent disorders. Binding affinities toward the ligand-binding domains (LBDs) of estrogen receptor α (ERα), estrogen receptor β (ERβ), androgen receptor (AR), and glucocorticoid receptor (GR) were assessed, together with inhibitory effects against aldo-keto reductases AKR1C3 and AKR1C4, key enzymes in steroid metabolism. LC-MS/MS revealed distinct polyphenolic profiles, and PCA linked composition to biological activity.

LC-MS/MS analysis revealed distinct polyphenolic profiles, with the 70% EtOH extract enriched in quinic (500.77 ± 3.02 ng/mL d.w.) and cinnamic acids (94.45 ± 0.69 ng/mL d.w.), while the H_2O extract contained higher levels of protocatechuic (300.65 ± 2.02 ng/mL d.w.) and *p*-hydroxybenzoic acids (83.76 ± 0.89 ng/mL d.w.); amentoflavone was detected at low levels in both extracts [1]. Neither extract bound ERα, ERβ, or AR, whereas selective GR binding was observed, strongest for the 70% EtOH extract and comparable to prednisolone. Both extracts inhibited AKR1C3 and AKR1C4, with the H_2O extract showing the highest activity, in some cases exceeding ibuprofen (70.32% and 62.37%, respectively). Overall, the H_2O extract demonstrated the most potent dual AKR1C3/AKR1C4 inhibitory profile, highlighting the prominent role of polar constituents in AKR inhibition. PCA linked AKR inhibition to *p*-hydroxybenzoic and protocatechuic acids, while GR binding correlated with cinnamic, quinic, *p*-coumaric, and caffeic acids.

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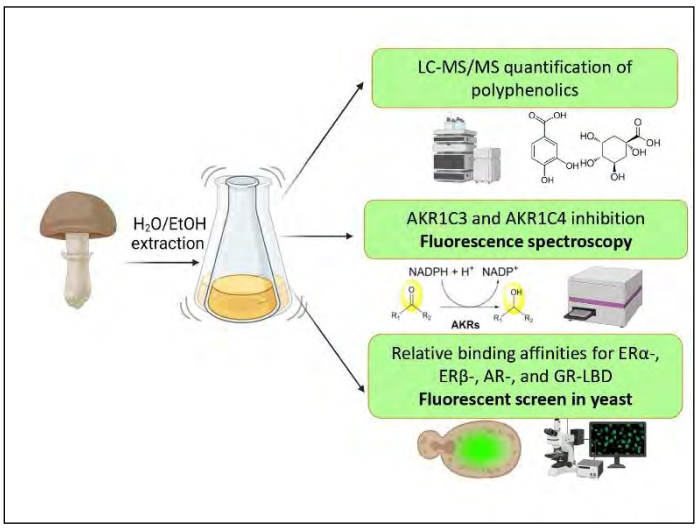

PRIPRAVA I KARAKTERIZACIJA ČVRSTE FORMULACIJE LIJEK-POLIMER EKSTRUDIRANJEM

PREPARATION AND CHARACTERIZATION OF A SOLID DRUG-POLYMER FORMULATION

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Poli(laktid-*ko*-glikolid) (PLGA) kopolimeri privlače pažnju kao nosači za lokalnu dostavu lijeka zbog svoje biokompatibilnosti i biorazgradivosti [1]. Lokalna dostava je način dostave lijeka koji zaobilazi gastrointestinalni trakt i djeluje direktno na mjestu primjene uz istodobno smanjenje nuspojava [2]. Pronalazi primjenu i u kirurgiji, gdje polimer pomaže zarastanju i fiksiranju tkiva uz istodobno oslobađanje lijeka [1]. Za pripravu čvrste formulacije lijek-polimer korišten je ekstruder pri temperaturi namješavanja do 130 °C, brzinama kontrarotacijskih vijaka do 60 min^{-1} i vremenima namješavanja do 5 min. Udio lijeka u formulaciji varirao je od 1 do 20 mas. %. Priređnim formulacijama analizirana je molekulska masa, toplinska stabilnost i toplinski prijelazi kako bi se utvrdio utjecaj parametara namješavanja na svojstva formulacije, odnosno je li došlo do degradacije komponenata formulacije. Mehanička svojstva čvrstih formulacija karakterizirana su kidalicom te im je određena tvrdoća po Vickersu, što nam daje dodatan uvid u primjenska svojstva.

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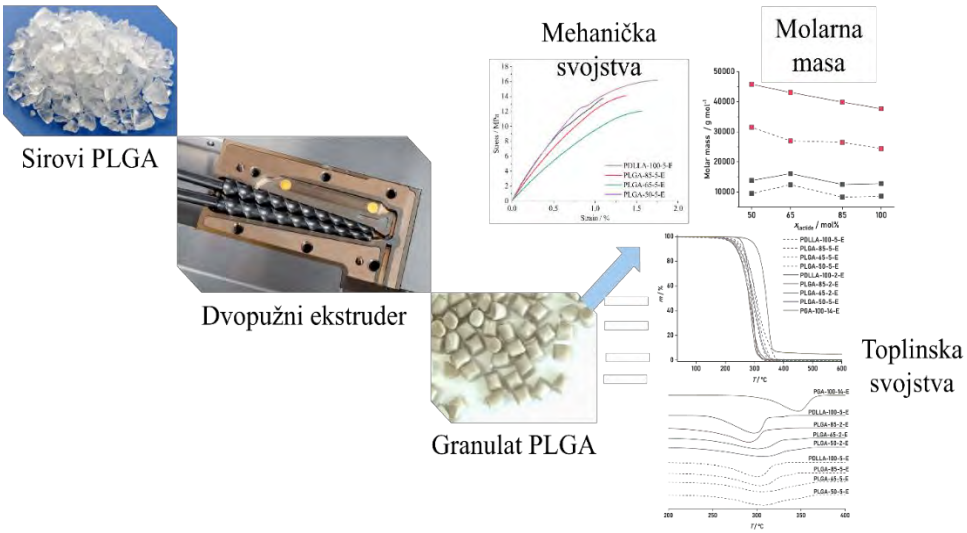

KINETIKA TOPLINSKE RAZGRADNJE PLGA KOPOLIMERA – UTJECAJ SASTAVA I MOLEKULSKE MASE

THERMAL DEGRADATION KINETICS OF THE PLGA COPOLYMER – EFFECT OF COMPOSITION AND MOLAR MASS

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Poly(lactic-co-glycolic acid) (PLGA) is a linear, biodegradable copolymer composed of randomly distributed lactide and glycolide units. Due to its biodegradability, biocompatibility, and ability to enable sustained drug release, PLGA is widely used as a drug delivery carrier [1]. Since polymer materials are often subjected to thermal processing during the preparation of drug delivery systems, factors such as processing temperature, atmosphere, and water content are crucial for optimizing the procedure, underscoring the importance of comprehensive characterization [2].

The thermal degradation of polymers can be described by kinetic equations, through which activation energy, pre-exponential factor, and reaction mechanism are evaluated [3]. To determine the thermal degradation kinetics of PLGA copolymers, isoconversional methods are used to calculate activation energies without assuming a specific reaction model, with the most widely used approaches being Friedman, Flynn–Wall–Ozawa, Kissinger–Akahira–Sunose, and Criado methods [4].

In this study, PLGA copolymers with varying compositions (50–100% PLA) and molar masses were thermally characterized using thermogravimetric analysis (TGA) at four heating rates (2, 5, 7, and 10 K·min^{-1}). It was found that the thermal degradation of PLGA may follow a multi-step process, with changes in activation energy and reaction mechanism depending on lactide content and molar mass.

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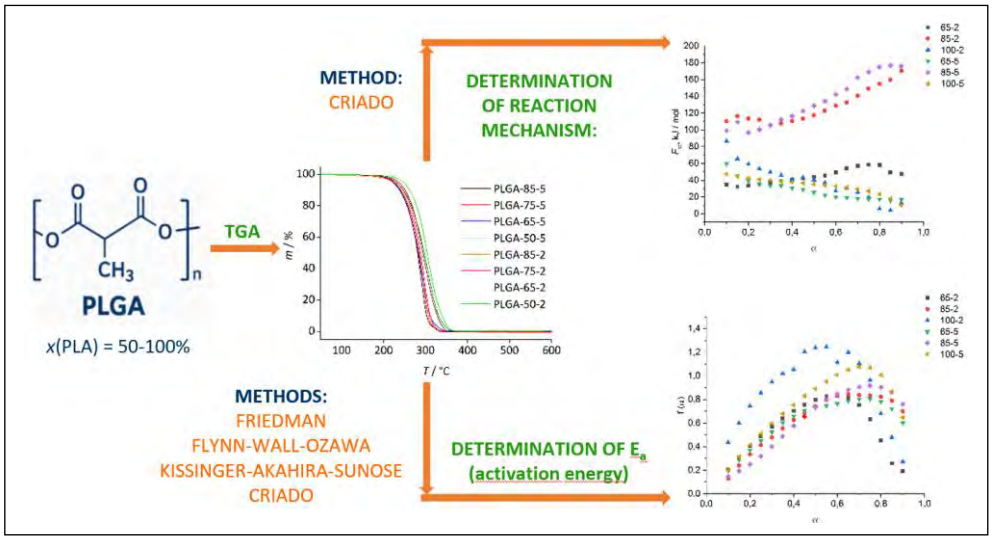

PRINTING SOLUTIONS FOR SENSING PROBLEMS

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Advancements in printing technologies have opened the way towards miniaturization of analytical devices and facilitated use of a wide variety of materials for their production. 3D printing has enabled low-cost production of modularized microfluidic systems, while 2D printing technologies, notably state-of-the-art screen printing and emerging inkjet printing, have simplified the production and use of planar, flexible, and disposable electrochemical sensors. While combining these printing technologies to produce functional microfluidic analytical devices is no simple task, facilitated detection of important analytes for process monitoring, clinical biomarkers or environmental pollutants is certainly a rewarding result [1].

In this work, a new approach to constructing an integrated microfluidic sensing system will be presented. By combining 3D printing technologies for modular cell design and 2D-fabricated electrochemical sensors, we assembled a 3D-printed flow cell that enables *in operando* hot swapping of a planar printed three-electrode system, which allows monitoring the process of interest that could not typically be tracked continuously. In our case, continuous monitoring of methylene blue reduction is prevented by strong adsorption of the analyte on the electrode surface, and it is circumvented by exchanging the sensor without disrupting the flow. Interelectrode reproducibility is key for such system and was tested by hot swapping electrodes at different flow rates, with and without electrochemical preconcentration. Optimized flow measurements yielded a linear response in the concentration range 0.01-0.07 μM, with excellent sensitivity (-65.59 ± 3.76 μA/μM) compared to batch calibrations, and with interelectrode relative standard deviation of only 1.87%. This system could be successfully utilized for tracking processes without disassembling the system, using only small amounts of sample for discrete measurements, reducing losses, and facilitating environmental monitoring or flow synthesis of expensive compounds.

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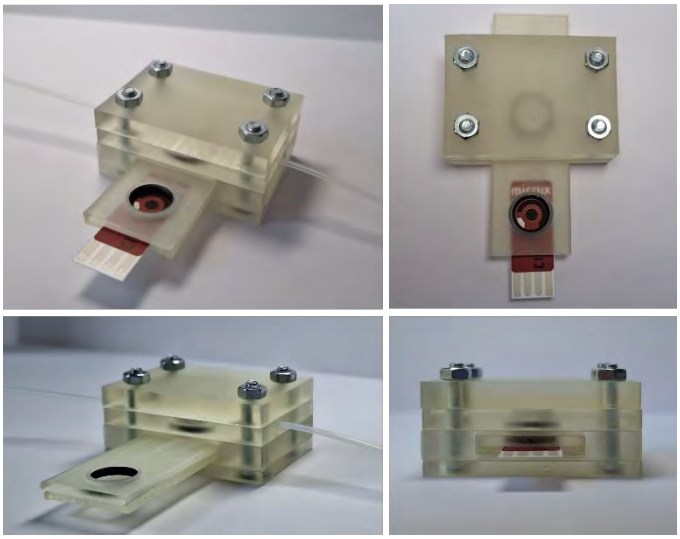
This work was supported by the Croatian Science Foundation under grants UIP-2020-02-9139, HRZZ-DOK-NPOO-2023-10-1144, HRZZ-DOK-2021-02-5999, and HRZZ-IP-2022-10-8004.



RAZVOJ 3D-TISKANIH KOMPOZITA NA TEMELJU BIORAZGRADLJIVOG POLIMERA I KALCIJEVIH FOSFATA

DEVELOPMENT OF 3D-PRINTED COMPOSITES BASED ON BIODEGRADABLE POLYMER AND CALCIUM PHOSPHATES

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The 3D hydrogel printing process represents a state-of-the-art approach in preparation of polymer-based materials used in tissue engineering applications, due to the possibility of fabricating hydrogel scaffolds with dimensions and geometries tailored to a target application [1]. Although polymer-based inks enable printing of controlled 3D architectures, such constructs often lack the mineral phase required for bone tissue regeneration. In order to form bioactive hydrogel-based scaffolds, calcium phosphate minerals, such as hydroxyapatite, can be incorporated into chitosan-based inks [2]. A key challenge during printing is the stabilization of the deposited strands and overall shape fidelity. Because extrusion printing relies on sequential deposition, a viscous solution is usually a suboptimal candidate due to its inability to retain form or shape. To achieve a stable printed structure, various crosslinking agents are used. Most commonly used crosslinking agents, such as glutaraldehyde or genipin, can introduce cytotoxic effects [3]. In order to avoid cytotoxicity, we propose a physical crosslinking *in situ* to obtain a stable structure with precise dimensions and shape.
In this work, we prepared a chitosan/hydroxyapatite (CHT/HAp) composite ink as a feedstock material for 3D printing of hydrogel structures. Parameters such as chitosan concentration (1–3%), acetic acid concentration (0.5–1%), and weight fraction of HAp (0–30%) were varied to optimize the ink's properties. To produce stable and defined structures, parameters such as printing gauge size (20-25 G), printing speed (6–8 mm/s), printing pressure (150–230 kPa), strand height (0.150–2.270 mm) and NaOH bath concentration (0.07–0.5 M) were investigated. The composite hydrogels were printed using an additive manufacturing process into a circular shape with a continuous linear infill rotated by 90° every layer, a radius of 10 mm, an infill distance of 2.1 mm and an outline distance of 1 mm directly into the NaOH bath to achieve physical crosslinking *in situ*. The resulting composite scaffolds were characterized by scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDS), X-ray diffraction (XRD), and Fourier transform infrared spectroscopy (FTIR), while the bioactive properties were investigated in simulated body fluid for 21 days. Physical crosslinking enabled the formation of a stable strand deposition and shape retention with a high level of control over printing fidelity. XRD and FTIR confirmed the successful incorporation of hydroxyapatite into the polymer matrix, while the bioactivity test indicated the deposition of calcium phosphate crystals on the surface of the printed material. Overall, the use of physical crosslinking *in situ* offers a cytocompatible oriented approach for fabricating 3D-printed CHT/HAp hydrogels.

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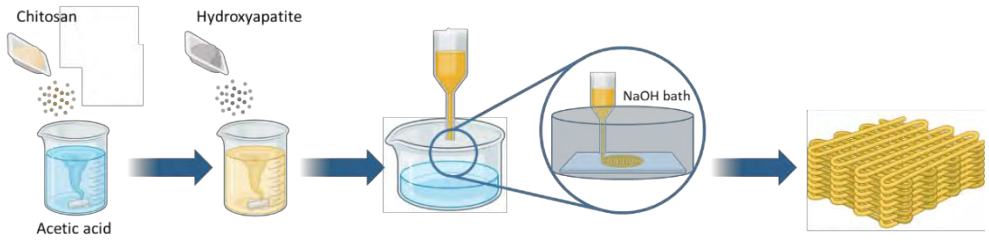

INFLUENCE OF STARCH BOTANICAL ORIGIN ON THE PROPERTIES OF THERMOPLASTIC STARCH AND ITS BLENDS

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The globally increasing polution due to highly durable and hardly degradable plastics has led to growing interest in the biodegradable biopolymers. Starch is one of the most widely studied biopolymers, mainly due to its availability, low cost, perfect biocompatibility, and complete biodegradability. It is employed in the food industry, as a packaging material in agriculture, and in the pharmaceutical and cosmetics industries [1]. Native starch cannot be processed by standard protocols due to high molecular weight combined with strong hydrogen bonds. However, it is possible to convert the native starch to thermoplasticized starch (TPS) using low molecular weight plasticizers such as glycerol or citric acid. TPS is usually prepared by solution casting, melt-mixing or their combination [2].
In this work, we prepared four TPS's from four different source plants (wheat, corn, tapioca, and potato; see figure - upper row). We compared their homogeneity (see figure - middle row), thermomechanical and micromechanical properties (see figure - bottom row), rheology, and processing properties. We applied the same preparation protocol to all four starches in three different laboratories (in the Czech Republic, Croatia, and Poland) to verify the reliability and reproducibility. For two selected starches with the most different morphology – the highly homogeneous wheat starch and the least plasticized potato starch – we compared also the properties of their blends with polycaprolacon, as the TPS/PCL blends are widely used in technical applications [3]. The botanical origin of starch influenced the morphology, homogeneity and processing properties of TPS, exhibited a minor impact on the mechanical properties of TPS, but the final mechanical properties of TPS/PCL blends were the same within the experimental error.

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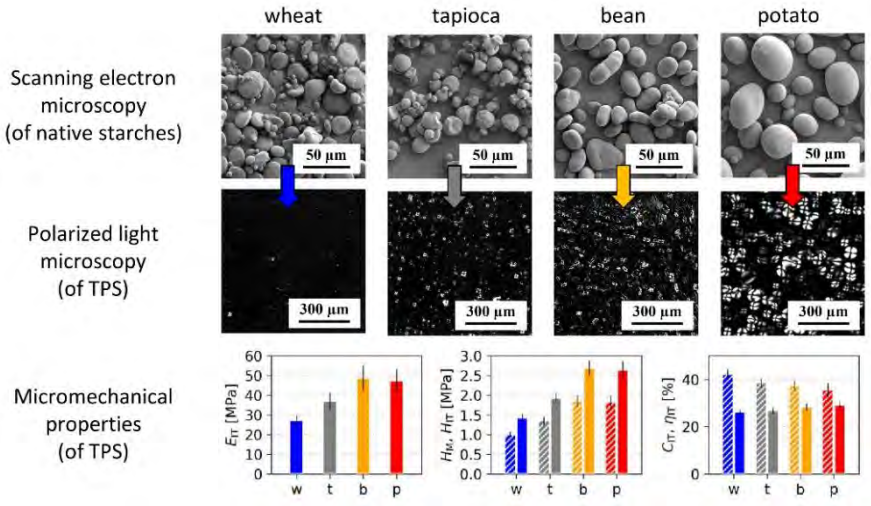
This work was supported by Technology Agency of the Czech Republic, program NCK, project TN02000020.



NOVEL APPROACH OF GENERATING MOLYBDENUM OXIDE THIN FILMS VIA SPARK PLASMA ABLATION DEPOSITION

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Spark plasma ablation deposition (SPAD) is an innovative and green method for generating nanoparticles in a fast and simple way, where by controlling a few parameters, it is possible to convert any solid and (semi)conductive material into nanoparticles. SPAD can generate metal oxide nanoparticles in a reactive atmosphere by either filtration, diffusion or impaction. Molybdenum oxide (MoO_3) has versatile applications in many fields such as electronics, catalysis, sensors, energy-storage units, field emission devices, superconductors, thermal materials, etc.
Molybdenum oxides generally show stable structure with a bandgap around 2.9–3.1 eV, providing unique electronic properties that facilitate efficient gas adsorption and high catalytic activity [1].
The aim of this work is to develop MoO_x thin films as active materials for applications, such as gas sensing or photocatalytic degradation of pollutants. The frame of applicability builds on their tuneable oxidation states, high surface reactivity and compatibility with miniaturized and flexible sensor platforms. Molybdenum oxide thin films were prepared by spark discharge generator (SPAD–SDG) varying the carrier gas and the time of the substrate exposition. Consequently, it was found that structural and morphological properties of MoO_x thin films were influenced by the temperature of the subsequent annealing.
Crystalline composition of MoO_x films was determined by X-ray diffraction (XRD). Raman spectroscopy was used for further elaboration of the thin film properties. The morphology and topography of the thin films were examined by scanning electron microscopy (SEM) and atomic force microscopy (AFM) along with cross-sections prepared by focused ion beam–Scanning Electron Microscopy (FIB–SEM).

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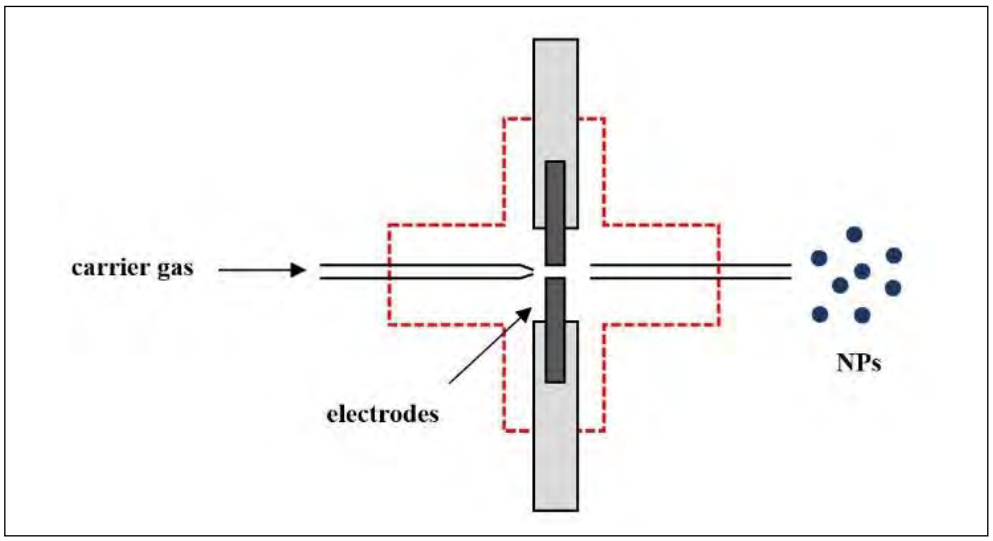

IMPACT OF ACID HYDROLYSIS ON THE STRUCTURE AND PROPERTIES OF THERMOPLASTIC STARCH

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Acid hydrolysis (AH) was employed to enhance the processability of thermoplastic starch (TPS), which is hindered by the strong interactions among starch molecules with extremely high molecular weight [1]. Wheat starch was partially hydrolyzed for different durations (AH times: 0, 1, 2, and 4 h), neutralized, dried, and plasticized using our two-step protocol [2]. AH mainly targeted the amorphous regions, reducing their molar mass and viscosity. During processing, the softer matrix in the AH-treated starches caused minimal disruption of the semicrystalline lamellae, leading to a slightly coarser structure observed by polarized light microscopy (PLM) and increased crystallinity measured by wide-angle X-ray scattering (WAXS), both of which became more pronounced with increasing hydrolysis time. The softer, less viscous amorphous phase produced by AH was counterbalanced by a higher fraction of stiffer crystalline domains, resulting in similar rheological and micromechanical properties regardless of AH time. During the melt mixing, the shorter chains generated by AH acted as lubricants, facilitating the starch mixing and leading to a reduced torque and processing temperature, as evidenced by *in situ* measurements in the kneading chamber. Overall, these results indicate that controlled acid hydrolysis is an effective strategy to facilitate TPS processing while preserving satisfactory mechanical performance.

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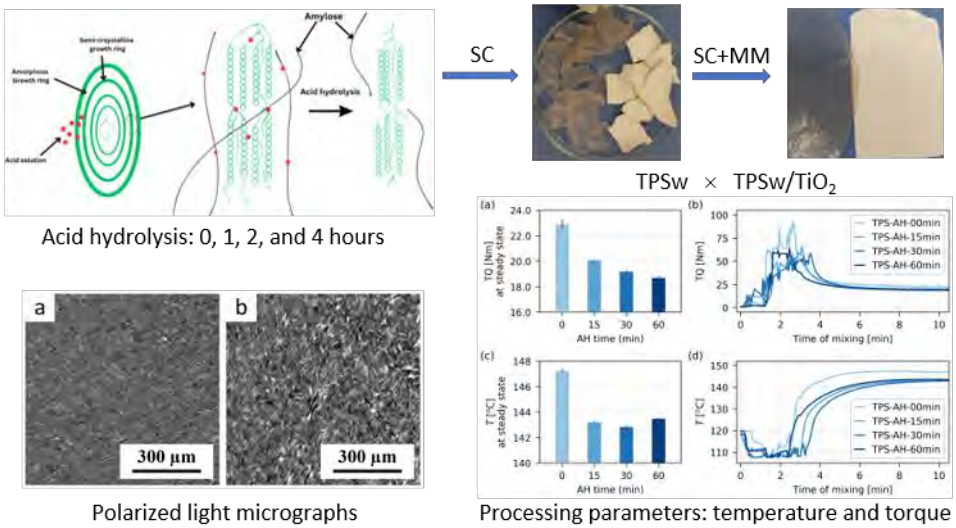
[2] A. Ostafinska et. al., Int. J. Biol. Macromol. (2017) 273-282.

This work was supported by the Technology Agency of the Czech Republic, program NCK, project TN02000020.



Acid hydrolysis: 0, 1, 2, and 4 hours

Polarized light micrographs

Processing parameters: temperature and torque

PRIMJENA INFRACRVENE SPEKTROSKOPIJE U ODREĐIVANJU SASTAVA PLGA POLIMERA

APPLICATION OF INFRARED SPECTROSCOPY IN DETERMINATION OF PLGA POLYMERS' COMPOSITION

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Poznavanje kemijskog sastava poli(D,L-laktida) (PDLLA) i poli(laktid-*ko*-glikolida) (PLGA) važno je zbog njihove široke primjene u farmaceutskoj industriji [1]. Primjena tih polimera je široka zahvaljujući njihovoj biokompatibilnosti, biorazgradivosti i prikladnim mehaničkih svojstvima [2,3]. Za određivanje sastava PLGA polimera se mogu primijeniti infracrvena spektroskopija s Fourierovom transformacijom (FTIR) i nuklearna magnetska rezonanca (NMR) [1].
U usporedbi s NMR tehnikom, prilikom primjene FTIR tehnike ne koriste se deuterirana otapala za pripremu uzoraka, potrošnja energije po uzorku je niža i oprema za analizu je ekonomski prihvatljivija. Nadalje, tehnika je nedestruktivna, što je posebno važno ako su na raspolaganju male količine uzorka. Radi razvoja zelenije, ekonomičnije i pristupačnije metode za određivanje sastava PLGA polimera, provedena su ispitivanja infracrvenom spektroskopijom i razvijeno je nekoliko empirijskih metoda određivanja molarnih udjela glikolida i laktida u PLGA polimerima, kako bi se utvrdilo mogu li se FTIR tehnikom dobiti rezultati po pouzdanosti, preciznosti i točnosti slični onima dobivenim NMR tehnikom.

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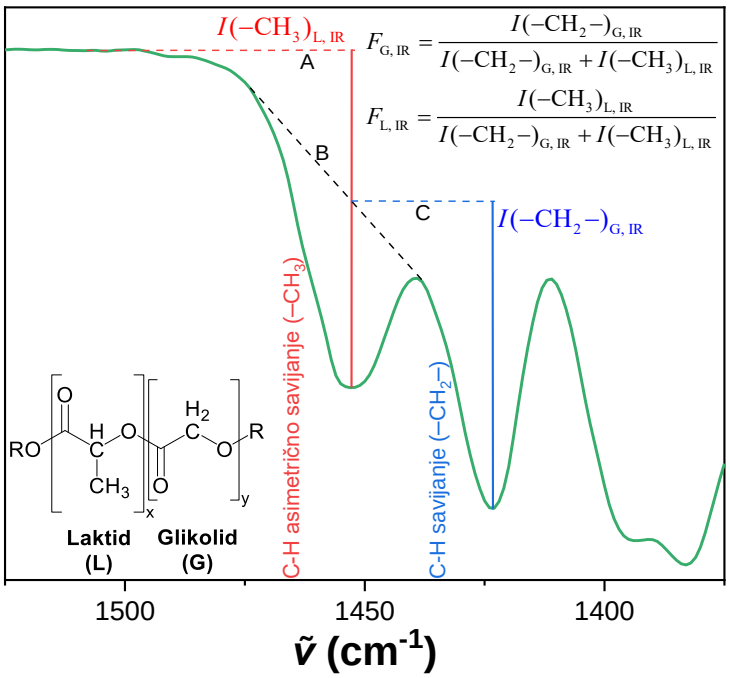

IMPACT OF BORATE BIOACTIVE GLASS ON THE STRUCTURE AND PROPERTIES OF CHITOSAN-BASED SCAFFOLDS

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Bone tissue engineering represents a promising strategy for the regeneration of large bone defects by developing bioactive materials that provide structural support while promoting cell integration and bone regeneration. Among inorganic biomaterials, bioactive glasses have been extensively investigated due to their ability to bond directly to bone and stimulate osteogenesis, while borate-based bioactive glasses (BBG) have gained increasing attention for their enhanced degradation rate and ability to promote angiogenesis and tissue regeneration [1]. However, their high solubility can negatively affect cellular response. To diminish a rapid dissolution, BBG nanoparticles can be incorporated into a stable polymer matrix [2].

In this study, mesoporous borate bioactive glass nanoparticles doped with silver (Ag^{+}) and cobalt (Co^{2+}) ions were investigated as an inorganic phase for composite scaffold fabrication. The doped BBG nanoparticles exhibited bioactive properties, antibacterial activity against *E. coli* and *S. aureus*, and good cytocompatibility at low concentrations. Highly porous chitosan/BBG composite scaffolds were prepared by direct mixing and freeze-drying, with the process optimized by varying BBG content (0 – 20 wt%). To obtain stable composite scaffolds, two types of crosslinking were explored: a physical crosslink using NaOH neutralization (at different concentrations and incubation time), and a chemical crosslink using genipin at different genipin-to-chitosan ratios (0.5 – 2%). The effects of fabrication parameters on scaffold structure and stability were investigated. Changes in morphology and pore architecture resulting from variations in BBG content, neutralization time, and crosslinking method were analysed by SEM. The incorporation, distribution, and relative content of borate bioactive glass within the chitosan matrix were evaluated using FTIR, TG, and SEM-EDX, while porosity analysis was used to assess the suitability of the scaffolds for bone tissue engineering applications.

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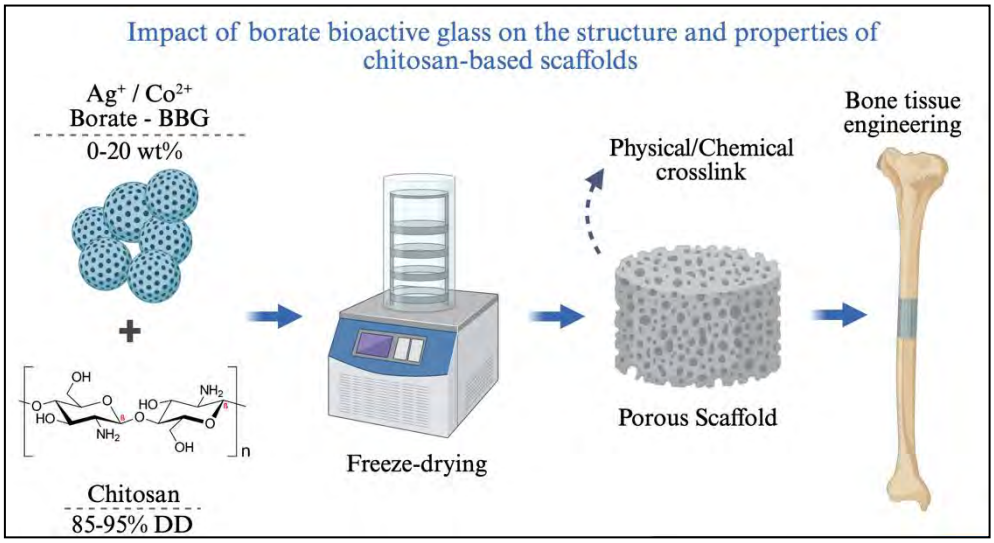

CALCIUM -OXYGEN BATTERIES: RISE OF NEXT-GENRATION OF MULTIVALENT ENERGY STORAGE SYSTEM

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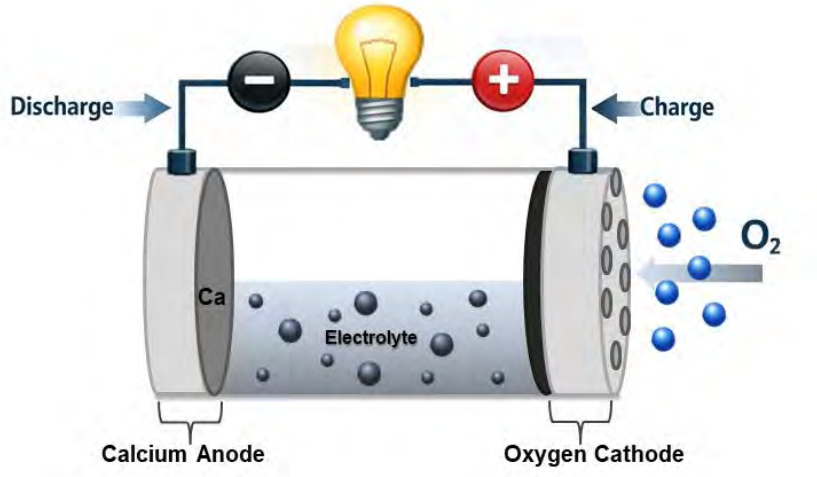
The current electronics and automotive market are dominated by batteries as primary energy storage devices. Rapid development in recent years has driven alternative approaches to battery design and encouraged the exploration of technologies beyond lithium-ion. Among these, multivalent batteries, utilizing calcium, magnesium, zinc and aluminum as anode materials, have attracted significant attention. Among them, calcium is particularly promising due to low reduction potential (-2,89 V vs. SHE), ionic size comparable to sodium, volumetric capacity comparable to lithium, high abundance and high capacity due to two electron charge transfers. The integration of calcium anode with high performance cathode, such as oxygen, could yield exceptional gravimetric and volumetric capacity, as well as superior energy and power densities. However, finding suitable electrolytes remains critical challenge. Such electrolytes must enable reversible calcium electrodeposition without parasitic corrosion processes, while simultaneously supporting both the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER).
This work provides conceptual overview of calcium-oxygen batteries from the fundamental perspective, addressing the key scientific challenges and progressing toward practical application and testing. Standard electrochemical techniques, including cyclic voltammetry, electrochemical impedance spectroscopy and chronoamperometry were employed to investigate behavior of calcium anode and phenomena related to electrodeposition. The same methodology was applied to examine ORR/OER in organic media. The electrolyte system was evaluated for stability using multiple characterization, including Fourier -transform infrared (FTIR) and Raman spectroscopy.
Finally, these insights are combined to demonstrate the operational feasibility of the functional calcium- oxygen battery. The presented framework highlights critical research direction toward the development of calcium-oxygen batteries as viable next-generation multivalent energy storage systems.

This work was funded by the European Union within the project NPOO.C3.2.R3-I1.04.0187: Development of new materials and advanced innovative technologies for the production of lithium-ion batteries.



PRIPRAVA KOMPOZITA POLISTIRENA I LIGNINA – UTJECAJ NA TOPLINSKA I MEHANIČKA SVOJSTVA

PREPARATION OF POLYSTYRENE-LIGNIN COMPOSITES: EFFECTS ON THERMAL AND MECHANICAL PROPERTIES

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Sve veće količine otpadnih termoplasta potiču istraživanja vezana uz ponovnu obradu i mogućnosti poboljšanja svojstava reciklata [1]. Polistiren je među najzastupljenijim potrošnim plastikama, a istraživanja su pokazala kako reciklirani polistiren pokazuje smanjenu molekulsku masu i toplinsku stabilnost zbog degradacije iz prethodnih ciklusa prerade [2]. Kako bi se poboljšala mehanička svojstva reciklata može se koristiti lignin kao bio-punilo [3], no njegova interakcija s polistirenom nije još detaljno istražena. U ovom radu ispituje se utjecaj lignina i procesnih parametara namješavanja u talini na molekulsku masu, toplinska i mehanička svojstva recikliranog polistirena.
Kompoziti su pripremljeni s različitim udjelima lignina (1 – 10 mas. %) i pri različitim vremenima (5 – 60 min) i brzinama miješanja (25 – 100 min^{-1}) u laboratorijskom ekstruderu-mikseru. Diferencijalno pretražna kalorimetrija (DSC) pokazala je kako prilikom duljih vremena miješanja T_g kompozita opada. Pad T_g znači veću pokretljivost lanaca koja može biti zbog degradacije polimera prilikom pripreme. Gel permeacijskom kromatografijom (GPC) potvrđen je pad molekulske mase kompozita pripravljenih pri duljem trajanju namješavanja. Povećanje udjela lignina dodatno snižava T_g. Rezultati pokazuju da udio lignina i različite vrijednosti parametara obrade utječu na pad molekulske mase, toplinsko ponašanje i mehanička svojstva recikliranog polistirena, što je uz razumijevanje međuodnosa sasatava i svojstava, važno za ponovnu primjenu kompozita na osnovi polimernih reciklata.

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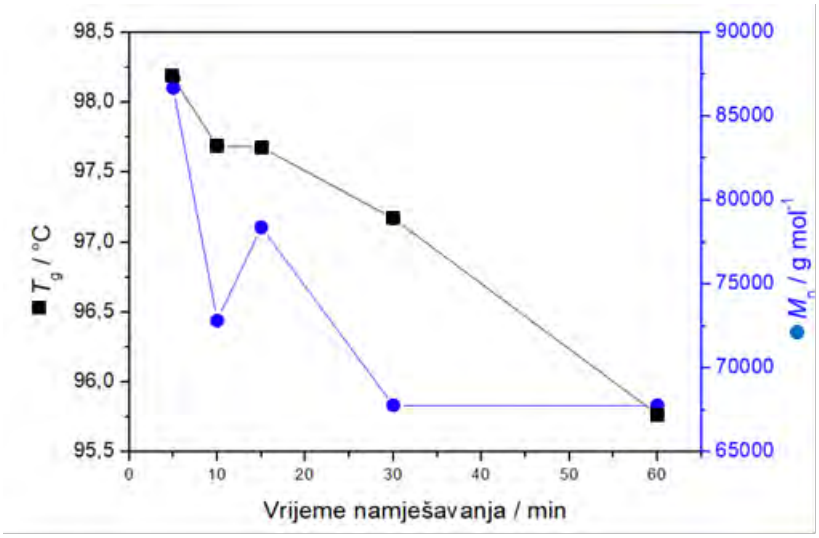

POLISAHARIDNE OKOSNICE USMJERENE STRUKTURE ZA REGENERACIJU TETIVA

POLYSACCHARIDE SCAFFOLDS WITH AN ORIENTED STRUCTURE FOR TENDON REGENERATION

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Tendons, highly aligned connective tissues responsible for transmitting force from muscle to bone, can be affected by various disorders, such as ruptures, overuse injuries, and inflammatory or degenerative conditions. Due to their low vascularity, tendons have a limited self-healing capacity, which often results in the formation of less organized, mechanically weaker scar tissue that is prone to reinjury and partial loss of function [1]. To address these limitations, it is necessary to stimulate a repair process that promotes the regeneration of the injured tendon tissue. A practical approach involves biomimetic scaffolds made from biocompatible and biodegradable polymers, such as chitosan, which serve as temporary frameworks for cell adhesion and promote tissue regeneration. To create an oriented microchannel structure and enhance the scaffold's stability, chitosan can be cross-linked with zinc ions [2]. In addition to stabilizing the chitosan matrix, zinc ions are convenient cross-linkers because they promote cellular activity and stimulate the expression of collagen type I, a key marker of tendon regeneration [3]. Additional impregnation of chitosan scaffolds with alginate, which forms a polyelectrolyte complex with chitosan, enables controlled modification of the scaffold's functional properties [4]. Thus, in this work, chitosan–zinc scaffolds were prepared *in situ* to obtain an oriented microchannel structure. Subsequently, the lyophilized scaffolds were impregnated with alginate solutions of different concentrations (0.1 and 0.5 wt.%), washed to remove excess alginate, and freeze-dried. Zinc was detected using energy-dispersive X-ray spectroscopy, while successful alginate impregnation was verified by attenuated total reflectance Fourier-transform infrared spectroscopy. Surface and cross-sectional morphologies were investigated by scanning electron microscopy, and microchannel dimensions were estimated using ImageJ software. Absorption capacity was measured in phosphate-buffered saline (PBS) at 37 °C at different time points. Lysozyme-induced degradation of the scaffolds at 37 °C was assessed by monitoring mass loss over time, and morphological changes during degradation were evaluated using scanning electron microscopy. Overall, the obtained results demonstrate that the prepared scaffolds possess the structural characteristics required for tendon tissue engineering applications.

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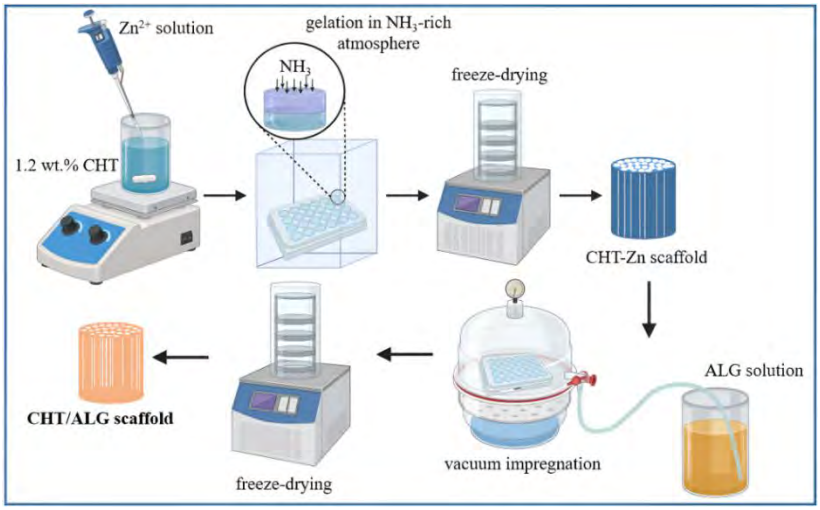

POSTERSKA IZLAGANJA
POSTER PRESENTATIONS

Biokemijsko inženjerstvo
Biochemical engineering

ZELENO ELEKTROISPREDANJE BIORAZGRADIVIH POLIMERA

GREEN ELECTROSPINNING OF BIODEGRADABLE POLYMERS

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Driven by superior processability and economic viability, polymeric membranes have emerged as pivotal tools in advanced separation technologies, water treatment, and biomedical fields [1]. However, the conventional fabrication of these materials is frequently hindered by a reliance on toxic organic solvents, which compromises both environmental safety and biocompatibility [2]. To reconcile high-performance engineering with ecological stewardship, a protocol was established for the electrospinning of natural and synthetic biodegradable polymers using exclusively benign, "green" solvents.

Initial efforts were focused on the precise tuning of solution viscosity to ensure fundamental spinnability and stable jet initiation. Subsequently, to navigate the complex multi-variable landscape of the electrospinning process without resorting to inefficient trial-and-error, a systematic Design of Experiment (DoE) approach was employed. Utilizing Design-Expert software (State-Ease), the intricate interactions between applied voltage, flow rate, needle size, and tip-to-collector distance were statistically modeled.

The optimization process was driven by the performance of the final solid product; critical response variables included the membrane width and length, as well as the enhancement of rheological properties (mechanical integrity). Finally, optical microscopy was utilized as a validation tool to confirm the morphological quality of the resulting micro- and nanofibers. This work demonstrates that by integrating green chemistry with computational statistics, mechanically robust and high-yield biomaterials can be produced, satisfying the rigorous demands of modern medicine while adhering to sustainable manufacturing principles.

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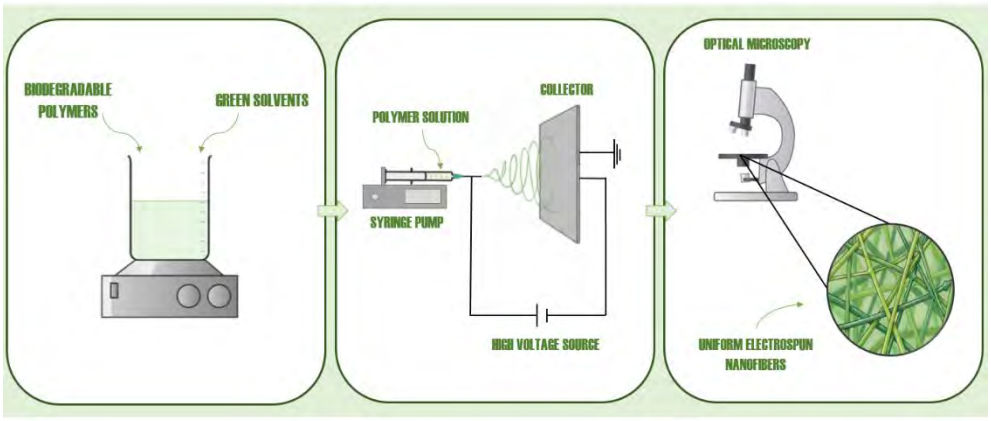
This paper was funded by the Croatian Science Foundation through the project IP-2024-05-4339 entitled " Coffee ring' effect in 'Lab on a Chip' environments in the development of new drug formulations." leader prof. Ernest Meštrović.



FLUID FLOW CHARACTERIZATION IN A 3D-PRINTED MILLIREACTOR WITH IMMOBILIZED GLUCOSE DEHYDROGENASE

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Enzymes are increasingly being investigated for sustainable energy applications, including biohydrogen production, where highly specific biocatalysts convert renewable biomass into clean fuel. However, when enzymes are removed from their natural biological environment, they often lose activity and structural stability, which poses a major limitation for large-scale industrial applications. Enzyme immobilization in flow systems is an effective strategy to improve biocatalyst stability and reusability while enabling precise control of reaction conditions. In this study, fluid flow behavior in 3D-printed millireactors with immobilized glucose dehydrogenase (GDH) was investigated to evaluate the influence of reactor geometry and immobilization strategy on catalytic performance. Rectangular and modified millireactor designs were fabricated and coupled with different GDH immobilization approaches, including bead-based entrapment and hydrogel immobilization on reactor surface. Computational fluid dynamics (CFD) [1] simulations were used to characterize flow profiles, velocity distribution and potential dead zones, and were validated by experimental measurements. The modified millireactor exhibited more uniform flow patterns and reduced dead volume compared to the rectangular design. These improved hydrodynamic characteristics resulted in enhanced enzymatic performance, with the modified reactor showing superior results when GDH was immobilized on both the top and bottom surface. The results demonstrate a clear correlation between fluid flow characteristics, millireactor geometry, and enzyme immobilization strategy, highlighting the importance of hydrodynamic optimization in the design of efficient enzymatic millireactors.

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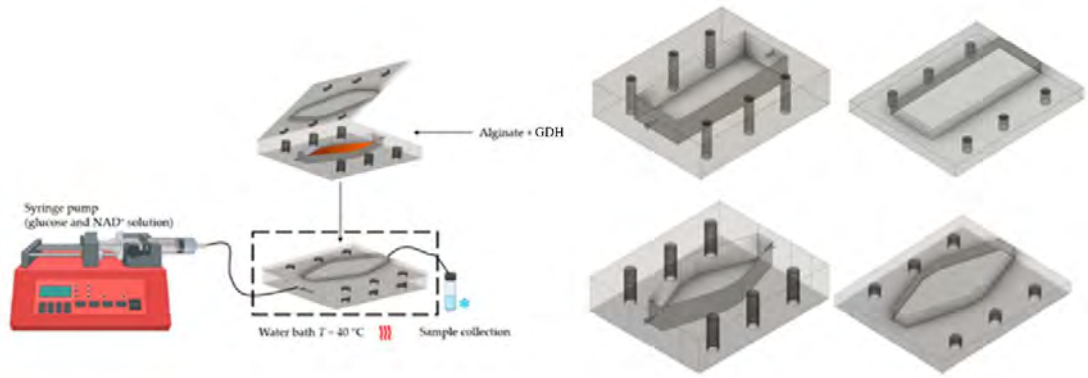

SCREENING OF PUTATIVE NEURAMINIC ACID SYNTHASE HOMOLOGUE LIBRARY FOR CHEMOENZYMATIC SYNTHESIS OF *N*-PROPIONYLNEURAMINIC ACID

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Sialic acids are a nine-carbon sugar family, and they are terminal glycan moieties that modulate diverse molecular recognition interactions [1]. Access to defined non-natural analogues could prove as useful as they have the potential to exhibit biological activity.
N-acetylneuraminic acid synthases from the organism Neisseria meningitidis (NmNeuS; EC 2.5.1.56) catalyze the irreversible metal-dependent aldol addition of phosphoenolpyruvate (PEP) with N-Acetyl-d-mannosamine (ManNAc) to form N-acetylneuraminic acid (Neu5Ac) [2]. Our prior studies of this enzyme have demonstrated its promiscuity towards the sugar substrate that can be leveraged for the synthesis of novel products.
In this work, in vitro screening of a commercial metagenomic library of putative N-acetylneuraminic acid synthase homologues (PNH; Prozomix®) and NmNeuS was done by using the chemically synthesized N-propionyl-d-mannosamine (ManNProp) as the substrate to identify enzymes capable of producing Neu5Prop. HPLC analysis was used to quantify the reaction outcome, reported as substrate conversion and apparent product yield. This study's preliminary investigations demonstrate high conversions and substrate promiscuity of the tested enzymes, underlining their potential for generating non-natural sialic acid analogs. This highlights the opportunities for expanding the biocatalytic toolbox in the synthesis of sialic acid analogues with potential pharmaceutical relevance.

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This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 956631.

KINETIČKA KARAKTERIZACIJA RAZGRADNJE DIKLOFENAKA KORIŠTENJEM ENZIMA LAKAZE

KINETICAL CHARACTERIZATION OF DICLOFENAC DEGRADATION USING THE ENZYME LACCASE

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Farmaceutici su skupina onečišćujućih tvari koje privlače sve više pozornosti zbog česte prisutnosti u okolišu. Njihova široka primjena dovodi do kontinuiranog unošenja u vodene ekosustave, uglavnom putem komunalnih otpadnih voda i neučinkovitih sustava pročišćavanja. Među njima se ističe diklofenak kao nesteroidni protuupalni lijek čija su perzistentnost i toksičnost u okolišu potvrđene brojnim istraživanjima [1]. S obzirom na ograničenu učinkovitost konvencionalnih metoda obrade otpadnih voda u uklanjanju farmaceutika, raste interes za biološke pristupe temeljene na primjeni enzima. Enzimi omogućuju specifičnu, učinkovitu i ekološki prihvatljivu razgradnju organskih onečišćivala. Posebnu pažnju privlači lakaza, oksidoreduktaza koja sadrži više atoma bakra i katalizira oksidaciju širokog spektra fenolnih i aromatskih spojeva, uz istodobnu redukciju molekularnog kisika do vode. Kinetička karakterizacija lakaze ključna je za razumijevanje njezine učinkovitosti i specifičnosti prema pojedinim supstratima, uključujući diklofenak [2]. U ovom radu proučavana je enzimatska razgradnja diklofenaka katalizirana lakazom, uz ispitivanje utjecaja koncentracije enzima, dostupnosti kisika i ponovljenih ciklusa oksidacije. Rezultati su pokazali da je diklofenak kemijski stabilan u odsutnosti enzima, dok se u prisutnosti lakaze uspješno razgrađuje. Dostupnost otopljenog kisika nije bila ograničavajući čimbenik procesa, a kinetika razgradnje opisana je Michaelis-Menteničinim modelom te su procijenjeni i kinetički parametri. Validacija matematičkog modela provedena pri različitim koncentracijama enzima pokazala je da biekponencijalni model najbolje opisuje deaktivaciju lakaze. Pri svim ispitivanim koncentracijama enzim je postupno gubio aktivnost tijekom uzastopnih ciklusa, ponajviše zbog akumulacije razgradnih produkata.

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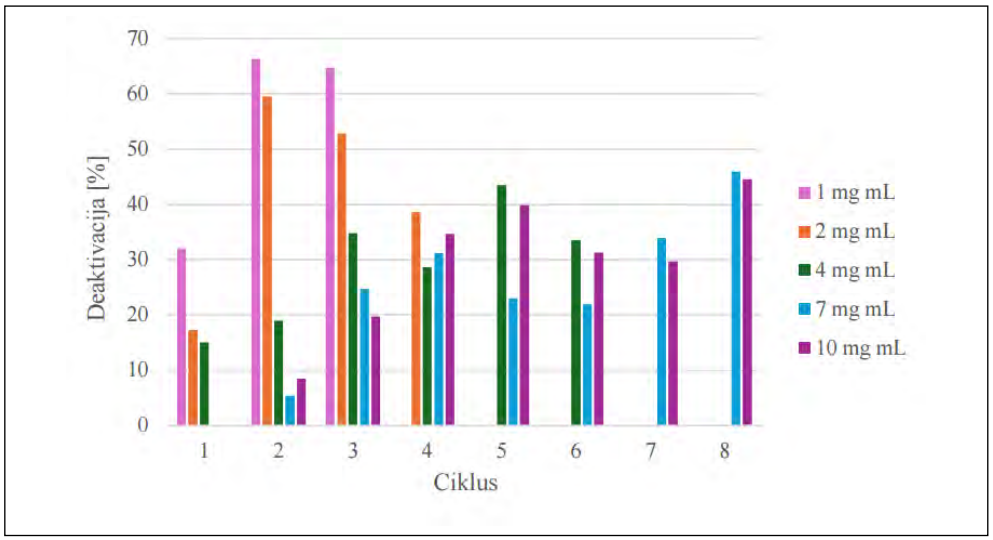

DES-MEDIATED INTENSIFICATION OF Ω-TRANSAMINASE-CATALYZED SYNTHESIS OF FURFURYLAMINE

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Furfurylamine (FA) is an important biobased chemical produced from furfural (FUR), which is obtained from hemicellulosic sugars. FA is widely used in the production of polymers, resins, solvents, and pharmaceutical intermediates, making the development of sustainable synthesis methods increasingly relevant. Traditional chemical routes to FA often suffer from low selectivity, harsh reaction conditions, and the use of external reducing agents. Because of these limitations, ω-transaminases (ω-TAs) have emerged as a more selective and environmentally friendly alternative for the amination of FUR. Despite their advantages, current ω-TA-based processes still face several drawbacks. Many systems require a large excess of amine donor to drive the reaction, and substrate concentrations typically remain low due to the poor solubility of FUR in aqueous media. In addition, FUR can form a Schiff base with amine donors under acidic conditions, reducing the amount of free substrate available for transamination. Recently, it has been shown that high yields can be achieved under equimolar donor–acceptor conditions, addressing the issue of donor excess [1]. However, the problem of low substrate loading continues to limit the scalability of the process.

To tackle this challenge, we explored the use of deep eutectic solvents (DESs) as alternative reaction media. DESs are considered sustainable and tunable solvents that can improve substrate solubility while remaining compatible with biocatalysts [2]. In this study, six different DESs were selected to balance two essential requirements: increasing FUR solubility and maintaining conditions suitable for ω-TA activity, while avoiding side reactions such as Schiff base formation. Using DES-based media, we showed that ω-TA-catalyzed conversion of FUR to FA can be performed at 100 mM substrate concentration, an order of magnitude higher than what is typically achievable in aqueous buffer, while still using equimolar donor–acceptor ratios. The DES improved FUR solubility and preserved sufficient enzyme activity to enable efficient FA formation at elevated substrate levels, demonstrating a promising approach for process intensification. Overall, these results highlight DES-based medium engineering as a valuable strategy for improving the sustainability and scalability of biocatalytic transamination. By enabling higher substrate loadings under mild and atom-efficient conditions, DESs provide a promising platform for developing greener and more industrially relevant routes to FA.

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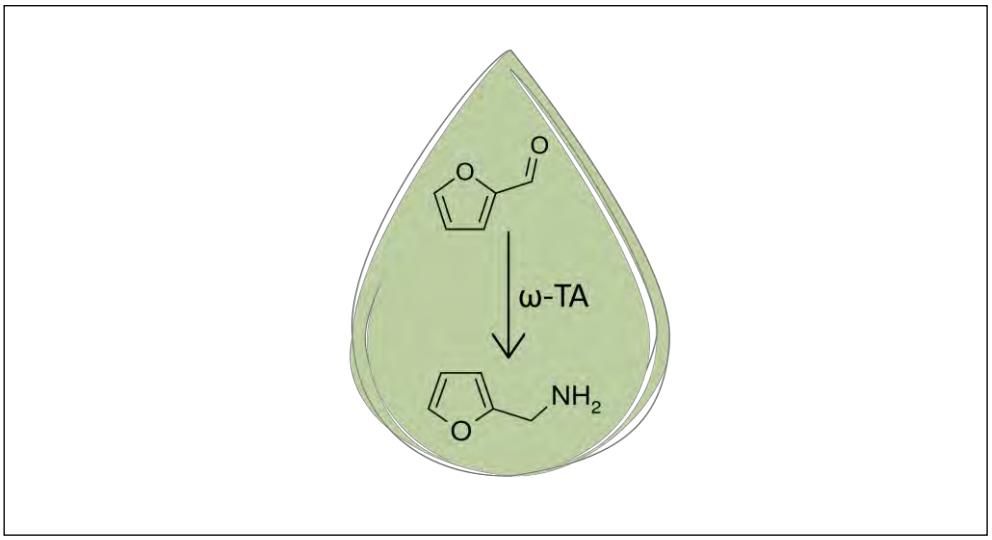

NUCLEOFUGALITIES OF THE TRIPHENYLPHOSPHINE

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Quaternary phosphonium salts (QPSs) are a fundamentally class of organophosphorus compounds, which have been applied as important reagents in synthetic organic chemistry, in medicinal chemistry, phase-transfer catalysts, ionic liquids, and in coordination chemistry [1]. More recently, phosphonium salts have begun to be explored as anti-cancer agents as well as in drug delivery as a result of their low cytotoxicity against normal human cells and good stability [2].
The leaving group abilities (nucleofugalities) of triphenylphosphine (Ph_3P) have been derived from the S_N1 solvolysis rate constants of the corresponding ferrocenyl-X-phenylmethyltriphenylphosphonium salts (Scheme 1.) by applying the *Linear Free Energy Relationship* (*LFER*) equation: $\log k\ (25\ ^\circ C) = s_f\,(E_f + N_f)$ [3]. In this equation k is a first order rate constant for S_N1 reaction at 25°C, s_f (slope of the log k/E_f correlation line) and N_f (nucleofugality, negative intercept on the abscissa of the log k/E_f correlation line) are nucleofuge specific parameters, while E_f is the electofugality parameter of the corresponding ferrocenylphenylmethyl cations determined earlier [4]. This method makes feasible estimating the solvolytic reactivity in a given solvent of any substrate constituted from an electrofuge of known E_f parameter and a nucleofuge of known s_f and N_f parameters.
On the nucleofugality scale developed in line with *LFER* equation triphenylphosphine is the weakest neutral nucleofuge (the poorest neutral leaving group). Because of solvation in the reactant ground state, the reactivity of phosphonium salts decreases as the polarity of the solvent increases. Impact of the phenyl group in ferrocenylphenylmethylphosphonium salts on stabilization of the positive charge is leveled by the α-ferrocenyl group and due to the substituents on the phenyl ring (X = H, 4-Cl, 3-F, 3-Br, and 3-Cl on Scheme 1) have small impact on its stability.

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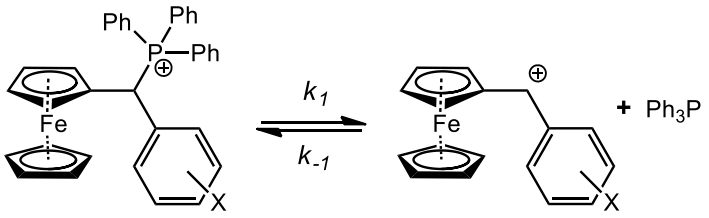

X = H, 4-Cl, 3-F, 3-Br, 3-Cl
Ph = phenyl

UNLOCKING THE ROLE OF MICROBIAL ENZYMES IN SUSTAINABLE BIOREMEDIATION

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The remarkable metabolic diversity of microorganisms, along with their ability to synthesise functionally diverse enzymes, underpins modern bioremediation strategies. Particular interest is given to autochthonous bacterial isolates which, due to their adaptation to environmental conditions, possess a wide range of enzymatic systems essential for degrading environmental pollutants. This study aimed to characterise autochthonous bacterial isolates and assess their potential for application in bioremediation processes based on their metabolic activity. Two bacterial isolates were obtained from the environment and analysed using a combination of classical microbiological techniques (differential staining, biochemical assays such as API 20E and API 50CH) and advanced identification by MALDI-TOF mass spectrometry. Identification revealed that the isolates belong to the genus *Bacillus*, specifically *Bacillus megaterium* and *Bacillus subtilis*. The biochemical profiles of the isolates indicated the presence of enzymes from the groups hydrolases, dehydrogenases, reductases, isomerases, and kinases, demonstrating well-developed metabolic pathways directly involved in the enzymatic degradation of diverse organic substrates. The results of this study confirm that autochthonous bacterial isolates of the genus *Bacillus* possess substantial biochemical potential, making them promising candidates for the development of effective enzyme-mediated bioremediation strategies.

EXPLORATION OF NOVEL HYDRAZINE SYNTHETASES FOR THE SYNTHESIS OF NITROGEN-NITROGEN BONDS

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Nitrogen–nitrogen (N–N) bond formation represents a significant challenge in chemical synthesis due to the high electronegativity and poor reactivity of nitrogen atoms. Nevertheless, nature routinely overcomes these limitations by evolving diverse enzymatic strategies. To date, over 300 natural products containing N–N bonds [1] have been identified, many of which exhibit a range biological activities, including antiviral, antibacterial, and anticancer effects. The increasing number of N–N bond-containing drugs approved by the U.S. Food and Drug Administration (FDA) in recent years highlights their growing relevance in the pharmaceutical industry, particularly in the treatment of cancer and cardiovascular diseases [2,3].

While traditional chemical synthesis of hydrazine and its derivatives are well-established, these methods are often constrained by safety risks, harsh conditions, instability, toxicity, and significant safety risks that limit industrial scalability. In contrast, biocatalytic systems offer a sustainable and operationally attractive alternative for N–N bond formation under mild, environmentally friendly conditions. Nature demonstrates this potential by generating a variety of linear and cyclic hydrazines ($R_2N–NR_2$) and related derivatives including hydrazides. Enzymes such as the piperazate synthase KtzT, which catalyzes the formation of L-piperazic acid [5], and hydrazine synthetases like Apy9 [6], which generate linear hydrazine intermediates, illustrate nature's enzymatic ingenuity in N–N bond biosynthesis. Despite their importance, these enzymes remain insufficiently characterized, limiting their translation into engineered processes.

This project aims to bridge that gap by elucidating the catalytic mechanisms of hydrazine synthetases through comprehensive biochemical and structural characterization. In parallel, we will apply directed enzyme engineering to expand their substrate scope and enhance stability and reactivity. By integrating enzymology with principles of bioprocess development, this work aims to broaden the biocatalytic toolbox for sustainable N–N bond formation applying nature's strategies for safer, greener, and more innovative approaches that support a sustainable pharmaceutical industry.

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PEKTINI EKSTRAHOVANI IZ VOĆNIH TROPOVA KAO FUNKCIONALNI SASTOJCI HRANE

PECTINS EXTRACTED FROM FRUIT POMACES AS FUNCTIONAL FOOD INGREDIENTS

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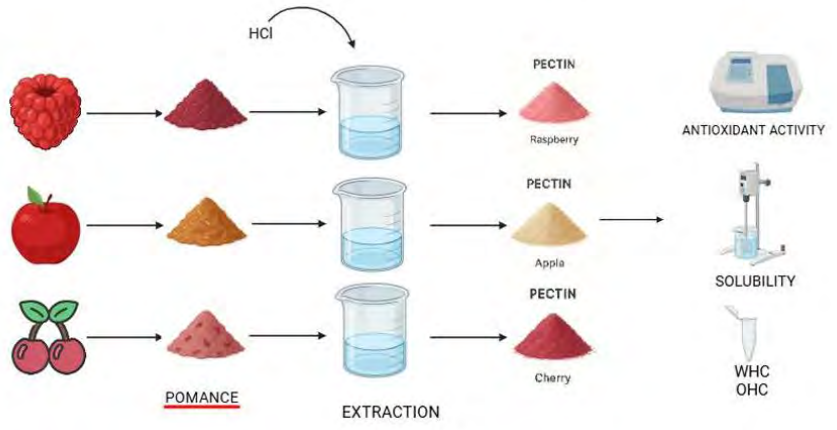
The Zero Waste concept is becoming increasingly relevant in today's era of mass production in which we strive not only to reduce waste but also to find valuable applications for industrial by-products. During the production of fruit juices, a considerable quantity of fruit pomace is generated as a by-product, and is recognized as a valuable source of pectin. Pectin is a structural polysaccharide in plants that is mainly composed of galacturonic acid and is widely used in the food industry as a gelling, thickening, and stabilizing agent. It is essential in the production of jams and jellies and also improves the texture and viscosity of beverages and dairy products. Additionally, it is utilized as a fat replacer in low-calorie foods and serves as a source of soluble dietary fiber. In this study, pomaces remained after juice production from raspberry, sour cherry, and apple were used as raw materials for pectin extraction. Pectin was extracted using a conventional hot-acid method. The extracted pectin from different sources were evaluated for their functional properties, including water-holding capacity, oil-holding capacity, and solubility, as well as for their antioxidant activity. Our results showed that the highest pectin yield was from apple pomace, reaching approx. 9% calculated on a dry matter basis. Apple pectin also demonstrated complete (100%) solubility and exhibited the highest water-holding capacity. The strongest in vitro antioxidant activity was determined for pectin extracted from raspberry pomace. All extracted pectins were capable to hold more than 1 g oil/g. Considering all of these, pectins extracted from used fruit pomaces showed excellent functional and biological properties, and could be considered as promising ingredients for the applications in food industry.



ISPITIVANJE UTJECAJA RAZLIČITIH AKTIVACIJSKIH SREDSTAVA NA IMOBILIZACIJU ENZIMA LAKAZE

INVESTIGATION OF THE INFLUENCE OF DIFFERENT ACTIVATION AGENTS ON LACCASE IMMOBILIZATION

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Onečišćenje voda farmaceutskim spojevima postaje sve veći ekološki problem zbog njihove postojanosti, biološke aktivnosti i potencijalno štetnog djelovanja na vodene organizme i ekosustave. Farmaceutski ostaci često dospijevaju u okoliš putem otpadnih voda jer konvencionalni sustavi pročišćavanja ne uspijevaju u potpunosti ukloniti takva mikroonečišćivala. Jedan od često prisutnih farmaceutika u okolišu je diklofenak, nesteroidni protuupalni lijek, čije se povišene koncentracije bilježe u površinskim i podzemnim vodama diljem svijeta [1]. Zbog njegove otpornosti na razgradnju u klasičnim uvjetima, istražuje se primjena alternativnih metoda za njegovo uklanjanje, među kojima se ističe enzimatska razgradnja pomoću oksidativnih enzima kao što je lakaza. Lakaza je oksidaza koja sadrži bakar i pokazuje sposobnost razgradnje širokog spektra aromatskih spojeva, uključujući farmaceutske kontaminante. Unatoč tome, primjena slobodne lakaze ograničena je njenom nestabilnošću i nemogućnošću višekratne uporabe, zbog čega se često pribjegava različitim metodama stabilizacije kao što je imobilizacija [2].

U ovom radu provedena je sinteza i funkcionalizacija magnetskih nanočestica obloženih silikom, na koje je zatim imobilizirana lakaza uz pomoć različitih aktivacijskih sredstava. Pritom su ispitivani utjecaji pH te vrste i koncentracije aktivacijskih sredstava na učinkovitost imobilizacije, očuvanu katalitičku aktivnost te stabilnost. Dobiveni imobilizirani sustavi korišteni su za razgradnju diklofenaka u modelnim uvjetima, a učinkovitost procesa praćena je spektrofotometrijski te pomoću HPLC-a.

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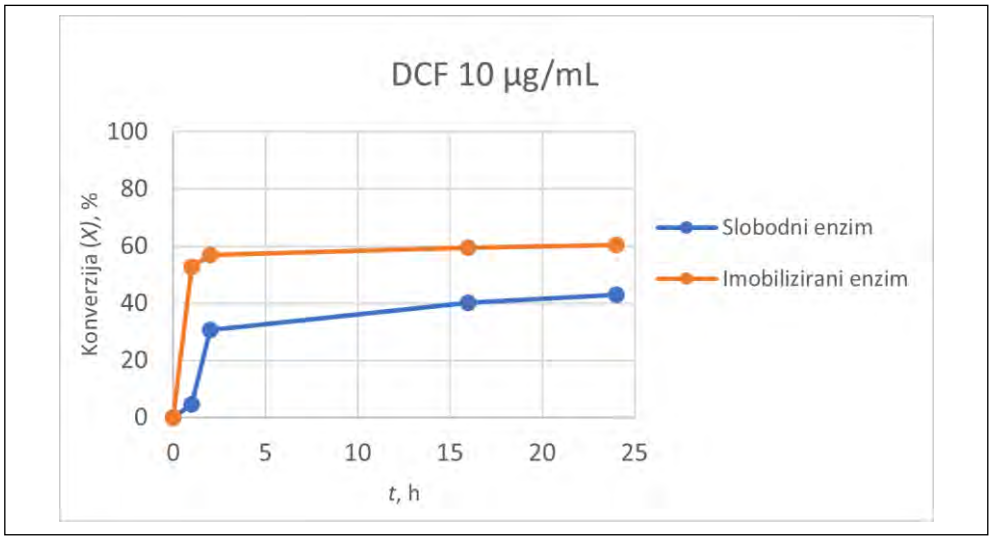

DIZAJN I IZRADA SUSTAVA *LUNG-ON-A-CHIP* S INTEGRIRANIM SENZORIMA, MEMBRANOM I HIDROGELNIM KOMPONENTAMA

DESIGN AND FABRICATION OF A *LUNG-ON-A-CHIP* WITH INTEGRATED SENSORS, MEMBRANES AND HYDROGELS

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Due to ethical concerns, regulatory restrictions, and the long duration of animal studies, there is an increasing demand for alternative testing methods. Traditional in vitro models also have significant limitations, particularly their inability to adequately mimic the complex conditions of living organisms. These challenges have led to the development of advanced in vitro systems, such as organ-on-a-chip technologies [1]. Organ-on-a-chip systems are biomimetic three-dimensional microsystems that replicate key aspects of human organ physiology. The lungs, the primary organ of the respiratory system, enable oxygen uptake from the atmosphere. Gas exchange occurs in the pulmonary alveoli, the basic functional units of the lungs. Their specialized structure is defined by the alveolar epithelial layer, which interfaces with the internal lung environment and the external atmosphere, serving as the first line of defense against inhaled particles, toxins, and pathogens [2]. *Lung-on-a-chip* (LOC) models have proven especially valuable for studying lung physiology, respiratory diseases, and drug efficacy under controlled laboratory conditions. At the core of LOC systems is the alveolar–capillary barrier, as it represents the critical interface between air and fluid in the human lungs [3]. To achieve physiological relevance, the model should reproduce as many key features of the alveolar–capillary barrier as possible, including the appropriate cell types, a controlled medium flow that mimics blood circulation through the capillaries, breathing frequency, and the cyclic stretching and relaxation of lung tissue [4]. Therefore, the aim of this research was to develop a functional *lung-on-a-chip* model as a platform for future biomedical studies. Using state-of-the-art methods such as CAD design, 3D printing, and electrospinning, a compact device was fabricated in which the basal membrane between epithelial and endothelial cell layers is mimicked by an electrospun polycaprolactone (PCL) membrane. Connective tissue was simulated by applying a hydrogel layer onto the membrane. Airflow and cyclic membrane stretching were generated through controlled air suction and release in the upper chamber, while a regulated medium flow in the lower chamber mimicked blood circulation. Integrated sensors were to monitor pH, oxygen concentration, and selected inhaled drugs, enabling evaluation of the system's functionality. By this approach, we propose a reliable and physiologically relevant *in vitro* model of the human lung, capable of accurately simulating respiratory functions and responses, advancing respiratory biomedical research [5, 6].

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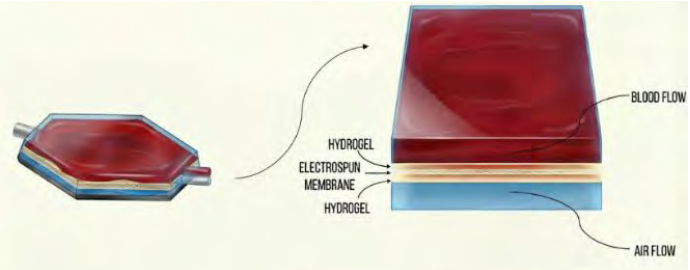
This work was funded by the Croatian Science Foundation through the project IP-2024-05-4339 entitled " Coffee ring' effect in 'Lab on a Chip' environments in the development of new drug formulations." leader prof. Ernest Meštrović.



KINETIC CHARACTERIZATION OF PestE ENZYME IN SYNTHESIS OF *N*-TRANS-FERULOYLTYRAMINE IN WATER-BASED SYSTEM

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N-trans-feruloyltyramine (*N*-FT) is a member of the hydroxycinnamic acid amide group, which are secondary metabolites produced by various plants [1]. Extensive studies have shown that it possesses antioxidant, antidiabetic, anticancer, neuroprotective and anti-inflammatory properties [2,3]. The small quantities of *N*-FT present in plants make direct extraction impractical, so alternative methods for producing larger amounts have been explored. Enzymatic synthesis has emerged as an environmentally friendly way to produce *N*-trans-feruloyltyramine, achieving good yields under milder conditions [4]. Certain promiscuous hydrolases/acyltransferases have been shown to synthesise amides in aqueous solutions, one of which is the extremely thermostable PestE enzyme from *Pyrobaculum calidifontis* VA1 [5,6]. Using PestE's acyltransferase activity, it is possible to produce *N*-trans-feruloyltyramine in a water-based medium, without cofactors or large quantities of organic solvents [7].
The PestE enzyme was kinetically characterised in the synthesis of *N*-trans-feruloyltyramine. In this study, results from kinetic characterization of this enzyme will be presented. The acquired data can be used as a basis for the development of the mathematical model of the process and reaction optimization.

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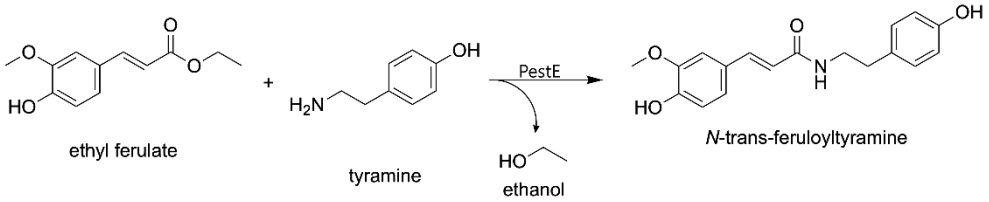

EVALUATION OF DEEP EUTECTIC SOLVENT–BASED AQUEOUS TWO-PHASE SYSTEMS PERFORMANCE FOR FERULIC ACID EXTRACTION

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Ferulic acid is a valuable phenolic compound widely recognized for its antioxidant, antimicrobial, and functional properties, which has stimulated growing interest in the development of efficient and environmentally benign extraction techniques. Conventional extraction methods often rely on large volumes of organic solvents, elevated temperatures, and multiple purification steps, which can limit selectivity and sustainability. In this context, aqueous two-phase systems (ATPS) based on deep eutectic solvents (DES) represent a promising green alternative for the selective extraction and separation of ferulic acid. The use of DES in ATPS offers several distinct advantages for ferulic acid extraction. First, DES are characterized by low volatility, tuneable polarity, and strong hydrogen-bonding capacity, which can be tailored to improve the affinity toward phenolic compounds such as ferulic acid. Second, the aqueous nature of ATPS provides a mild extraction environment, minimizing degradation of thermolabile compounds and reducing energy consumption. Third, the biphasic system enables simultaneous extraction and preliminary purification in a single step, thereby simplifying downstream processing. In addition, the incorporation of ethanol into the salt-rich phase improves system flexibility and may facilitate future solvent recovery and recycling.

In the present study, an ATPS composed of a DES-rich phase and an inorganic salt phase was investigated for its potential to extract ferulic acid. The upper phase consisted of various choline chloride–based DES formulated with different hydrogen bond donors, including fructose, glucose, maltose, sucrose, and xylose, prepared at selected molar ratios and concentrations. The lower phase was formed by potassium hydrogen phosphate (K_2HPO_4) dissolved in 50% (v/v) ethanol, serving as a salting-out agent to promote phase separation and enhance solute partitioning. The influence of DES composition, molar ratio, and concentration on phase formation and extraction performance was systematically evaluated. The results showed that the ATPS containing ChCl:Fruc (2.5:1) with 30% water achieved an extraction efficiency of 92.34%, followed by the ATPS containing ChCl:Glc (2:1) with 30% water, which resulted in an extraction efficiency of 71.99%. All other analysed systems exhibited extraction efficiencies below 50%. This study provides fundamental insights into the feasibility of DES-based ATPS as a sustainable platform for ferulic acid extraction. The results obtained from phase behaviour analysis and extraction experiments will contribute to the rational design of green separation systems and support the development of scalable, low-impact processes for the recovery of high-value phenolic compounds.

MECHANOCHEMICAL NUCLEOSIDE PHOSPHORYLATION

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The quest for life's origins centers on the mechanisms by which random abiotic interactions assemble into self-organizing biological systems. According to the RNA-world hypothesis, early life was based on RNA oligomers; however, the formation of these molecules first required overcoming the binary chemical contradiction of the "Phosphate Problem" and the "Water Problem". While phosphorus is vital for biological functions, such as energy transfer and the structural integrity of nucleic acids, its availability during the Hadean Eon (4.5 to 4.0 billion years ago) was limited by the low solubility of common minerals like apatite [1]. Paradoxically, water, though essential for life, drives chemical equilibrium toward hydrolysis rather than polymerization [2]. Phosphorylation is a "gateway" condensation reaction; because a water molecule is released, the process is thermodynamically unfavourable in dilute aqueous solutions. Consequently, the synthesis of proto-RNA relied on the formation of kinetically stable phosphate ester bonds under low-water-activity conditions. During this period, which overlaps with the Prebiotic Era, planetary bombardment was at its peak, suggesting that the flux of phosphorus-rich meteoritic minerals was a primary factor for prebiotic reactions [3].
In our work, phosphorylation and meteoritic flux are simulated by mechanochemical processing of solid mixtures containing nucleosides and prebiotically plausible phosphate and urea-rich compounds using a mixer mill [4]. In this context, urea acts as a condensing agent [5], which combined with mechanical and thermal energy, enables the formation of stable phosphate ester bonds by bypassing both the "Phosphate Problem" and the "Water Problem". Additionally, increasing the reaction temperature enhances the reaction yield and the amount of nucleoside 5′-monophosphate, the primary building block for modern and likely prebiotic RNA. To further advance these findings, our future research will refine these synthetic methods by tuning experimental conditions to simulate the Hadean environment better. Incorporating factors such as a reducing atmosphere or high-energy ionizing radiation would allow for more precise reconstruction of early Earth's conditions.

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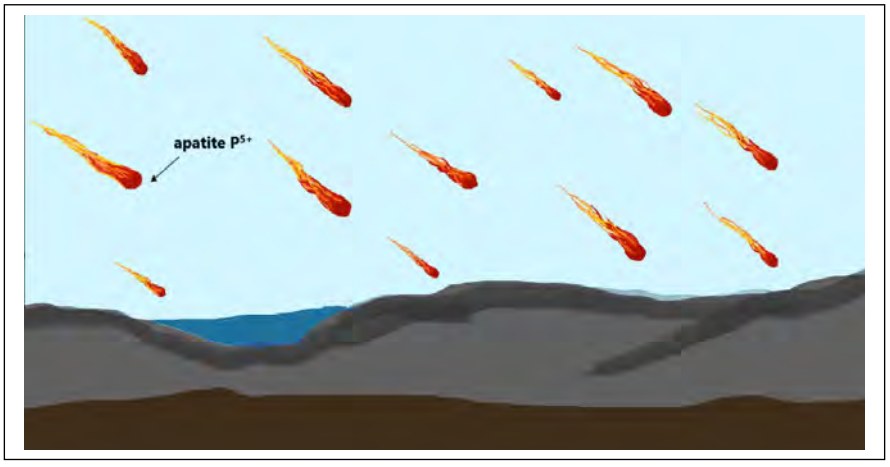

SMIČNO NAPREZANJE U KRVOTOKU: KRITIČAN IZAZOV ZA UČINKOVITOST NANOLIJEKOVA

SHEAR STRESS IN BLOODSTREAM: A CRITICAL CHALLENGE FOR NANOMEDICINE PERFORMANCE

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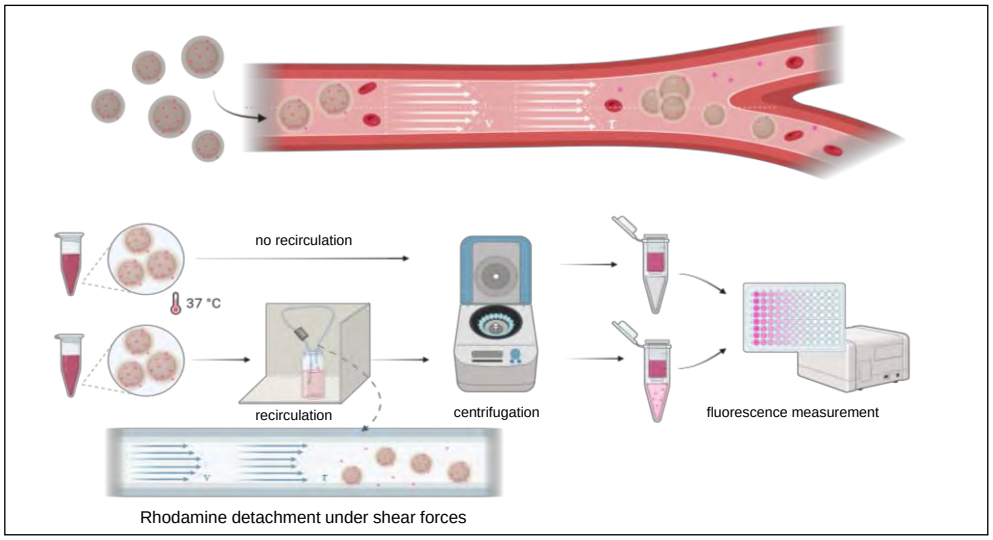
Nanomedicine has the potential to transform cancer therapy by enabling precise delivery of therapeutic agents to diseased tissues while minimizing systemic side effects. However, nanoparticles are continuously exposed to dynamic mechanical forces in the bloodstream, particularly shear stress, which can significantly influence their stability, surface chemistry, and overall performance. Understanding how nanoparticles behave under physiologically relevant shear conditions is therefore essential for the rational design of drug-delivery systems. In this study, Pluronic F127 nanoparticles were functionalized with rhodamine using click chemistry, enabling the formation of a covalent and stable fluorescent label. This approach ensures attachment of the dye while allowing non-specific interactions to be efficiently removed through washing. The fluorescent nanoparticles were then subjected to controlled shear stress using a recirculation setup consisting of narrow tubing and a pump, which allowed precise modulation of flow rates and shear levels to mimic key features of blood flow. Our findings demonstrate that shear stress might have a measurable impact on nanoparticle stability. Fuorescence analysis revealed that shear stress promotes partial detachment of the covalently attached rhodamine from the nanoparticle surface. Furthermore, increased shear levels led to an elevated polydispersity index (PDI), indicating a broader size distribution and suggesting that mechanical forces may contribute to particle deformation or aggregation. These changes highlight the importance of evaluating nanoparticle formulations under realistic conditions rather than relying solely on static characterization. Future work will extend this investigation to nanoparticles carrying different conjugates, including peptides and antibodies, and will examine their behaviour across a broader range of shear values. Such insights will support the development of more resilient and predictable nanocarrier systems for clinical applications.



DESIGN OF AN ENZYMATIC CASCADE FOR THE BIOSYNTHESIS OF L-PIPERAZIC ACID

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L-piperazic acid is a six-membered cyclic hydrazino acid and an important molecular scaffold that is a component of various pharmaceuticals [1]. The conventional synthesis of this compound is a complex, multi-step procedure that is carried out under harsh conditions. Enzymatic synthesis offers an alternative approach that overcomes the limitations of the conventional route [2,3]. The investigated cascade reaction utilizes L-ornithine as the starting compound. In the first step, a flavin-dependent N-hydroxylating monooxygenase (NMO) attaches a hydroxyl group to the δ-amino group of L-ornithine [4]. In this reaction, NADPH is utilized by the NMO as a source of reducing equivalents to reduce the flavin cofactor to enable repetitive utilization. Due to the high cost of NADPH cosubstrate, it is necessary to regenerate it over the course of the reaction. This is achieved with the use of a formate dehydrogenase (FDH) that has been engineered for greater affinity towards $NADP^+$. This enzyme oxidizes formate to carbon dioxide and simultaneously reduces $NADP^+$ to NADPH [5]. In the second step of the reaction, the N-hydroxylated amino acid undergoes cyclization to L-piperazic acid by a piperazate synthase [3]. In this work, the kinetics of the reactions catalyzed by these enzymes were investigated by using the initial reaction rate method. The activity of these enzymes was investigated at varying concentrations of the substances that are involved in the cascade reaction to estimate the values of parameters such as K_M, V_m and K_i. The obtained parameters were utilized to develop a mathematical model of the investigated reaction.

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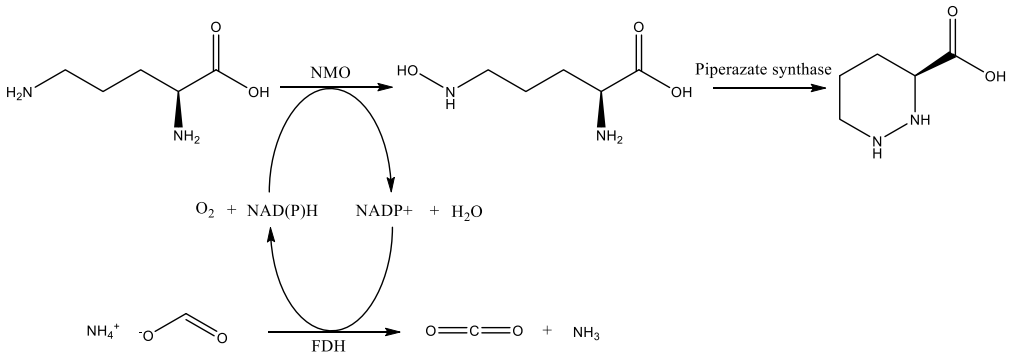

ADDITION OF ENCAPSULATED *LACTOBACILLUS HILGARDII* IN PEA PROTEIN FOR OBTAINING KOMBUCHA BEVERAGE WITH PROBIOTIC PROPERTIES

Katarina Žarko, Tara Budimac, Aleksandra Ranitović, Olja Šovljanski, Dragoljub Cvetković, Ana Tomić, Teodora Marić, Zita Šereš

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Kombucha is a traditional beverage, which is usually prepared by fermenting sweetened black tea using a symbiotic consortium of acetic acid bacteria (AAB) and yeast. Kombucha exhibits several functional properties such as antioxidant, antimicrobial, anticancer, etc. However, its probiotic potential is limited due to low and variable concentrations of lactic acid bacteria (LAB) and their number most often does not reach the specified criteria. LAB should be able to survive sometimes harsh conditions during fermentation, storage and passing through the gastrointestinal tract, to exhibit health benefits. Several methods of microencapsulation of probiotic microorganisms are widely used to improve their viability. The aim of this work was to enhance the probiotic properties of kombucha beverage by incorporating encapsulated *Lactobacillus hilgardii* into the fermentation system. The probiotic culture was encapsulated in pea protein by lyophilization method and added at the beginning of kombucha fermentation. Encapsulation in pea protein protected the cells under acidic and oxidative conditions, enabling their survival throughout the process. Obtained results indicated a slightly higher titratable acidity in samples enriched with encapsulated *L. hilgardii* compared to the control. The number of viable LAB remained stable during fermentation, with 7.28 log CFU/mL on the final day, exceeding the recommended minimum level for probiotic products defined as 6-7 log CFU/mL. The growth of native yeasts and acetic acid bacteria was not negatively affected. These findings suggest that pea protein-based encapsulation is a promising strategy for the development of kombucha with improved probiotic properties.

This research was funded by the Republic of Serbia program of the Ministry of Science, Technological Development and Inovation, grant numbers: 451-03-66/2024-03/200134 and 451-03-65/2024-03/200134.

KARAKTERIZACIJA EUTEKTOGELOVA NA BAZI OSMOLITA ZA STABILIZACIJU PROTEINA

RHEOLOGICAL CHARACTERISATION OF EUTECTOGELS BASED ON OSMOLITES FOR PROTEIN STABILISATION

Martina Železnjak[1], Matija Cepanec[2], Kristina Radošević[1], Nikolina Mustač Čukelj[1], Marina Cvjetko Bubalo[1], Marko Rogošić[2], Ivana Radojčić Redovniković[1]

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Proteini igraju ključnu ulogu u industrijama poput prehrambene, biotehnološke, kozmetičke i farmaceutske čineći temelj za napredak u terapiji i razvoju lijekova. Niskotemperaturna eutektička otapala (engl. *deep eutectic solvents*, DESs) su niskotoksična, biorazgradiva i visoko prilagodljiva otapala koja učinkovito stabiliziraju biomolekule poput proteina. Ova otapala također pokazuju antioksidativna i antimikrobna svojstva, što ih čini pogodnim za primjenu u isporuci lijekova. U prijašnjim istraživanjima istaknuo se potencijal DES-ova temeljenih na osmolitima, Osmoliti su male molekule koje se u stanicama proizvode kao odgovor na vanjske stimulanse, a pripisuje im se se nekoliko bioloških funkcija, među kojima je najizraženija povećanje termodinamičke stabilnosti makromolekula bez ugrožavanja njihove izvorne funkcionalnosti, zbog čega je njihova stabilizacijska uloga zanimljiva za industriju. DES-ove čije su komponente osmoliti nazivamo osmoDES-ovima [1]. Takvi tzv. osmoDES-ovi mogu se primijeniti kao netoksični stabilizacijski medij, koji otvara nove mogućnosti za primjenu proteina u biotehnologiji i medicini, osobito u uvjetima povišenih temperatura ili drugih destabilizirajućih faktora [2]. Međutim, postojeće tekuće formulacije proteina i dalje se suočavaju s izazovima poput smanjene stabilnosti tijekom skladištenja i primjene, što potiče intenzivna istraživanja usmjerena na razvoj stabilnijih formulacija koje omogućuju sigurniju, učinkovitiju i kontroliraniju dostavu lijekova.

Eutektogelovi su relativno nov pojam koji se odnosi na polimerne mreže mekih materijala čiji je sastav temeljen na komponentama DES-a. Inkorporacijom DES-ova u polimerne mreže dobivaju se gelovi s mehaničkim svojstvima konvencionalnih gelova te stabilizacijskim svojstvima DES-ova [3]. Eutektogelove na bazi osmolita istražujemo kao potencijalne nosače za oralnu ili transdermalnu administraciju proteina, nudeći jedinstvenu kombinaciju termodinamičke stabilnosti i strukturnih svojstava prilagođenih isporuci. Karakterizacija eutektogelova fokusirana je na svojstva ključna za prolaz kroz biološke barijere, uključujući reološko ponašanje (viskoznost i tiksotropija, važne za transdermalnu primjenu i prolaz kroz gastrointestinalni trakt), kao i sposobnost gela da zaštiti protein od degradacije primjerice uslijed niskog pH u želucu ili enzimske aktivnosti. Daljnji koraci istraživanja usmjereni su na ispitivanje u kojoj mjeri sinergija osmolita i polimernog skeleta u eutektogelovima može predstavljati potencijalni put prema razvoju stabilnih i učinkovitih proteina za primjenu bez injekcije. Stoga, cilj ovog rada je karakterizirati nove eutektogelove na bazi osmolita, s posebnim naglaskom se na njihova ključna svojstva (poput reoloških i strukturnih), kako bi se procijenio njihov potencijal kao nosača za stabilnu i učinkovitu neinvazivnu dostavu proteina.

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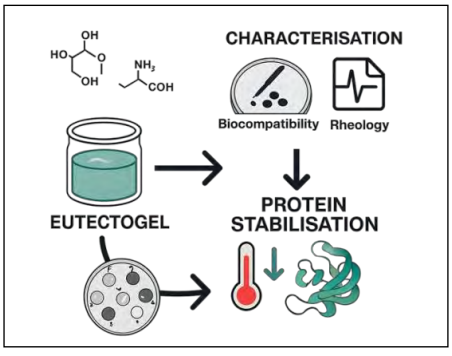
Ovaj rad financiran je sredstvima Hrvatske zaklade za znanost u sklopu projekta IP-2024-05-9948.



Ekoinženjerstvo
Environmental engineering

VALORIZATION OF AGRO-INDUSTRIAL WASTE FOR PHB BIOPOLYMER PRODUCTION USING ACID HYDROLYSIS AND SUBMERGED FERMENTATION

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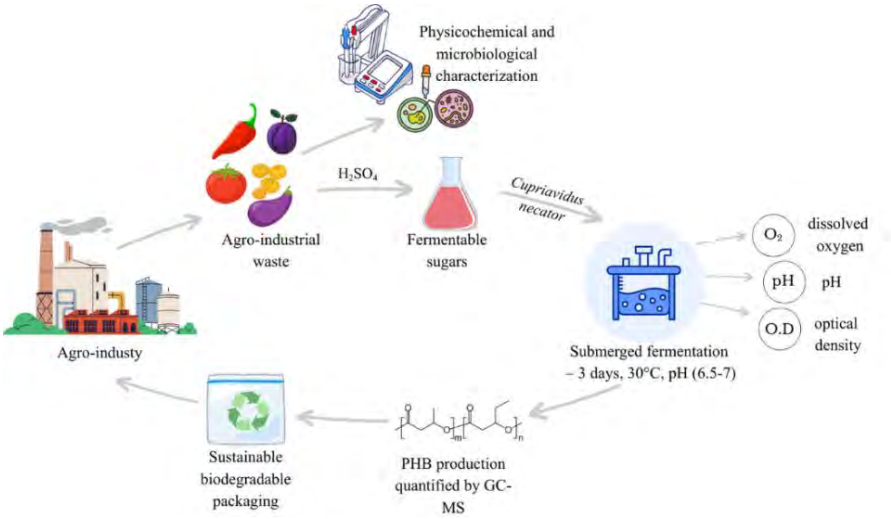
Conventional synthetic plastics present an increasing environmental concern due to their persistent degradation, potential toxicity and extensive use of non-renewable resources. As a sustainable alternative, biodegradable polymers such as poly(3-hydroxybutyrate) (PHB) have gained significant attention. PHB is a biopolymer naturally synthesized by microorganisms and can be produced from low-cost renewable substrates such as agro-industrial residues. Such residues represent valuable biological resources rich in carbohydrates, proteins, and other organic compounds which could be suitable for biotechnological conversion. [1] In this study, a mixture of various agro-industrial wastes (chickpeas, plums, eggplants, peppers, and tomatoes) was prepared and evaluated as a substrate for PHB production through submerged fermentation (SmF). To assess its suitability for SmF, the waste mixture underwent physicochemical and microbiological characterization, followed by acid hydrolysis to release fermentable sugars. These sugars were subsequently used as the carbon source in the SmF process. Fermentation was carried out in a bioreactor over three days at 30°C, with the pH maintained between 6.5 and 7.0, using the bacterial strain *Cupriavidus necator*. The medium initially contained 4.83 g/L of sugar, and additional feed was added continuously to maintain a consistent carbon concentration. Process performance was monitored by measuring optical density, pH, and dissolved oxygen to track microbial growth and PHB accumulation. The resulting biomass contained 60% PHB, as determined by GC-MS analysis. Overall, the results demonstrate that agro-industrial residues can be effectively valorized for PHB production, contributing both to waste reduction and the development of sustainable biodegradable packaging materials.

[1] L. Getino et al., Microorganisms 12 (2024) 2028.

Financira Europska unija NextGenerationEU *This research was carried out 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-I1.04.0059) financed by the National Recovery and Resilience Plan (financed by the European Union, NextGenerationEU).*



RAZVOJ ANALITIČKE METODE ZA ODREĐIVANJE KANCEROGENIH I MUTAGENIH POLICIKLIČKIH AROMATSKIH UGLJIKOVODIKA U PM_{10} ČESTICAMA

DEVELOPMENT OF AN ANALYTICAL METHOD FOR THE DETERMINATION OF CARCINOGENIC AND MUTAGENIC POLYCYCLIC AROMATIC HYDROCARBONS IN PM_{10} PARTICLES

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Policiklički aromatski ugljikovodici (PAU) široko su rasprostranjeni spojevi poznati po svojim kancerogenim i mutagenim svojstvima. U okoliš dospijevaju procesima proizvodnje goriva, prirodnog plina, lakih i teških metala ili prirodnim putem prilikom šumskih požara i vulkanskih erupcija. Najčešći izvori PAU su izgaranje goriva u motornim vozilima, spaljivanje otpada i kućna ložišta na drvo i ugljen. Izgaranjem benzinskog goriva ispuštaju se PAU većih molekulskih masa, dok dizelska goriva emitiraju PAU manjih molekulskih masa. U okolišu su prisutni vezani na organske i anorganske čestice u tlu, na PM_{10} čestice u zraku ili kao slobodne molekule u zraku. Iz navedenih razloga u Državnom hidrometeorološkom zavodu (DHMZ), kao i u ovom radu, pratila se koncentracija većeg raspona molekulskih masa PAU (od benzo[*a*]antracena do benzo[*g,h,i*]perilena) u PM_{10} česticama.
U ovom istraživanju optimirana je i validirana metoda za određivanje PAU u PM_{10} česticama na plinskom kromatografu spregnutom sa spektrometrijom masa (GC-MS). Razvoj metode uključivao je optimizaciju pripreme uzoraka, uvođenje postupka ubrzane ekstrakcije otapalom i optimizaciju metode GC-MS. U postupku pripreme uzoraka uvedeni su novi unutarnji standardi, postupak ekstrakcije optimiran je s obzirom na temperaturu ekstrakcije, volumen otapala i broj ciklusa ekstrakcije. U metodi GC-MS optimirani su uvjeti rada promjenom kolone, protoka pokretne faze, temperature ubrizgavanja uzorka i kolone. Određeni su optimalni uvjeti postupka ekstrakcije: temperatura ekstrakcije od 90 °C, volumen otapala 75 % volumena ćelije i 3 ciklusa ekstrakcije. Primjenom nove kolone (*Select PAH*) i nove otopine unutarnjeg standarda (*PAH Mix 9 deuterated*) postignuta su bolja iskorištenja u odnosu na prethodno korištenu kolonu i unutarnje standarde. Validacija metode provedena je ispitivanjem selektivnosti, linearnosti, ponovljivosti i istinitosti. Na temelju rezultata validacije pokazano je da se metoda može primjenjivati za analizu PAU u realnim uzorcima PM_{10} čestica prikupljenih na postaji Puntijarka u Zagrebu i dostavljenih u Državni hidrometeorološki zavod.

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HIGH-EFFICIENCY BIODEGRADATION OF LEACHATE BY ACTIVATED SLUDGE CONSORTIA

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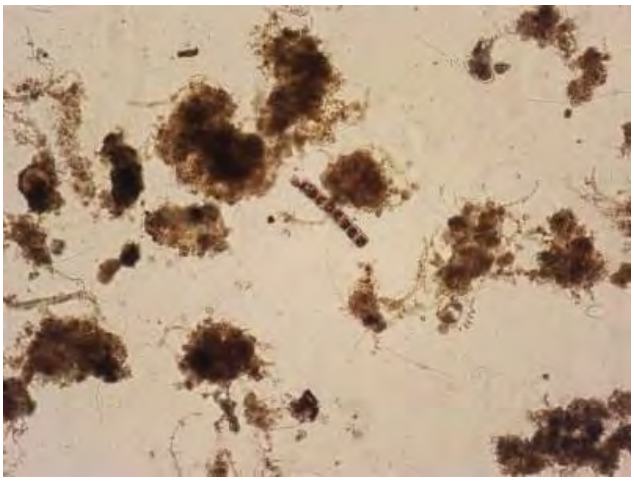
Wastewater treatment is a major global challenge as drinking water becomes an increasingly valuable natural resource. Consequently, legislative frameworks impose strict environmental protection measures and requirements for the treatment of such water. Bioremediation technology uses microorganisms to transform or remove pollutants from the environment. These approaches improve the efficiency of wastewater purification by supporting the sustainable removal of organic contaminants.

In this study, the biodegradation potential of a model leachate sample was investigated using activated sludge under batch, aerobic conditions. The chemical oxygen demand (COD) of the leachate was 17 212 mg/L. The organic matter content of the activated sludge was high, at 0.87 ± 0.09. Dissolved oxygen ranged from 0.03 to 5.80 mg/L, and the pH averaged 6.30 ± 1.47. Microbiological analyses confirmed active growth of heterotrophic bacteria at 8.8 ± 0.4 log cfu/mL. The organic matter removal efficiency was 85 ± 1%. The results demonstrate the significant potential of biological technologies for treating contaminated wastewater. These processes offer a viable alternative to conventional methods and provide environmentally friendly solutions for environmental protection.



MOLECULARLY IMPRINTED TiO_2 BASED PHOTOCATALYST FOR TORASEMIDE REMOVAL FROM WATER

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The rapid development of technology has enabled the development of numerous pharmaceutically active compunds, significantly improving human quality of life. However, this progress has also contributed to their widespread presence in the environment. Various pharmaceuticals are found in soils, sediments, groundwater, surface water, and especially in wastewater, entering the environment through household use and improper disposal. Considered emerging pollutants, pharmaceuticals pose a significant risk to ecosystems and human health due to their biological activity and persistence in the environment. One of the most commonly used processes for removing organic pollutants from wastewater is photocatalysis. TiO_2 photocatalysts are most frequently used due to their stability, efficiency, and low cost. However, a drawback of these photocatalysts is their low affinity and selectivity toward the target compound. This study investigated the preparation of molecularly imprinted TiO_2 based photocatalyst for torasemide removal from water. Torasemide imprinted TiO_2 photocatalyst was tested to enhance degradation efficiency by improving the recognition and adsorption of torasemide. To evaluate the selectivity and efficiency of the imprinted photocatalyst, non-imprinted TiO_2 photocatalyst was also prepared.

This study was supported by the Croatian Science Foundation under the project number HRZZ-IP-2022-10-4400 entitled Development of molecularly imprinted polymers for use in analysis of pharmaceuticals and during advanced water treatment processes (MIPdePharma).

GREEN SYNTHESIS OF ZnO NANOPARTICLES USING GRAPE POMACE EXTRACT AND THEIR APPLICATION IN THE PHOTOCATALYTIC DEGRADATION OF METFORMIN

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The widespread use of pharmaceuticals in both human and veterinary medicine has resulted in their accumulation in aquatic environments, where they pose increasing ecological risks. Metformin (MET), a commonly prescribed first-line therapy for type 2 diabetes is of particular concern [1]. Advanced oxidation processes offer a promising solution, with heterogeneous photocatalysis emerging as particularly effective due to its eco-friendly nature, use of renewable solar energy, and ability to generate highly reactive species capable of degrading persistent pollutants [2]. Heterogeneous photocatalysis relies on semiconductor materials as catalysts, and recent research increasingly promotes the use of green photocatalysts synthesized from plant extracts. Such bio-derived materials not only reduce the use of hazardous chemicals but also support principles of green chemistry and circular economy, especially when catalysts are produced from agricultural waste as demonstrated in this study [3]. The aim of this study was the green synthesis of ZnO nanoparticles using grape pomace extract and the investigation of their efficiency in the photocatalytic degradation of MET (influence of catalyst loading) from an aqueous suspension under simulated solar irradiation. Firstly comparison between photolytic and photocatalytic degradation was performed. After 3 h of irradiation, the photocatalytic process showed higher MET degradation efficiency when newly synthesized ZnO nanoparticles obtained from grape pomace extract were used as the photocatalyst. Considering the optimized experimental conditions, in the presence of newly synthesized ZnO nanoparticles based on grape pomace extract (1.0 mg/mL), 17% of substrate was removed, after 180 min of irradiation. Based on the obtained results it can be concluded that the photocatalytic process is more effective than simple photolytic process. Also, the results confirmed that the newly synthesized ZnO nanoparticles based on grape pomace extract are suitable and effective for the photocatalytic degradation of MET.

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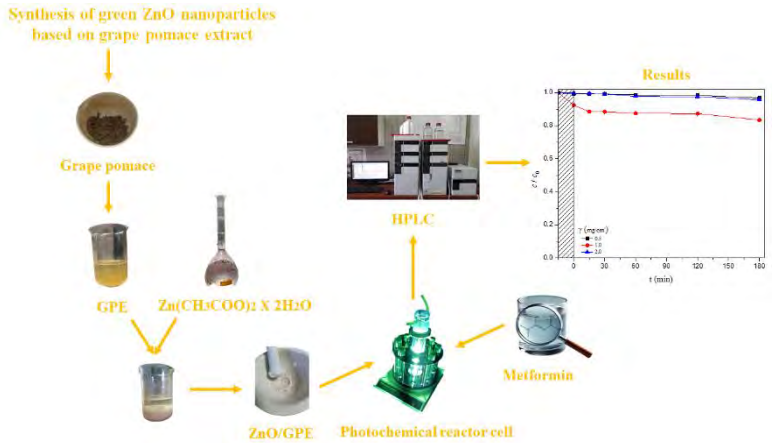
The authors gratefully acknowledge the financial support of the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Grants Numbers: 451-03-137/2025-03/ 200125 and 451-03-136/2025-03/200125).



ODREĐIVANJE ANTIMIKROBNIH SVOJSTAVA ADITIVA

DETERMINATION OF ANTIMICROBIAL ACTIVITY OF ADDITIVES

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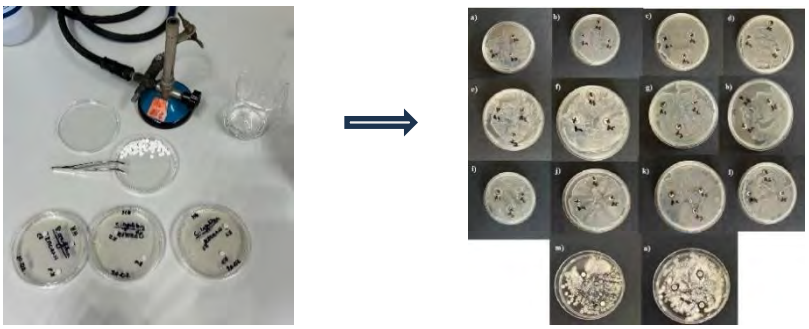
Budući da je jedan od ključnih problema današnjice rezistencija mikroorganizama, mnoga istraživanja usmjerena su na proučavanje antimikrobnih svojstava raznih aditiva. Različite industrije kao što su prehrambena, poljoprivredna, kozmetička te farmaceutska tragaju za novim rješenjima u suzbijanju rasta mikroorganizama. Neki od antimikrobnih aditiva koji se danas koriste su nanočestice srebra, timol i kitozan. Iako se u prošlosti nisu toliko upotrebljavali, ljudi su primijetili antimikrobna svojstva kod srebra, biljaka koje kao glavni sastojak sadrže timol te kod kitozana koji se dobiva iz hitina, rožnate tvari koja čini vanjski oklop člankonožaca.
Cilj ovog rada bio je odrediti antimikrobna svojstva navedenih aditiva pri šest različitih masenih udjela protiv 5 bakterija i 3 gljive. Ispitivanje je provedeno u laboratoriju, a za eksperimentalno određivanje antimikrobne aktivnosti korištena je disk difuzijska metoda. Nanočestice srebra inhibirale su rast bakterija *Enterococcus faecalis, Staphylococcus aureus, Bacillus subtilis, Escherichia coli* i *Pseudomonas aeruginosa*, te rast gljive *Penicillium funiculosum*. Za gljivu *Candida lipolytica* nanočestice srebra nisu pokazale inhibicijsko djelovanje. Kod *Aspergillus niger* uočava se izostanak zona. Provođenjem eksperimenta s timolom, uočeno je inhibicijsko djelovanje za *Enterococcus faecalis, Candida lipolytica, Staphylococcus aureus i Escherichia coli*. Za bakteriju *Pseudomonas aeruginosa*, uočeno je inhibicijsko djelovanje samo pri najvećoj koncentraciji timola, dok za *Bacillus subtilis* te *Penicillium funiculosum* timol ne pokazuje nikakvo inhibicijsko djelovanje. Kod gljive *Aspergillus niger* uočava se izostanak zona. Ispitivanjem antimikrobnih svojstava kitozana, uočeno je inhibicijsko djelovanje samo za bakterije *Escherichia coli* te *Staphylococcus aureus.*

Financira Europska unija NextGenerationEU *Ovo istraživanje provedeno je u sklopu projekta „Proizvodnja i razvoj kompostabilne ambalaže iz otpadne biomase za pakiranje industrijski prerađenih prehrambenih proizvoda" (NPOO.C3.2.R3-I1.04.0059) financiranog iz Nacionalnog plana oporavka i otpornosti (financiranog od strane Europske unije, NextGeneration EU).*



INFLUENCE OF PRETREATMENT ON REVERSE OSMOSIS MEMBRANE FLUX DURING TEXTILE WASTEWATER TREATMENT

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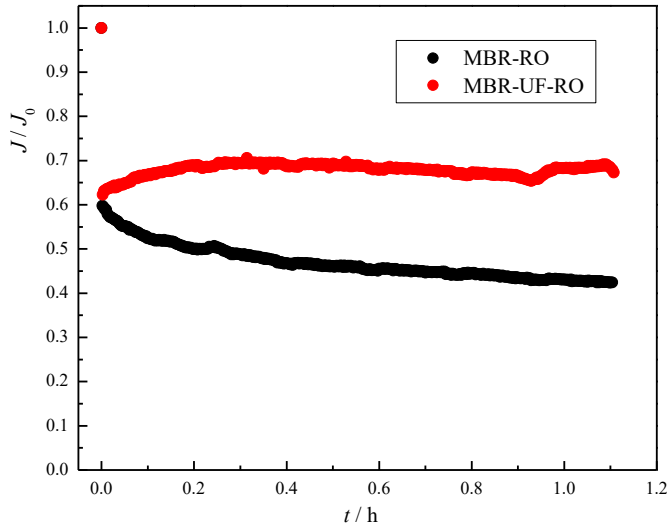
The textile industry consumes large amounts of water (drinking water or groundwater) for its wet processes. As a result, a large volume of textile wastewater (TWW) is generated, which is extremely toxic and highly polluted due to the presence of acids, alkalis, auxiliaries, salts, dyes, and other substances. This leads to high levels of chemical oxygen demand (COD), suspended solids (SS), color, electrical conductivity, turbidity, and more.
Real TWW was sampled at a textile factory in Croatia and was first treated with a membrane bioreactor (MBR). The MBR permeate was then treated with (1) reverse osmosis (RO) and (2) ultrafiltration (UF) followed by RO. During MBR treatment, the mixed liquor suspended solids were 9.74±0.34 g/L, and the hydraulic retention time was between 11 h and 13 h. The UF membrane used was GH (Veolia, France), and the RO membrane was XLE (Dupont FilmTec, USA). The working pressure for UF and RO were 10 bar and 14 bar, respectively. The flux for UF and RO was measured every 10 seconds using mass balance over 1 h.
The initial flux (with demineralized water) of the RO membrane was 139 L/(m^2·h) and 137 L/(m^2·h) for MBR-RO and MBR-UF-RO systems, respectively. For both systems, the flux decreased at the beginning of the treatment by 40% and 35%, respectively. For the MBR-RO system, the flux decreased continuously during the 1 h treatment by up to 55%, while for the MBR-UF-RO system, the flux remained constant during the 1 h treatment. These results show that UF, as an additional treatment step, reduced fouling in the final RO step, which is important for the membrane's lifetime.

This research was funded by the NATO Science for Peace and Security Programme under grant id. G6087 and Croatian Science Foundation project DOK-NPOO-2023-10-8063.



INTEGRATED ULTRASONIC AND ENZYMATIC PRETREATMENT OF AGROINDUSTRIAL WASTE FROM PLUMS FOR THE BIOSYNTHESIS OF POLYHYDROXYALKANOATES USING SOLID STATE FERMENTATION

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The excessive accumulation of non-degradable plastics represents one of the leading environmental challenges of the modern era. Combined with the depletion of fossil fuel reserves, this has created an urgent need for intensive research and application of sustainable and biodegradable materials [1]. As a result, polyhydroxyalkanoates (PHA) have been developed - polyester compounds of hydroxyalkanoates synthesized by microorganisms which are stored intracellularly, under nutrient limited conditions [2]. Their biodegradability, biocompatibility and similarity to synthetic polymers make PHA a promising alternative for conventional plastics [3]. To achieve efficient PHA biosynthesis with minimal energy consumption, the use of solid state fermentation (SSF) for microbial cultivation is being explored [4]. Furthermore, to reduce the overall production cost of PHA, agroindustrial waste rich in lignocellulosic compounds is increasingly being used as a nutrient source [1].

In this study, valorization of plum biomass waste for PHA biosynthesis using *Cupriavidus necator* had been investigated. To increase the availability of reducing sugars, the substrate was pretreated using ultrasonic pretreatment and enzymatic hydrolysis, during which various processing variables were examined. After determining the optimal pretreatment parameters, the pretreated substrate was subjected to SSF. Efficiency of pretreatment as well as the amount of produced PHA were compared with the results obtained from fermentation of the untreated substrate. Throughout the experiment, physicochemical and microbiological parameters were continuously monitored. After fermentation, extraction and characterization of the synthesized PHA were performed. Results indicated that pretreatment significantly increased sugar availability, which in turn lead to higher PHA accumulation during fermentation (2.92 %) in comparison with the untreated substrate (1.72 %). This study confirmed the importance of pretreatment for improving PHA production processes.

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Financira Europska unija NextGenerationEU *This research was carried out 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-I1.04.0059) financed by the National Recovery and Resilience Plan (financed by the European Union, NextGenerationEU).*

VALORIZATION OF PLUM WASTE WITH THE AIM OF OBTAINING POLYHYDROXYALKANOATES BY SUBMERGED FERMENTATION

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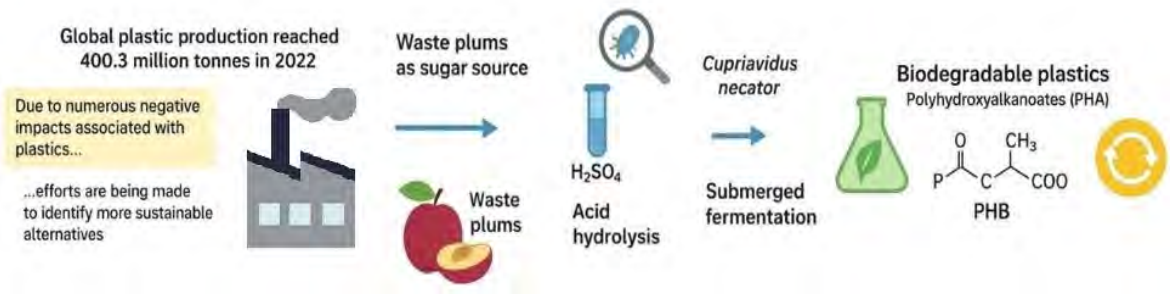
The environmental burden associated with conventional plastics, particularly their poor degradability and the release of micro- and nanoparticles into ecosystems, has intensified the search for sustainable alternatives. Polyhydroxyalkanoates (PHAs), biodegradable polymers naturally synthesized by microorganisms, represent a promising solution [1]. This study investigated the production of PHA using submerged fermentation (SmF), with waste plums serving as a cost-effective and lignocellulosic-rich carbon source. Comprehensive physicochemical and microbiological characterization of the raw biomass revealed a pH of 4.590, electrical conductivity of 1523 µS/cm, glucose content of 81.45 mg/$g_{dry\ matter}$, moisture content of 68.15%, volatile matter of 97.03%, COD of 353.14 mg/$g_{dry\ matter}$, and a C/N ratio of 49.27/1. Microbial analysis showed 1.97×10^8 bacterial cells and 1.52×10^9 yeasts, while molds were not detected. To increase fermentable sugar availability, the biomass underwent acid hydrolysis with 2% sulfuric acid, resulting in a sugar concentration of 333.59 mg/$g_{dry\ matter}$ and COD of 494.62 mg/$g_{dry\ matter}$. Submerged fermentation was carried out using *Cupriavidus necator*, with an initial sugar concentration of 4 g/L, followed by continuous feeding over three days. The fermentation pH remained between 6.5 and 7.0, and optical density increased from 1 to 4, indicating successful microbial growth. The resulting biomass contained approximately 60% PHA. These findings demonstrate the potential of waste plums as an efficient carbon source for PHA production and highlight the feasibility of integrating agricultural residues into biopolymer manufacturing processes.

[1] B. McAdam et al., Polymers 12 (2020) 2908.

Financira Europska unija NextGenerationEU *This research was carried out 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-I1.04.0059) financed by the National Recovery and Resilience Plan (financed by the European Union, NextGenerationEU).*



CHARACTERISATION OF BREWER'S SPENT GRAIN AND SPENT COFFEE GROUNDS FOR SUSTAINABLE BIOPROCESS SYSTEMS

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Brewer's spent grain (BSG) and spent coffee grounds (SCGs) pose a significant challenge due to the large volume of waste produced and its environmental impact. BSG constitutes up to 85% of total waste from the brewing industry, while millions of tonnes of SCGs are generated globally each year. Although these substrates are rich in fibre, protein, polysaccharides, and bioactive compounds, they are often disposed of in landfills, contributing to greenhouse gas emissions and waste management issues [1]. Biological treatment of these substrates offers solutions within the circular bioeconomy, reducing environmental impact and creating added value [2]. Recent research highlights the need to develop systems capable of processing large quantities of these substrates sustainably [3].
The aim of the study was to characterise BSG and SCG substrates through physicochemical and microbiological analyses. In the prepared eluates, the results show a high volatile solids (VS) content of 86 ± 1 g/L and a pH of 5.9 ± 0.9, with bacterial and fungal counts of 5.2 ± 4.4 and 2.7 ± 0.7 log cfu/mL, respectively. The development of integrated waste processing technologies for the sustainable utilisation of large quantities of BSG and SCG paves the way for innovative waste management solutions and a reduction of the ecological footprint.

[1] K. A. Luna et al., Fermentation 11 (2023) 366-372.
[2] M. Pettinato et al., Chem. Eng. Trans. 105 (2023) 56-63.
[3] A. Becze et al., Molecules 29 (2024) 4983-4990.

WASTEWATER TREATMENT THROUGH MICROBIAL BIOSORPTION

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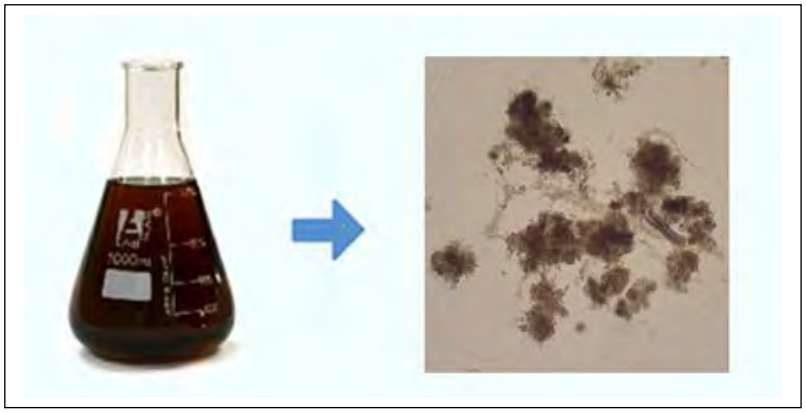
Biosorption uses the natural ability of microorganisms to bind organic pollutants from contaminated environments. The process depends on the metabolic activity of microorganisms to sorb and degrade complex organic compounds. Compared to conventional methods, it offers significant advantages in availability, efficiency, and cost-effectiveness. Waste sludge is increasingly recognised as a resource, particularly for its potential as a biosorbent in water treatment, which aligns with the principles of the circular economy.
In this study, the biosorption of organic substances in leachate using activated sludge was investigated under submerged and batch conditions. The concentration of organic load exceeded 15,000 mg COD/L. The dissolved oxygen and bacterial content were 1.87 mg/L and 8.6 log cfu/mL, respectively. The organic fraction (VSS) in total suspended solids (TSS) was 0.88. The biosorption efficiency was approximately 16% after 90 minutes. The integration of activated sludge in wastewater treatment enables biomass recycling through sustainable resource management and the implementation of solutions for environmental protection.



OPTIMIZACIJA BIORAZGRADNJE ANTIVIROTIKA LOPINAVIRA AKTIVNIM MULJEM

OPTIMIZATION OF THE BIODEGRADATION OF THE ANTIVIRAL LOPINAVIR USING ACTIVATED SLUDGE

Dora Lastovčić, Ivona Zirn, Tijana Jezerčić, Luka Večenaj, Viktorija Martinjak, Matija Cvetnić, Marinko Markić, Tomislav Bolanča, Dajana Kučić Grgić, Šime Ukić

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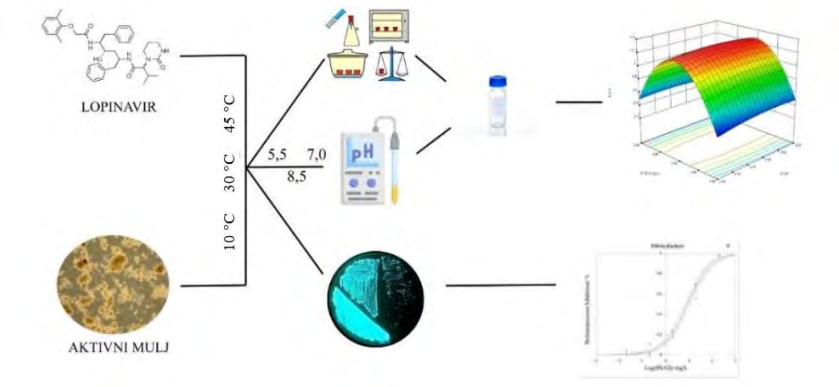
Svrha ovog rada bila je optimizirati uvjete biorazgradnje SARS-CoV-2 antivirotika lopinavira primjenom aktivnog mulja. Posljedica koronavirusa, osim povećanog broja oboljelih i umrlih, preopterećenja zdravstvenih sustava te ekonomske krize, jest i pojava prekomjerne količine antivirotika u otpadnim vodama. [1] Proces obrade otpadnih voda uključuje, uz mehaničke i kemijske metode obrade, i biološku obradu, u kojoj mikroorganizmi razgrađuju organske tvari, dušikove i fosfatne spojeve, deterdžente te mikroonečišćujuće tvari, uključujući i antivirotike, pri čemu aktivni mulj igra ključnu ulogu. [2] U ovom radu istraživano je u kojim uvjetima aktivni mulj postiže najveću učinkovitost u biorazgradnji antivirotika lopinavira provedbom 27 eksperimenata. Proučavani parametri su temperatura, pH i koncentracija biomase mulja kako bi se odredili optimalni uvjeti procesa. Uzorci su uzimani na početku pokusa te nakon 2, 4, 6, 8, i 24 sata, a tijekom eksperimenta praćeni su koncentracija antivirotika, koncentracija otopljenog kisika, vodljivost, pH, MLSS (ukupna suspendirana čvrsta tvar), MLVSS (udio organske tvari u suspendiranoj tvari), MLNSS (udio anorganske tvari u suspendiranoj tvari) te mikroskopska analiza aktivnog mulja. Također je određivana ekotoksičnost otopine antivirotika primjenom bakterije *Vibrio fischeri*, dok je koncentracija antivirotika praćena tekućinskom kromatografijom ultravisoke djelotvornosti (UHPLC). Provedeni eksperimenti, usmjereni na kontrolirano i optimalno uklanjanje lopinavira pomoću aktivnog mulja, pružaju ključne informacije o sudbini ovog antivirotika u okolišu te njegovim ekotoksikološkim posljedicama.

[1] A. Haileamlak. Ethiop J Health Sci. 31(6) (2021) 1073-1074.
[2] R. Wang i sur., J Hazard Mater. 457 (2023) 131694.

Ovaj rad izrađen je u sklopu istraživačkog projekta Okolišni aspekti SARS-CoV-2 antivirotika (IP-2022-10-2822) financiranog od Hrvatske zaklade za znanost.



DETERMINATION OF THE ECOTOXICITY OF CHEMICAL WARFARE AGENT SIMULANTS BY *Vibrio fischeri*

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Manufacturing weapons, destroying infrastructure, and releasing hazardous chemicals pose significant environmental threats. Chemical warfare agents (CWAs) are highly toxic compounds developed for military use to incapacitate, seriously injure, or kill. CWAs can contaminate water infrastructure systems and military water supplies used for drinking, cooking, washing, and showering, leading to oral, dermal, and inhalation exposure [1]. In this study, the ecotoxicity of dimethyl methylphosphonate (DMMP), a simulant of the G-class nerve agents, and 2-chloroethyl ethyl sulfide (2-CEES), a simulant of the blister agent sulfur mustard, was determined using the bacterium *Vibrio fischeri*. Due to its high sensitivity to toxic substances and rapid response, *Vibrio fischeri* enables fast and reliable ecotoxicity assessment. The aim of this study was to assess the ecotoxicity of CWA simulants to improve understanding of their environmental impact.

[1] B. J. Lukey et al., CRC Press (2007).

This research was funded by the NATO Science for Peace and Security Programme under grant id. G6087 and Croatian Science Foundation project DOK-NPOO-2023-10-8063.

ODREĐIVANJE PRIKLADNOG DESORBENSA PLA/nZVI KOMPOZITA NAKON UKLANJANJA Cr(VI) i As(V) IZ VODE

DETERMINATION OF A SUITABLE DESORBENT FOR PLA/nZVI COMPOSITES AFTER REMOVAL OF Cr(VI) AND As(V) FROM WATER

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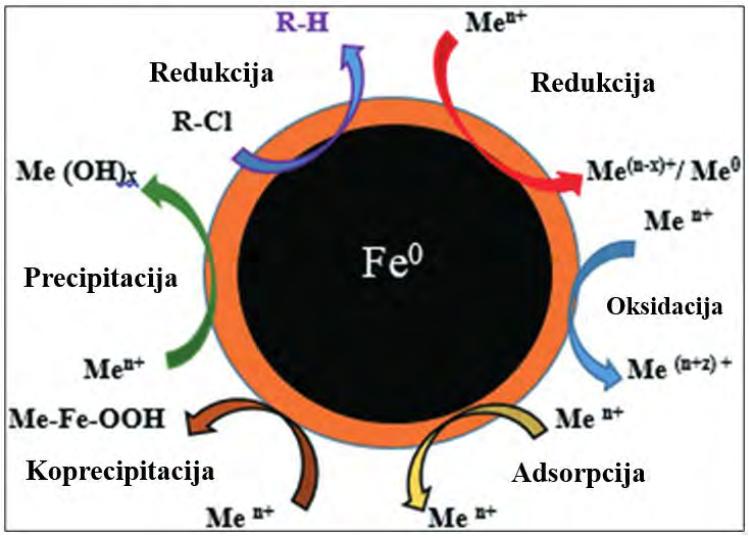
Neutralne željezove nanočestice (*eng. nano zerovalent iron*, nZVI) poznate su po vrlo visokoj reaktivnosti i izraženoj sposobnosti uklanjanja niza organskih te anorganskih onečišćivala. Njihova struktura jezgra–ljuska omogućava im više mogućih mehanizama uklanjanja onečišćivala iz otpadnih voda, koji su prikazani na slici 1. Ipak, praktična primjena nZVI čestica ograničena je njihovom sklonošću aglomeraciji i brzoj sedimentaciji, što smanjuje dostupnu specifičnu površinu i učinkovitost. Kako bi se prevladala ova ograničenja i poboljšala stabilnost i funkcionalnost samih nanočestica vrlo često se pristupa modificiranju površine pomoću kelata, primjerice piridin-2,6-dikarboksilnom kiselinom (PDCA), oksalnom kiselinom (OA) i etilendiamintetraoctenom kiselinom (EDTA) ili inkorporacijom čestica u porozne nosače poput poli(mliječne kiseline) (PLA).

U ovom radu izrađeni su PLA/nZVI kompoziti sa nemodificiranim nZVI česticama te nZVI česticama modificiranim PDCA, EDTA i OA kelatima. Ispitana je učinkovitost niza potencijalnih desorbenasa; kiselina (sumporne i klorovodične), lužina (kalijeve i natrijeve), natrijeve soli EDTA, natrijeva karbonata te destilirane vode za desorpciju kroma i arsena adsorbiranih na PLA/nZVI kompozitima. Paralelno su uspoređivani procesi adsorpcije i desorpcije na čistim nZVI česticama i na PLA/nZVI kompozitima pri različitim koncentracijama desorbensa, s ciljem procjene dugoročne održivosti materijala i mogućnosti njegova višekratnog korištenja. Dobiveni rezultati pokazuju da su PLA/nZVI kompoziti vrlo učinkoviti za uklanjanje As(V), osobito pri ponovnoj uporabi kroz više uzastopnih ciklusa adsorpcije i desorpcije, pri čemu se EDTA pokazala kao najprikladniji desorbens za arsen. Nasuprot tome, pri uklanjanju Cr(VI) uočeno je smanjenje učinkovitosti već nakon drugog ciklusa, unatoč tome što je sumporna kiselina bila najučinkovitiji desorbens za krom, što upućuje na potrebu dodatnog optimiranja uvjeta desorpcije ili odabira prikladnijeg desorbensa. Na temelju dobivenih rezultata može se zaključiti da bi PLA/nZVI kompoziti mogli postati učinkovita alternativa za pročišćavanje voda, osobito ako se dodatno optimira postupak regeneracije nakon pročišćavanja, kako bi se omogućilo uklanjanje širokog spektra anorganskih onečišćivala iz otpadnih voda.

[1] S. Shad et al., Environ. Sci.: Water Res. Technol., 6 (2020) 3057–3065



MOLECULARLY IMPRINTED POLYMER FOR SORPTION OF VENLAFAXINE – KINETIC STUDY

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Pharmaceuticals are various compounds used to treat and prevent diseases in humans and animals, and their production and use have increased with the rapid development of technology and science. They have become one of the emerging pollutants of the 21st century, entering the environment through use, improper disposal, untreated wastewater, and other pathways. Although present in relatively small quantities, their environmental effects are still insufficiently researched, since some of them have already shown harmful and lasting impacts, such as bacterial resistance to antibiotics and endocrine disruptors. Methods for their removal are often impractical, making it necessary to develop more effective approaches, such as synthesizing selective materials imprinted with pollutant molecules, as investigated in this research. The sorption performance of a venlafaxine-imprinted polymer (MIP) was compared to a non-imprinted polymer (NIP) for the removal of venlafaxine, an antidepressant, from aqueous media. The time required to establish the sorption equilibrium between the sorbent and the solution (sorbate) was determined at different intervals over 24 hours. To describe the sorption kinetics, first and second order kinetic models and intraparticle diffusion were used. Experimental data indicate that both sorbents (MIP and NIP) require the same time, 24 hours, to reach sorption/desorption equilibrium, but the MIP sorbent has a higher equilibrium sorption capacity due to its greater selectivity achieved by molecular imprinting.

This study was supported by the Croatian Science Foundation under the project number HRZZ-IP-2022-10-4400 entitled Development of molecularly imprinted polymers for use in analysis of pharmaceuticals and during advanced water treatment processes (MIPdePharma).

REMOTE SENSING MONITORING OF THE ITALIAN MEDITERRANEAN COASTAL LAGOONS REVEALING POOR ECOLOGICAL CONDITIONS

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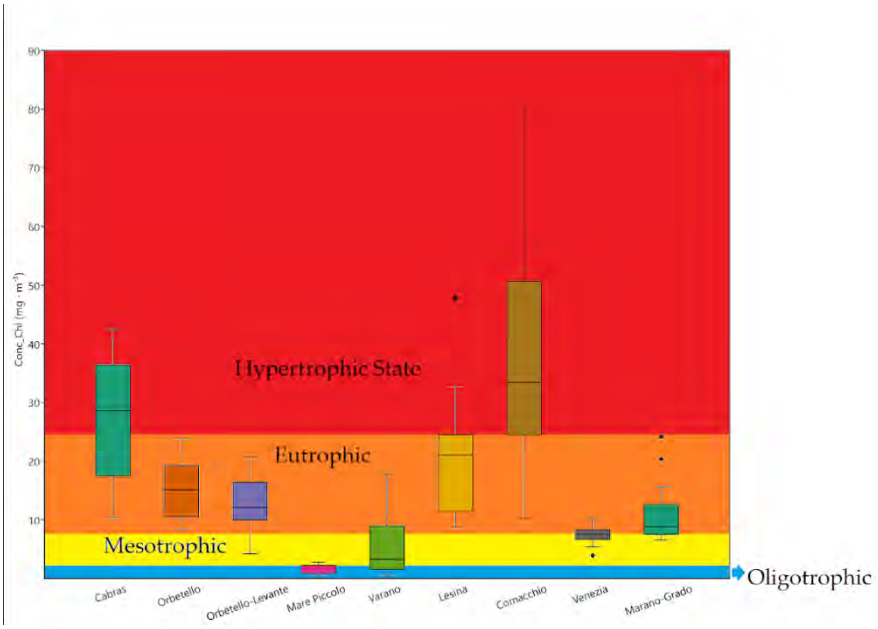
Coastal lagoons are geologically young, biodiversity-rich, and highly fragile ecosystems that provide important ecosystem services but are particularly vulnerable to nutrient enrichment, eutrophication, and algal blooms. In this study, nine Italian coastal lagoons larger than 10 km², most previously classified as having poor ecological status, were analysed to evaluate their trophic conditions over the period 2015–2025 using remote sensing techniques. Sentinel-2 satellite imagery was employed to derive automatic products of chlorophyll-a (Chl-a), total suspended matter (TSM), and water transparency (kd_z90max). Overall, Chl-a concentrations revealed predominantly eutrophic to hypereutrophic conditions across the lagoons, with values ranging from very low concentrations in Mare Piccolo (0.44 mg·m^{-3}), indicative of oligotrophic conditions, to extremely high levels in Comacchio (up to 80.81 mg·m^{-3}). Comacchio and Cabras lagoons consistently exhibited high Chl-a concentrations and low water transparency, reflecting chronic eutrophication. In contrast, Mare Piccolo maintained high transparency and low productivity. Significant long-term increases in Chl-a were detected in Varano and Cabras lagoons ($p < 0.05$), accompanied by rising TSM levels ($p < 0.01$) and decreasing transparency in Varano ($p < 0.05$). Most of the remaining lagoons showed no significant long-term trends but persisted in degraded trophic states. Overall, the results highlight the high vulnerability of Italian coastal lagoons to environmental degradation and the lack of recovery in many systems. Ecological conditions varied markedly among lagoons, from oligotrophic to chronically hypereutrophic. Suspended sediments primarily influenced water clarity, although algal blooms played a key role in some cases. Sentinel-2 imagery proved to be an effective and valuable tool for long-term monitoring, supporting environmental management and early detection of degradation trends.

[1] V. Pagliani et al., Phycology 5 (2025) 87.



STABILITY OF GLUCOSE DEHYDROGENASE AND HYDROGENASE IN DEEP EUTECTIC SOLVENTS

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Enzymes are widely used in biocatalytic processes due to their high specificity, efficiency, and environmentally friendly properties. However, their practical use is often limited by poor stability under industrial conditions, including variations in temperature, pH, and solvent environment. Deep eutectic solvents (DESs) have emerged as promising alternative media for biocatalysis, offering advantages such as low toxicity, tunable physicochemical properties, and the ability to stabilize biomolecules. They are composed of ammonium salts and hydrogen bond donors such as alcohols, carboxylic acids, amides, amines, or sugars that are not harmful to the environment or toxic. For these reasons, DESs are considered green solvents [1]. In addition to forming hydrogen bonds, DESs can accept and donate electrons and protons, which increases their ability to dissolve various materials [2]. The use of DESs as catalytic and reaction media yields promising results, with many enzymes exhibiting greater stability than in aqueous media. For example, glucose dehydrogenase (GDH) demonstrates up to 60 times greater stability in a glycerol-based solvent compared to the reference water buffer [3].

This study investigates the long-term stability of GDH and hydrogenase in various DESs to identify suitable media for biocatalytic applications. Enzyme stability was monitored over time intervals ranging from several hours to several weeks at three temperatures (4, 25, and 35 °C). The results demonstrate that specific DES formulations, depending on the temperature, effectively preserve enzyme activity over extended periods, while others lead to a rapid loss of activity and early-stage denaturation. These findings provide a basis for the rational selection of DESs and operating temperatures for enzymatic processes and for optimizing formulations of stable biocatalytic systems.

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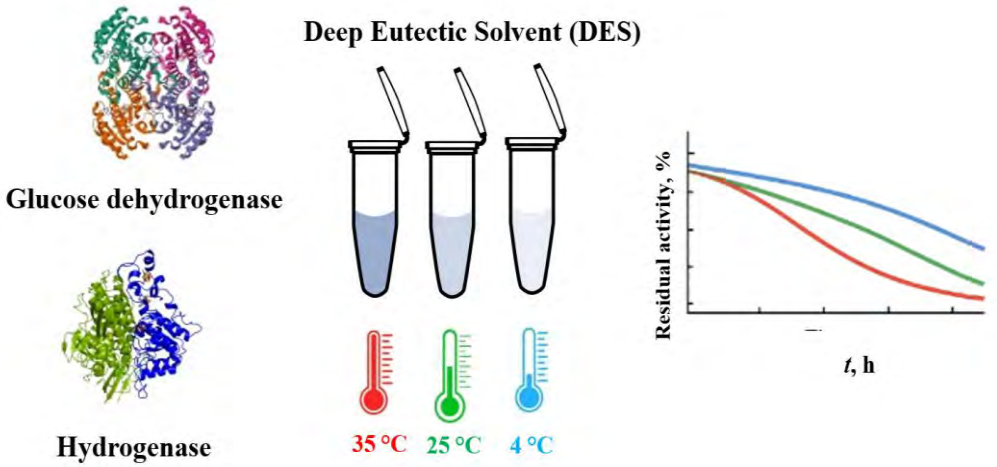
[2] A. Paiva et al., ACS Sustain. Chem. Eng. 2 (2014) 1063-1071.
[3] M. Radović et al., Front. Chem. 12 (2024) 1436049.



KOMPOZITI In_2O_3 S NANOMATERIJALIMA NA BAZI UGLJIKA ZA FOTOKATALITIČKU RAZGRADNJU PFAS-a

In_2O_3 COMPOSITES WITH CARBON-BASED NANOMATERIALS FOR ENHANCED PHOTOCATALYTIC PFAS DEGRADATION

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Poli- i perfluoroalkilne tvari (PFAS) u vodenom okolišu danas predstavljaju značajan globalni problem zbog svoje iznimne stabilnosti, široke rasprostranjenosti, otpornosti na konvencionalne metode obrade voda te potencijalne štetnosti za ljudsko zdravlje. Zbog vrlo jakih veza ugljik-fluor teško se uklanjaju uobičajenim postupcima, što naglašava potrebu za razvojem učinkovitijih tercijarnih procesa za njihovu razgradnju. Među dostupnim tehnologijama, fotokataliza se ističe kao obećavajući pristup, no zahtijeva razvoj i optimizaciju materijala pogodnih za tu primjenu [1,2]. U ovom istraživanju ispitan je potencijal različitih ugljikovih nanomaterijala za modifikaciju indijeva(III) oksida (In_2O_3) s ciljem poboljšanja fotokatalitičke razgradnje PFAS-a. Sintetizirane su dvije vrste ugljikovih kvantnih točaka (CQD) te reducirani grafen oksid (rGO), a njihova struktura potvrđena je primjenom nuklearne magnetske rezonancije, Ramanove spektroskopije, rendgenske difrakcije i infracrvene spektroskopije s Fourierovom transformacijom. Ovi materijali zatim su korišteni za pripremu serije kompozita s In_2O_3. Za CQD-In_2O_3 kompozite upotrijebljene su obje sintetizirane vrste CQD-a, dok je kod rGO-In_2O_3 sustava ispitan utjecaj različitih udjela reduciranog grafen oksida. Dobiveni kompoziti karakterizirani su rendgenskom difrakcijom, UV-Vis difuznom refleksijskom spektroskopijom i fotoluminiscentnom spektroskopijom. Fotokatalitička aktivnost svih uzoraka ispitana je na modelnom perfluoriranom spoju, perfluorooktanskoj kiselini (PFOA), čime je procijenjen utjecaj modifikacija ugljikovim nanomaterijalima na učinkovitost razgradnje u odnosu na čisti In_2O_3.

[1] Y. Wang et al., Environ. Int. 163 (2022) 107219.
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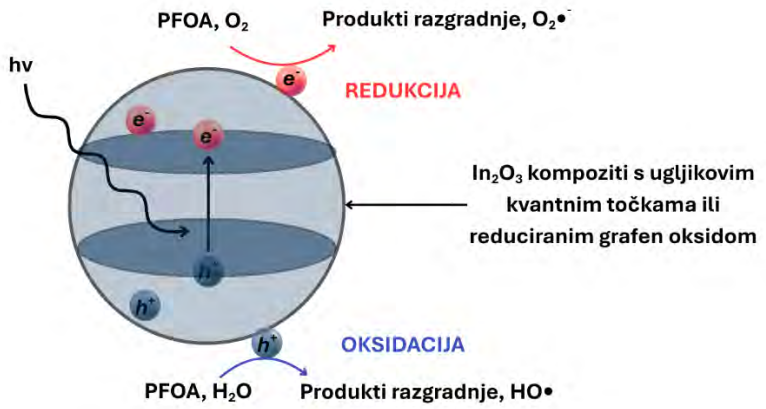
Zahvaljujem Hrvatskoj zakladi za znanost na financijskoj potpori kroz projekte MOBDOK-2023-1464 (Odlazna mobilnost asistenta) i SOL-MAT-CLEAN (IP-2025-02-8507), koji su omogućili provedbu ovog istraživanja. Također zahvaljujem Javnoj agenciji za znanstvenoraziskovalno in inovacijsko dejavnost Republike Slovenije (ARIS) na financijskoj potpori kroz projekt br. J2-4444.



LYOPROTECTANTS FOR IMPROVED FREEZE-DRYING SURVIVAL OF ENVIRONMENTAL BACTERIA ISOLATES

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Preserving environmental bacteria is essential for understanding ecosystem processes, monitoring environmental change, and maintaining cultures used in ecological and biotechnological research. However, long-term storage of microorganisms remains challenging, especially for strains that are difficult to cultivate or originate from fluctuating natural habitats [1]. Freeze-drying offers a practical approach for long-term preservation, but the survival of environmental isolates is limited by cellular stress caused by freezing and dehydration [2]. This study investigated the protective effects of six commonly used lyoprotectants on the survival of environmental Gram-negative bacteria subjected to freeze-drying. Survival rates were calculated by colony forming unit (CFU) counts before and after lyophilisation, with average initial cell densities of 1.3×10^9 CFU/ml and survival rates up to 46.8% for the most effective protectant. The findings demonstrate that selecting appropriate lyoprotectants can enhance the viability of environmentally derived bacteria, provide more reliable storage of microbial diversity and enabling future ecological and environmental applications.

[1] O. Prakash et al., Indian J. Microbiol. 60 (2020) 297–309.
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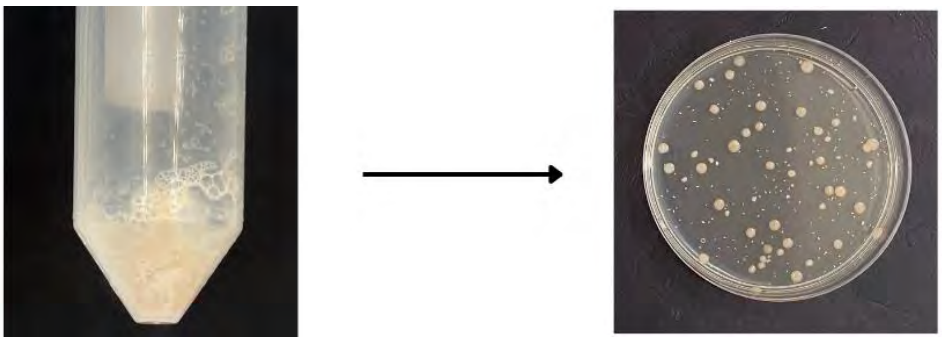

REMOVAL OF MICROPLASTIC PARTICLES OF PET AND PP THROUGH COAGULATION USING FERRATE(VI) IN AQUEOUS MEDIA

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Annual plastic production has exceeded 450 million tonnes, while plastic waste per capita has reached over 20 kg [1]. These figures are of great concern, especially given the risks that small plastic particles, known as microplastics (MPs, particle size range 1 µm to 5 mm), pose to organisms such as shellfish, fish, birds, and humans. The presence of MPs in aquatic ecosystems is a significant issue today [2]. Under the influence of environmental factors such as UV radiation, wind, and water, the polymer structure can change, a process often referred to as ageing. Ageing is commonly divided into abiotic and biotic categories, with biotic ageing being less common due to the limited bioavailability of polymers [3]. Common conventional MP removal methods, divided into three main groups – physical, chemical, and biological – are inadequate for the removal of MPs. Ferrate(VI) is considered a "green", eco-friendly removal method, combining oxidation and coagulation in its reduced state [4,5]. The aim of this work is to investigate the stability and activity of ferrate(VI) and to determine the possible use of ferrate(VI) for the removal of pristine and thermally aged PET and PP through the oxidation and coagulation process. The stability and activity of ferrate(VI) were tested at pH 5, 7, and 9 in Britton-Robinson buffer, and at ferrate(VI) concentrations of 2.5, 8.75, and 15 mM, using UV-visible spectroscopy and oxidation/reduction potential (ORP) measurements. The removal of thermally aged and pristine PET and PP, specifically the mass of precipitated microplastics, was examined under the same pH values in buffer solution and ferrate(VI) concentrations, using total organic carbon analysis in the dried, solid filter cakes of the samples. Optimal conditions were determined using the software Design Expert. 7.1.5. Results of the ANOVA analysis for the removal of MPs show that the optimal pH value is approximately neutral for all tested particles, while ferrate(VI) concentration may vary significantly. For example, the optimal pH for both pristine and aged PET is 7, while the optimal concentration is 2.5 mM for pristine PET and 14.61 mM for aged PET. The toxicity test of the filtrate after removal analysis was conducted on wheat (*Triticum aestivum*) by monitoring root and stem length.

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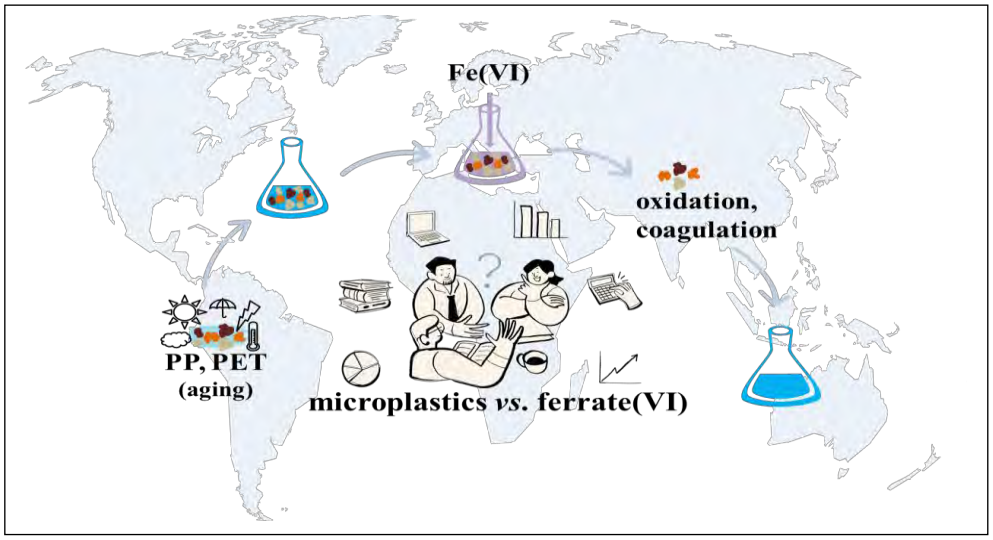

Kemijsko inženjerstvo
Chemical engineering

RAZVOJ FORMULACIJE NA OSNOVI PLGA POLIMERA ZA PRODULJENO OSLOBAĐANJE INDOMETACINA: OPTIMIZACIJA FORMULACIJE I *IN VITRO* TESTIRANJE

DEVELOPMENT OF A BIODEGRADABLE PLGA-BASED INJECTABLE FORMULATION FOR SUSTAINED RELEASE OF INDOMETHACIN: FORMULATION OPTIMIZATION AND *IN VITRO* RELEASE TESTING

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U ovom radu prikazan je razvoj formulacije za parenteralnu primjenu nesteroidnog protuupalnog lijeka indometacina, temeljene na biorazgradivim poli(laktid-*ko*-glikolid) (PLGA) kopolimerima [1]. Cilj formulacije je postizanje produljenog oslobađanja lijeka iz *in-situ* formirajućeg sustava, čime se omogućuje smanjenje učestalosti primjene i poboljšanje terapijske usklađenosti. Razvijena je *in vitro* metodologija oslobađanja, kojom se prati kinetika oslobađanja indometacina iz formulacija s različitim PLGA polimerima. Korištenjem PLGA kopolimera različitog sastava (omjer laktid:glikolid) i molekulske mase, pokazano je da se brzina oslobađanja može značajno modificirati – u rasponu od 2 tjedna do 3 mjeseca. Time se potvrđuje važnost racionalnog odabira polimernih komponenti u dizajnu sustava s kontroliranim otpuštanjem [2]. Formulacije su ispitane fizikalno-kemijskim metodama te je provedena karakterizacija morfologije depoa nakon injektiranja. *In vitro* testovi oslobađanja provedeni su u uvjetima koji simuliraju fiziološko okruženje, uz kontinuirano praćenje koncentracije oslobođenog lijeka.
Dobiveni rezultati potvrđuju da se primjenom PLGA polimera može precizno kontrolirati profil oslobađanja indometacina, što otvara mogućnosti za razvoj dugodjelujućih formulacija prilagođenih specifičnim terapijskim potrebama. Ovakav formulacijski razvoj predstavlja potencijalnu platformu za primjenu i drugih aktivnih tvari koje zahtijevaju produljeno djelovanje.

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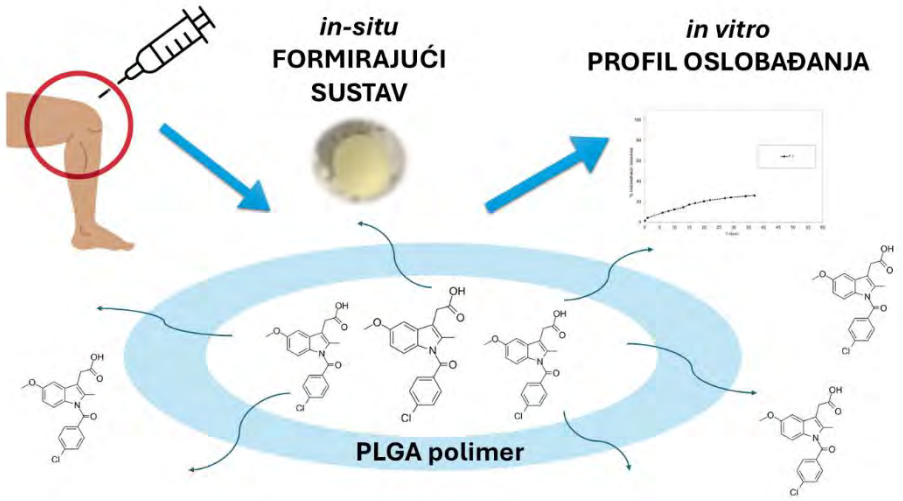

RAZVOJ FUNKCIONALNIH OBLIKA DODATAKA PREHRANI NA BAZI FERMENTIRANOG SOKA CRVENOG KUPUSA

DEVELOPMENT OF FUNCTIONAL DIETARY SUPPLEMENTS BASED ON FERMENTED RED CABBAGE JUICE

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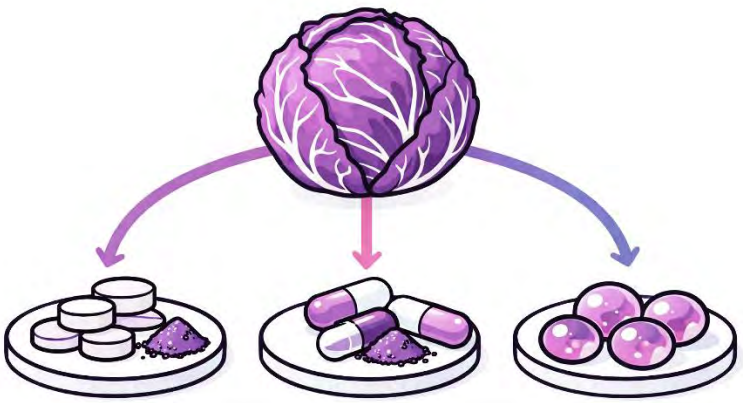
Prehrana ima ključnu ulogu u prevenciji kroničnih bolesti, no suvremeni način života sve više nameće potrebu za dodacima prehrani. Crveni kupus (*Brassica oleracea L. var. capitata f. rubra*), zahvaljujući visokom udjelu antioksidativnih fenolnih spojeva, predstavlja izvrsnu sirovinu za razvoj funkcionalnih proizvoda. U ovom radu istražena je mogućnost modifikacije fermentiranog soka od kupusa sa svrhom razvoja novih oblika funkcionalnih proizvoda prilagođenih lakšoj konzumaciji. Početna faza istraživanja obuhvatila je usporedbu fermentiranih sokova zelenog i crvenog kupusa pri različitim vremenima fermentacije. Analiza ukupnog sadržaja fenola, flavonoida i antioksidativne aktivnosti poslužila je kao kriterij za usporedbu sokova zelenog i crvenog kupusa. Rezultati su pokazali da je sok crvenog kupusa fermentiran 72 sata najpogodniji za daljnju modifikaciju te je stoga odabran za završnu formulaciju. Odabrani fermentirani sok crvenog kupusa potom je obrađen dvjema metodama: sušenjem raspršivanjem uz dodatak arapske gume te koncentriranjem u rotacijskom vakuum isparivaču. Procesom sušenja dobiven je prah koji je, uz primjenu pomoćnih tvari, formuliran u krute dozirne oblike – tablete i kapsule. Iz dobivenog koncentrata su, dodatkom želatine ili agar-agara, oblikovane polukrute kuglice. Analiza je potvrdila uspješno očuvanje bioaktivnih komponenti u tabletama i kapsulama, dok su kuglice na bazi agar-agara pokazale značajan potencijal, ali zahtijevaju dodatna istraživanja.



INFLUENCE OF IONIC LIQUIDS ON Ca^{2+}-SOLVENT INTERACTIONS FOR APPLICATION IN CALCIUM OXYGEN BATTERY SYSTEMS

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Ionic liquids have gained significant consideration in many research fields, including electrochemical conversion and storage devices, separation processes as well as materials synthesis and catalysis due to their high chemical and thermal stability, wide electrochemical window and low volatility. Their application often involves their incorporation into conventional electrolytes to improve the conductivity, stability and compatibility with the electrode materials [1]. Because of the high abundance of calcium, its low cost and high theoretical energy density, calcium-oxygen batteries are emerging as the next-generation energy storage technology. The development of these systems is hindered by sluggish oxygen reduction and evolution reactions (ORR/OER), as well as instability of calcium metal in conventional electrolytes [2]. To resolve these obstacles, better understanding of electrolytes and molecule interactions within is crucial. One of the possible directions for better understanding the molecule-ion interactions inside the electrolyte is using spectroscopic techniques such as Fourier transform infrared spectroscopy (FTIR), which enables the identification and interpretation of spectral changes within the electrolyte, hence giving deeper insight into the mechanisms underlying the modification of the physiochemical properties of the system. In this work, FTIR analysis was employed to determine the processes occurring within the electrolyte upon changes in its composition. Dimethyl sulfoxide was used as the organic solvent, while calcium tetrafluoroborate $Ca(BF_4)_2$, served as the electrolyte salt and was pre-dried to eliminate bound crystal water. The ionic liquid EMIM FSI (1-ethyl-3-methylimidazolium bis(fluorosulfonyl)imide) was used as an additive in concentrations of 1%, 10% and 30%.

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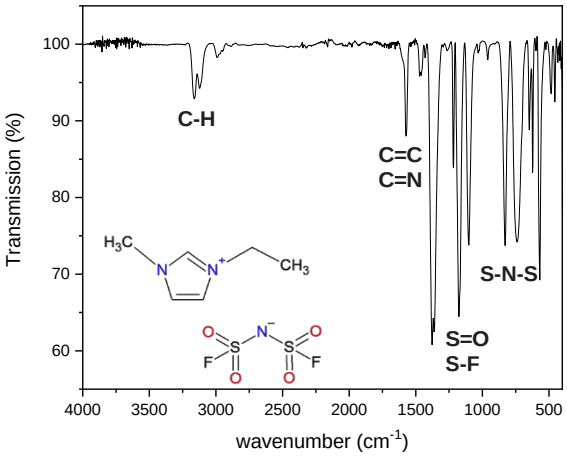
This work was financially supported by the project NPOO.C3.2.R3- I1.04.0187: Advanced innovative materials and technologies for lithium-ion batteries production.



PRIPRAVA HETEROSPOJEVA NA BAZI SREBROVOG MOLIBDATA

PREPARATION OF SILVER MOLYBDATE-BASED HETERO-COMPOUNDS

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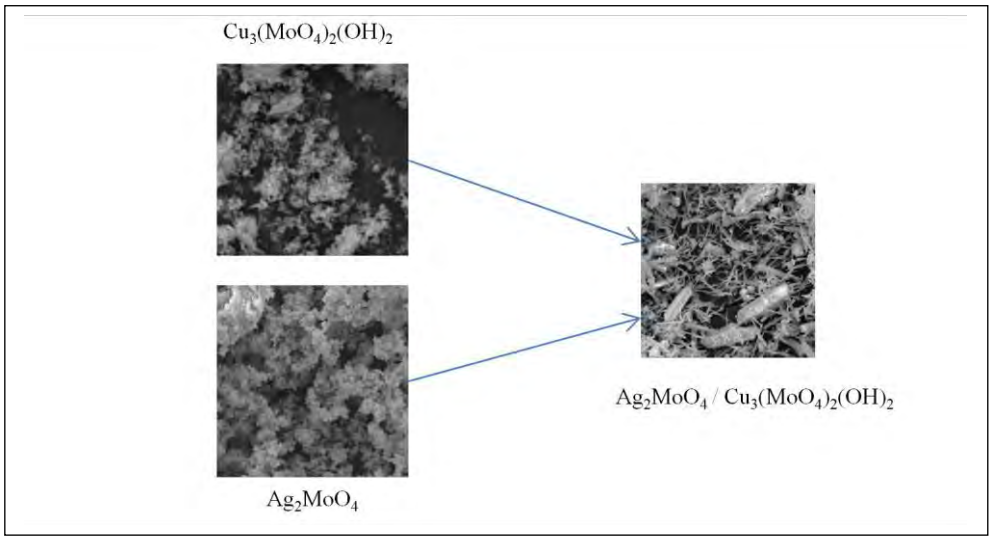
U ovom radu istražena je sinteza, strukturna i morfološka karakterizacija te fotokatalitička aktivnost materijala na bazi molibdata s ciljem dobivanja heterospojeva unaprijeđenih funkcionalnih svojstava. Heterospojevi su poluvodički materijali od posebnog interesa zbog poboljšanog prijenosa naboja i smanjene rekombinacije elektrona i šupljina, što rezultira povećanom fotokatalitičkom učinkovitošću. Srebrov molibdat (Ag_2MoO_4) u kombinaciji s drugim poluvodičem može tvoriti heterospoj tipa I, pri čemu se vodljiva i valentna vrpca jednog materijala nalaze unutar energetskog procjepa drugog. Takav raspored dovodi do nakupljanja elektrona i šupljina u istom materijalu, čime se olakšava njihova rekombinacija. Iako je takav energetski raspored povoljan za primjene poput fotodetektora, u fotokatalitičkim procesima brza rekombinacija može ograničiti učinkovitost. Zbog toga se Ag_2MoO_4 često kombinira s drugim materijalima kako bi se poboljšalo razdvajanje nositelja naboja. Heterospojevi su pripremljeni iz mehanokemijski i sonokemijski sintetiziranog Ag_2MoO_4 na koje je sonokemijskom metodom istaložen bakrov molibdat. Heterospojevi su pripremljeni u molarnim omjerima 1:1 i 3:1 srebrovog i bakrovog molibdata te je također pripremljen i uzorak čistog bakrovog molibdata. Nakon sonokemijske sinteze, produkti su isprani i centrifugirani radi uklanjanja nečistoća te na kraju osušeni. Svi dobiveni praškasti materijali detaljno su karakterizirani rendgenskom difrakcijom (XRD), pretražnom elektronskom mikroskopijom (SEM), UV-Vis difuznom refleksijskom spektroskopijom (DRS), termogravimetrijskom analizom (TGA), diferencijalnom pretražnom kalorimetrijom (DSC) i infracrvenom spektroskopijom s Fourierovom transformacijom (FTIR), čime su potvrđeni njihova struktura, morfologija i optička svojstva. Nadalje, ispitana je fotokatalitička aktivnost svih uzoraka i međusobno uspoređena.



DEVELOPMENT OF A MILLISYSTEM FOR CONTINUOUS EXTRACTION OF GLUCOSE DEHYDROGENASE

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Extraction of biologically active molecules requires systems that provide high selectivity, mild operating conditions, and preservation of biomolecular structure. Deep eutectic solvents (DESs) have emerged as alternative, environmentally friendly media that can enhance both the stability and catalytic activity of glucose dehydrogenase (GDH) and can also be used for its extraction in aqueous two-phase systems (ATPS). In addition to improving enzyme extraction, millisystems such as milliextractors, milliseparators and millireactors offer a versatile platform for conducting processes in single- or multiphase systems, providing precise control over reaction conditions and improved efficiency and scalability of the overall process [1].

This study describes the development of an integrated millisystem consisting of a milliextractor and a milliseparator for the continuous extraction of GDH using DESs as alternative, green solvents [2]. Building on previous research performed in batch extractors, artificial neural networks were used to predict the efficiency of various DES systems for simultaneous extraction and preservation of enzyme catalytic activity [2]. The model identified two DESs, Choline chloride : Urea (1:2, 20% H_2O (w/w) and Choline chloride : Urea (1:2, 40% H_2O (w/w), with the highest predicted potential, which were subsequently selected for further testing in a continuous milliextractor [3]. Within the milliextractor, the effects of residence time, ultrasound, operating temperature and channel diameter on extraction efficiency were investigated. Optimal performance was achieved at T = 25 °C and a channel diameter of 800 µm. In the following stage, the milliextractor was coupled with a milliseparator to enable continuous in-line phase separation, thereby improving overall process efficiency. Finally, a near-infrared (NIR) sensor was integrated into the milliseparator to enable real-time monitoring of extraction efficiency.

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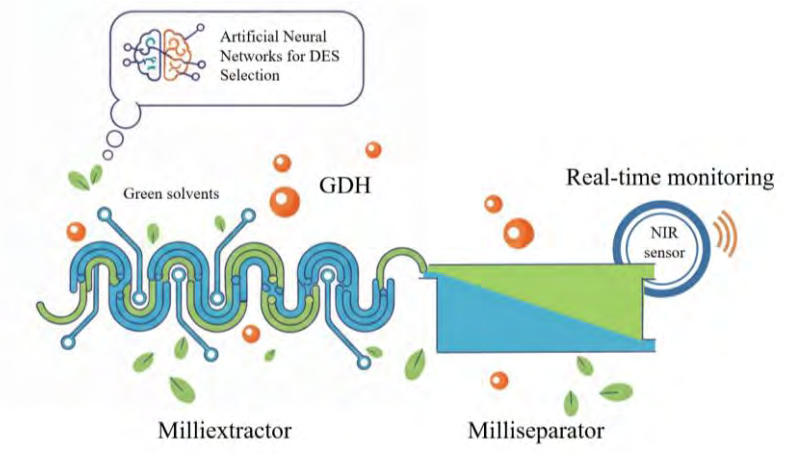

DETERMINATION OF SOLID-LIQUID EQUILIBRIUM IN HYDROPHOBIC EUTECTIC SOLVENT SYSTEMS BY DIFFERENTIAL SCANNING CALORIMETRY

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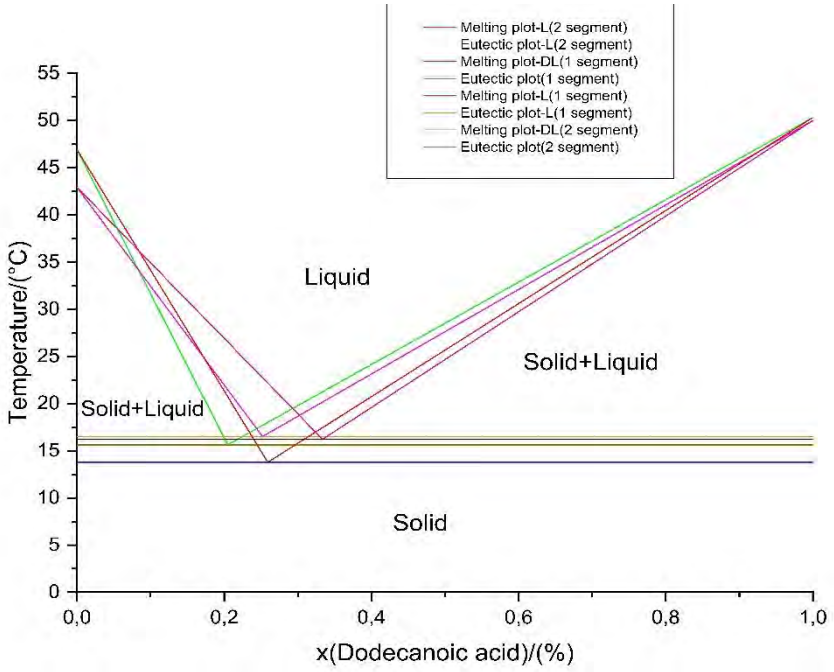
Research on nonaqueous deep eutectic solvents (DES) mostly involve hydrophilic DES systems due to their wide application (analytical sample preparation, energy storage, medication formulation, and biocatalysis, etc.), environmental friendliness, relatively easy preparation and good reproducibility. Hydrophobic DESs have attracted more recent interest as an alternative for application in systems requiring hydrophobic solvents, in the similar fields of use as their hydrophilic counterparts. To complicate the situation, hydrophobic DESs commonly involve organic molecules which come in the form of racemic mixtures, which may significantly complicate the thermograms and make their interpretation much more difficult. The first idea in characterizing a DES is the construction of the solid-liquid equilibrium phase diagram. In this study, phase diagrams were made for three DES systems: L-menthol – dodecanoic acid, L-menthol – thymol and thymol – dodecanoic acid. Unlike the common approach in the literature – melt mixing – DES systems were prepared by dissolving DES components in a common solvent: acetone, methanol and trichloromethane followed by the solvent evaporation, with an aim to reduce the consumption of main chemicals. The prepared DESs are then analyzed by the differential scanning calorimetry to construct phase diagrams for the systems. The results are compared with the COSMO-RS model predictions. The advantages and drawbacks are presented in light of the limited experimental dataset and the possibilities for further improvements are discussed.



CFD MODELING OF A DOUBLE-PIPE HEAT EXCHANGER

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Computational Fluid Dynamics (CFD) is a powerful tool for designing and analyzing thermal systems, such as double-pipe heat exchangers. However, the accuracy of CFD predictions depends not only on the appropriate selection of turbulence models, but also on the precise definition of the geometry and the quality of the computational mesh. In this work, heat transport and hydrodynamic behavior in a 1,5 m laboratory double-pipe heat exchanger (DPHE) with counter-current flow are analyzed. The DPHE consisted of an outer shell and an inner copper tube for the hot and cold fluid streams, respectively. An orifice plate is placed at the inner tube inlet to determine the flow rate, and temperature sensors are placed at the inlet and outlet of both tubes to determine the fluid temperatures. The CFD model of the DPHE is developed in Ansys Fluent 2024 R1. The Reynolds-Averaged Navier-Stokes (RANS) approach is adopted with the standard k-epsilon (k-ε) turbulence model. A structured computational mesh was carefully generated to ensure solution accuracy, comprising approximately 794,000 elements with high quality metrics, including an average orthogonal quality of 0.987 (minimum is 0.759) and an average skewness of 0.087 (maximum is 0.505). The primary objective of the simulation was to predict the heat transfer rate and analyze the pressure drop along with the velocity profiles within the DPHE. To validate the numerical results, a corresponding laboratory experiment was conducted where the inlet and outlet temperatures of both streams were measured. A direct comparison between the experimental data and the CFD predictions shows a close agreement, successfully validating the applied modeling methodology. This work confirms the reliability of the RANS k-ε approach implemented in ANSYS Fluent for this type of heat exchangers, providing a foundation for future design and performance optimization studies.

INFLUENCE OF ULTRASOUND IRRADIATION PULSE ON CRYSTAL GROWTH IN SONOCRYSTALLIZATION OF POTASSIUM SULPHATE

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Crystallization is classified as a fundamental separation operation, primarily employed to isolate a solid phase in its crystalline form from a mother solution. Due to its relatively low production costs and the ability to adapt to market demands, crystallization has become highly prevalent in the chemical industry. The crystallization process is initiated by nucleation, followed by the growth of nuclei and the formation of crystals, and concluded with the aging of the crystals. For crystallization to occur, the system must reach a state of supersaturation, which is often achieved by continuously cooling the saturated mother solution [1]. Recently, the use of ultrasonic energy during the crystallization process, known as sonocrystallization, has become increasingly common. It has been determined that the application of ultrasound to the mother solution can significantly affect process kinetics, particularly by influencing the width of the metastable zone and changes in system supersaturation over time. In essence, ultrasonic action in crystallization allows for greater process control, the production of high-quality crystals with improved characteristics, and high reproducibility [2]. Considering that crystallization takes place in a suspension, its efficiency is also greatly influenced by the implementation of mechanical stirring. It is essential to ensure a state of complete suspension within the crystallizer by using an appropriate impeller speed. This ensures optimal interfacial area, thereby intensifying the transfer phenomena within the system [3]. Due to these critical factors, this work investigates the combined influence of simultaneous ultrasonic action and mechanical stirring on the batch sonocrystallization of potassium sulphate. The study specifically examines the influence of the ultrasound pulse on crystal growth and the granulometric properties of potassium sulphate crystals obtained through batch crystallization with simultaneous ultrasonic irradiation and mechanical mixing. Crystallization was conducted by cooling the mother liquor at a speed of 6 °C h^{-1} in the crystallizer (V = 2.65 dm^3). Sonication was conducted at an amplitude of 20%, with five different ultrasound pulses applied (p = 0, 20, 50, 70, 100%). Mechanical mixing was ensured by using a straight blade turbine (4-SBT), with an impeller-to-tank diameter ratio equal to 0.43. The impeller speed corresponded to the minimum speed required to achieve the state of complete suspension ($N = N_{JS}$). Granulometric analysis of crystals during the crystallization process was performed using the laser diffraction method (*Horiba LA-300*). The results indicate a monomodal distribution of potassium sulphate crystals during the crystallization process for all applied pulsed irradiations. As the ultrasound pulse increased, the proportion of finer fractions increased, and overall, the median, mean, and mode of potassium sulphate crystal size decreased, indicating that ultrasound irradiation reduces crystal growth and therefore, the final size of the obtained crystals. Microscopic analysis showed less agglomeration and a more regular crystal form when ultrasound irradiation is applied, however, no significant effect was observed with an increase in ultrasound pulse.

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USPOREDBA I OPTIMIZACIJA TRIS–FENOL I TCA–ACETONSKE METODE ZA IZOLACIJU PROTEINA IZ LISTOVA VINOVE LOZE PRIMJENOM BOX–BEHNKEN DIZAJNA

COMPARISON AND OPTIMIZATION OF TRIS–PHENOL AND TCA–ACETONE METHODS FOR PROTEIN ISOLATION FROM GRAPEVINE LEAVES USING A BOX–BEHNKEN DESIGN

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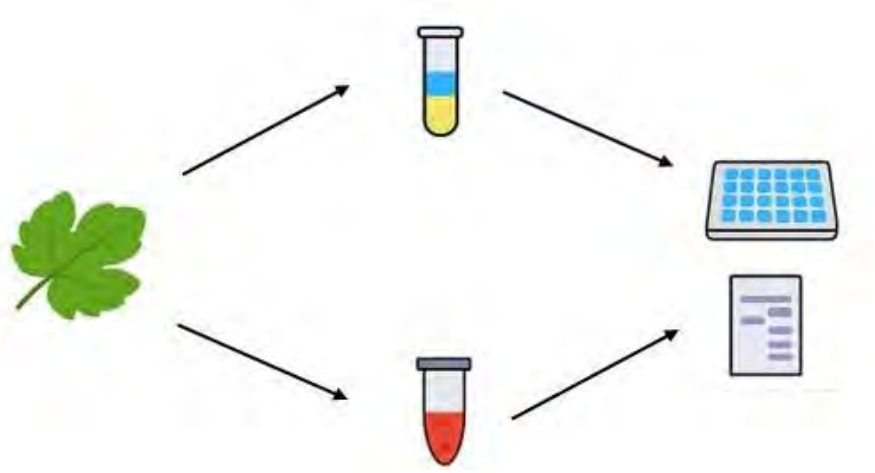
Izolacija ukupnih proteina iz biljnog tkiva, osobito iz listova vinove loze (*Vitis vinifera* L.), predstavlja značajan metodološki izazov zbog visokog udjela polisaharida, fenolnih spojeva i oksidativno aktivnih metabolita koji ometaju ekstrakciju, kvantifikaciju i naknadne proteomske analize. U cilju poboljšanja učinkovitosti i čistoće proteinskih ekstrakata provedena je optimizacija dvaju često korištenih protokola: Tris–fenol metode i TCA–acetonske precipitacije. Optimizacija je provedena primjenom Box–Behnken eksperimentalnog dizajna (BBD), pri čemu su odabrane ključne varijable kao što su masa uzorka, omjer mase uzorka i volumena ekstrakcijskog otapala te trajanje inkubacije te su sustavno varirane kako bi se identificirala njihova optimalna kombinacija. Kao primarni odgovor korišten je prinos ukupnih proteina određen BCA metodom, dok je kvaliteta izolata evaluirana SDS-PAGE elektroforezom. Rezultati ukazuju na jasne razlike između dvaju pristupa. Tris–fenol metoda dala je veći prinos i stabilniji proteinski profil, osobito kada su parametri optimirani unutar modela BBD. TCA–acetonska precipitacija pokazala se osjetljivijom na promjene eksperimentalnih uvjeta, uz učestaliju pojavu "*smearinga*" na gelu i slabiju topljivost proteina u denaturirajućim puferima. Box–Behnken analiza omogućila je identifikaciju statistički značajnih faktora te izradu prediktivnog modela, što je rezultiralo uspostavom optimalnih uvjeta za izolaciju proteina iz lisnog tkiva vinove loze. Ovi rezultati potvrđuju da kombinacija fenolne ekstrakcije i statističke optimizacije predstavlja robustan pristup za dobivanje proteinskih uzoraka pogodne čistoće i reproducibilnosti za daljnje *bottom-up* proteomske analize. Dobiveni model i optimirani uvjeti mogu poslužiti kao temelj za standardizaciju ekstrakcijskih protokola u studijama biljnih proteoma, osobito u istraživanjima metabolizma, biotičkog stresa i sortnih specifičnosti vinove loze.



PROPERTIES OF CHITOSAN/CARBOXYMETHYL CELLULOSE MULTILAYER PREPARED ON MODEL INTRAOCULAR LENSES MADE OF POLY(METHYL METHACRYLATE)

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Poly(methyl methacrylate) (PMMA) has long been established as a reference material for rigid intraocular lenses owing to its excellent optical clarity, biocompatibility, and long-term stability [1]. This study focuses on the physical and chemical characterization of model PMMA intraocular lenses and the formation of biocompatible polyelectrolyte multilayers, with emphasis on their surface and optical properties. Firstly, chemical composition of the model lenses was evaluated using attenuated total reflection infrared (ATR) FT-IR spectroscopy. Furthermore, surface morphology and roughness were then investigated by atomic force microscopy (AFM). After that, water contact angle was measured, while zeta potential analysis enabled determination of the surface potential. Finaly, the optical properties of PMMA lenses were assessed through UV–Vis spectroscopy. Such detailed characterization provides the critical foundation for understanding how substrate surfaces will interact with polyelectrolyte multilayer coatings. Polyelectrolyte multilayers (PEMs) are thin solid films formed by successive depositions of positively and negatively charged polyelectrolytes on solid substrates [2]. The properties of PEMs can be fine-tuned by changing the preparation conditions. In this study, chitosan and carboxymethyl cellulose polyelectrolyte multilayers were prepared on PMMA lenses using layer-by-layer (LbL) method. UV–Vis spectrophotometry measurements were carried to assess their optical properties. Tensiometry was used to track hydrophilicity changes during alternating polymer adsorption. Topography and roughness of PEMs were evaluated using AFM. Together, these measurements offer a comprehensive overview of the intrinsic properties of these biocompatible polyelectrolyte multilayers. The main objective of this study is to evaluate the suitability of chitosan/carboxymethyl cellulose polyelectrolyte multilayers as biocompatible surface coatings for PMMA-based intraocular lenses while preserving their optical performance. The study provides insight into multilayer formation and surface property modulation, as well as their potential influence on the optical characteristics of PMMA substrates.

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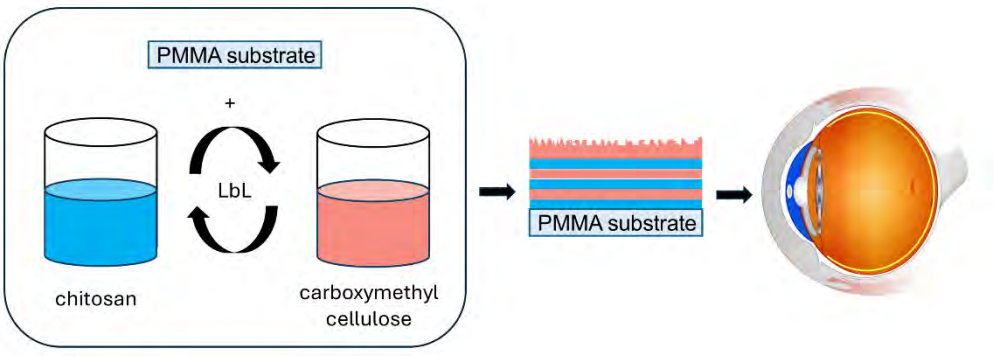
[2] G. Decher, Science 277 (1997) 1232–1237.



RAPID AND NON-DESTRUCTIVE MONITORING OF GDH ACTIVITY IN DEEP EUTECTIC SOLVENTS USING NIR SPECTORSCOPY AND ARTIFICIAL NEURAL NETWORKS

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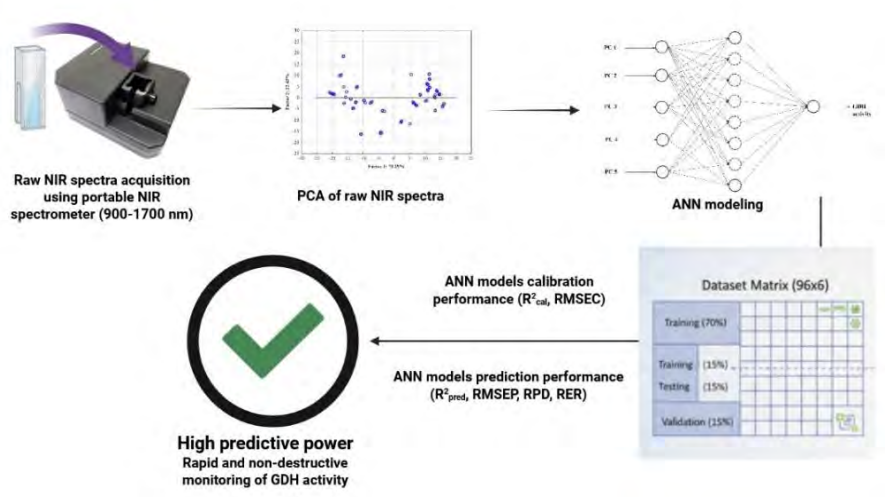
This study evaluated the applicability of Near-Infrared (NIR) spectroscopy combined with Artificial Neural Network (ANN) modeling to predict glucose dehydrogenase (GDH) activity after the extraction using aqueous two-phase systems (ATPS) based on deep eutectic solvents (DES). The activity of GDH in DESs is strongly influenced by the physicochemical properties of the solvent, resulting in complex and often nonlinear interactions. Rapid and reliable assessment of enzyme activity across a wide range of DES compositions is therefore essential for efficient process development and optimization. Conventional analytical methods are time-consuming and require extensive sample preparation, highlighting the need for alternative, non-destructive approaches capable of handling multivariate data. In this context, NIR spectroscopy combined with advanced chemometric and machine learning techniques represents a promising solution.

ANN models were developed using Statistica 14.0 (TIBCO Software Inc., CA, USA) to predict GDH activity across 32 selected DESs, based on raw spectra acquired with a portable NIR instrument (NIR-M-R2, InnoSpectra Technology, Taiwan) in the wavelength range 900 – 1700 nm. Model inputs consisted of factor scores from Principal Component Analysis (PCA); the first five components were selected as they accounted for 99% of the total sample variability. A 96×6 data matrix (96 samples; 5 input variables, 1 output variable) was utilized. For each output, 2,000 networks were developed using the backpropagation algorithm with the sum of squares as the error function. The dataset was randomly partitioned into calibration and prediction sets (70:30 ratio). Within the calibration set, a 70/15/15% split was applied for training, testing, and validation, respectively. To ensure robustness, cross-validation with random subsampling and a fixed random seed was employed. Model performance was evaluated using R^2_{cal}, $R^2_{cal,adj}$, and RMSEC, while predictive capability was assessed via R^2_{pred}, $R^2_{pred,adj}$, RMSEP, SEP, RPD, and RER. Results indicated that three MLP 5-6-1 models achieved high coefficients of determination during training and testing, successfully capturing the nonlinear relationships between spectral data and enzymatic activity. Although R^2 values slightly decreased during validation, the model utilizing an identity function in the output layer demonstrated superior generalization, achieving the highest $R^2_{validation}$ (0.8638) and the lowest prediction error. Furthermore, a high RPD (2.46) and satisfactory RER (8.05) confirmed the model's strong quantitative predictive power.

In conclusion, the integration of NIR spectroscopy and ANN modeling provides a reliable, non-destructive alternative to time-consuming analytical methods for estimating GDH activity in DES-based systems. These models represent an efficient tool for real-time monitoring and process optimization in biocatalytic and separation applications.



ETHANOL–WATER SOLVENT COMPOSITION EFFECTS ON BIFLAVONOID EXTRACTION FROM DIFFERENT GINKGO TISSUES

UTJECAJ SASTAVA OTAPALA ETANOL–VODA NA EKSTRAKCIJU BIFLAVONOIDA IZ RAZLIČITIH TKIVA GINKGA

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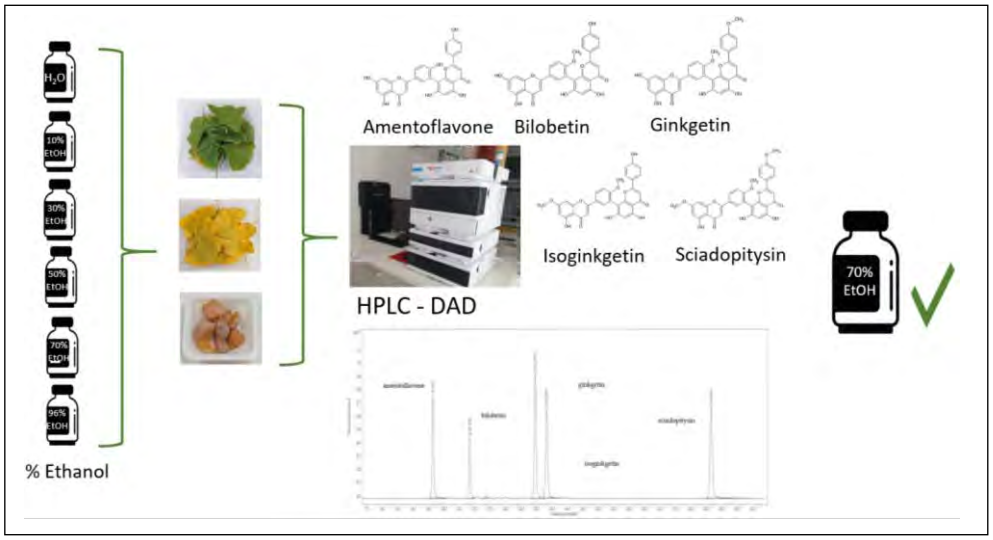
Ginkgo (*Ginkgo biloba* L.) is a medicinal plant rich in diverse bioactive compounds, but is particularly notable for accumulating biflavonoids which are not present in all plant species. Biflavonoids - dimers of flavonoids - are recognized as compounds with potential pharmacological applications in the treatment of various cancers, neurological and cardiovascular disorders, and as antiviral agents. Optimizing ethanol concentration is essential to maximize recovery of biflavonoids while minimizing solvent use, relevant for sustainable industrial applications. This study evaluated ethanol-dependent extraction from green leaves, yellow leaves, and sarcotesta using six ethanol concentrations (0, 10, 30, 50, 70, and 96%). Biflavonoids (amentoflavone, bilobetin, ginkgetin, isoginkgetin, sciadopitysin) were identified and quantified by HPLC-DAD. The highest total biflavonoid content was detected in yellow leaves, with sciadopitysin as the predominant biflavonoid, whose concentration reaching up to 5556.04 ± 225.07 µg/g dw in 96% ethanol. No biflavonoids were detected in water or 10% ethanol extracts, while 30% ethanol yielded low concentrations in yellow leaves. For total biflavonoids and for most individual biflavonoids the highest yields were obtained during extraction with 70–96% ethanol. Considering comparable extraction efficiency and lower toxicity, 70% ethanol was identified as the most suitable solvent.



CIRCULAR DRYING AND PYROLYSIS CONCEPT FOR SEWAGE SLUDGE USING RECYCLED BIOCHAR

KONCEPT KRUŽNOG SUŠENJA I PIROLIZE ZA OTPADNI MUT KORIŠTENJEM RECIKLIRANOG BIO-UGLJENA

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Sušenje mulja komunalnih otpadnih voda (MSS) predstavlja značajno energetsko/logističko usko grlo u upravljanju muljem. Cilj ovog rada bio je utvrditi može li biougljen (BC) djelovati kao strukturno pomoćno sredstvo za sušenje MSS-a u blagim uvjetima i kako se eksperimentalno uočeno poboljšanje sušenja može racionalizirati u ciklički, termički integrirani koncept procesa. Eksperimenti sušenja MSS/BC provedeni su pri 25 °C prirodnom konvekcijom s tri različita omjera mase MSS/BC (1:1, 2:1, 3:1) i kroz sekvencijalne cikluse ponovne upotrebe kako bi se simulirala recirkulacija BC-a. Optička mikroskopija, adsorpcija N_2 (BET) i ATR-FTIR korišteni su za karakterizaciju BC-a i mješavina MSS/BC. BC je pokazao heterogenu, fragmentiranu morfologiju i mikro-mezoporozna svojstva koja podupire djelovanje kao propusni skeletni okvir kada se dispergira unutar slojeva mulja. Spektroskopska analiza pokazala je da u miješanju prevladava fizičko/elektrostatsko povezivanje u odnosu na stvaranje novih kovalentnih veza između krutih tvari, analogno porozno-aditivnim mehanizmima za odvodnjavanje mulja i poboljšanje sušenja [1]. Povećani udio MSS-a smanjio je dostupnu poroznost i objasnio fizikalno-kemijskim principom uočeni trend smanjenja prinosa s većim opterećenjem mulja i cikliranjem. Dobivena eksperimentalna opažanja iskorištena su za formuliranje preliminarnog koncepta kružnog sušenja-pirolize u kojem bi se osušene mješavine MSS/BC podvrgle pirolizi radi pretvorbe, a dobiveni ugljen bi se recirkulirao na sušenje. Proveden je probir protoka mase i energije kako bi se utvrdilo je li toplinska integracija procesa izvediva, uključujući povrat topline pare putem toplinske pumpe, te kako bi se identificirali parametri osjetljivosti važni za povećanje opsega [2,3]. Preliminarni rezultati podupiru sušenje na niskim temperaturama poboljšano BC-om kao održiv proces koji omogućuje korak prema valorizaciji kružnog MSS-a i postavlja temelje za budući rad na validaciji koncepta korištenjem BC-a dobivenog iz MSS-a i izravno mjerenje energija u većem opsegu.

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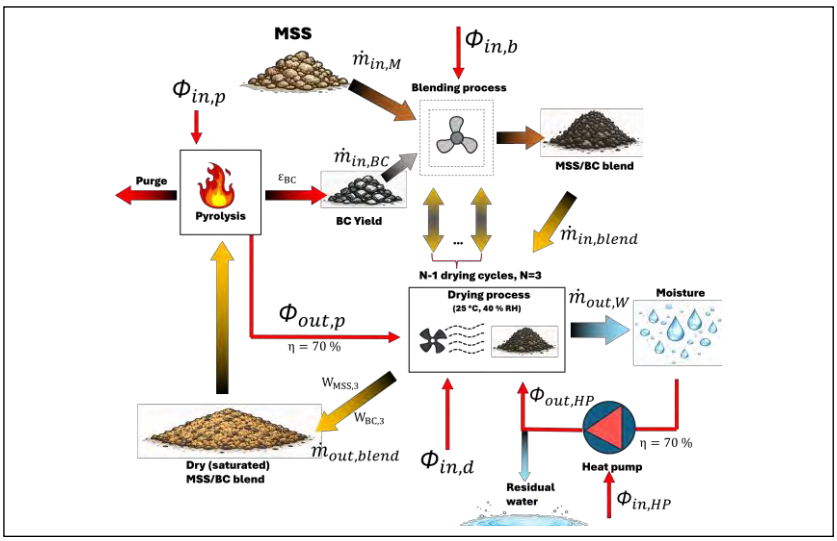

KOROZIJSKA ZAŠTITA UGLJIČNOG ČELIKA INHIBITORIMA NA BAZI BENZOATA

CORROSION PROTECTION OF CARBON STEEL BY BENZOATES

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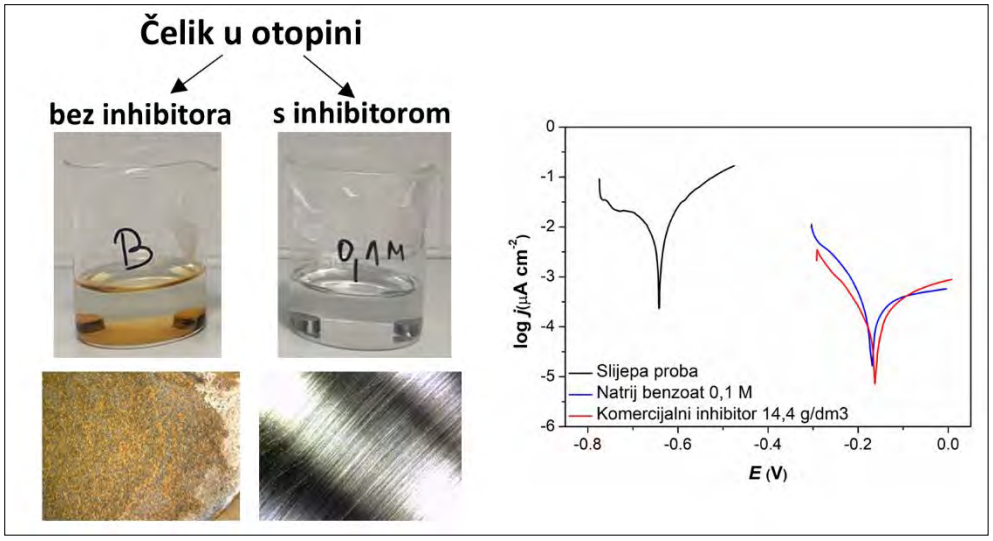
U ovom radu istraživano je djelovanje natrijeva benzoata kao inhibitora atmosferske korozije čelika. Iako je iz literature poznato da je ovaj spoj dobar inhibitor korozije te se može primijeniti kao parnofazni inhibitor, nije dovoljno istraženo koliko je inhibitorska djelotvornost određena elektrokemijskim ispitivanjima u korozivnim otopinama dobar pokazatelj inhibicije u parnoj fazi. Zbog toga su u ovom radu provedena ispitivanja njegovog inhibitorskog djelovanja u zaštiti ugljičnog čelika u simuliranoj kiseloj kiše. Ispitivanja su proveden elektrokemijskim tehnikama i gravimetrijskom metodom, kako bi se odredila optimalna koncentracija inhibitora. Ispitivanja su također provedena u parnoj fazi, u zatvorenom sustavu sa otopinom kisele kiše. Paralelna ispitivanja provedena su i sa komercijalnim inhibitorm na bazi benzoata, koji se preporuča za zaštitu čelika od atmosferske korozije. Dobiveni rezultati pokazuju da je moguće uspostaviti adekvatnu korelaciju između rezultata dobivenih u masi elektrolita i u parnoj fazi.



DIZAJN I KONSTRUKCIJA VISOKOUČINKOVITIH KALCIJEVO-KISIKOVIH BATERIJA

DESIGN AND CONSTRUCTION OF HIGH -PERFORMANCE CALCIUM-OXYGEN BATTERIES

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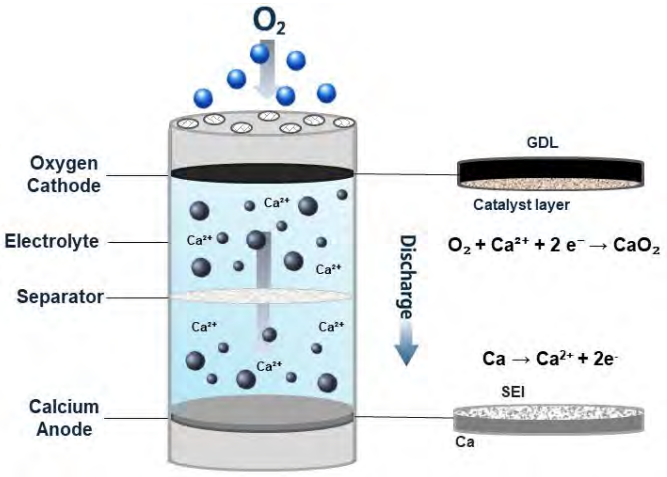
Metal-oxygen batteries have attracted significant attention as next-generation energy storage technologies owing to their exceptionally high energy and power densities. These systems are constructed with a metal anode, which provides battery-like storage, while the oxygen cathode is analogous to fuel cells. Among emerging multivalent anodes, calcium represents a promising metal anode alternative due to its reduction potential close to that of lithium, high abundance, low production cost, and ability to transfer two electrons per ion, enabling high volumetric and gravimetric energy density. However, the realization of rechargeable calcium-oxygen batteries remains a challenge to this day. Both the calcium anode and the oxygen cathode require optimized electrolytes and well-structured interfaces to achieve reversible operation. For calcium to achieve stable plating/stripping, it needs the formation of a stable solid electrolyte interphase (SEI), and efficient oxygen reduction and oxygen evolution reaction (ORR/OER) remain major obstacles. In this work, we constructed rechargeable calcium oxygen batteries through comprehensive materials and cell design strategy. We developed a new electrolyte that supports calcium reversible electrodeposition with formation of a stable and ionically conductive SEI at calcium metal interface. In parallel, we systematically optimized ORR/OER activity in organic electrolytes and identified an electrolyte capable of conducting both reversible reactions with addition of an ionic liquids as an electrolyte additive. Using all these advances, we assembled and evaluated a rechargeable calcium-oxygen battery under realistic operating conditions. Electrochemical testing demonstrated reversible cycling and promising performance, highlighting the potential of calcium-oxygen batteries as a high energy storage technology.

This work was funded by the European Union within the project NPOO.C3.2.R3-I1.04.0187: Development of new materials and advanced innovative technologies for the production of lithium-ion batteries.



UNAPREĐENJE SIGURNOSTI U KEMIJSKOM LABORATORIJU POMOĆU APLIKACIJE PROŠIRENE STVARNOSTI

ENHANCING CHEMICAL LABORATORY SAFETY THROUGH AUGMENTED REALITY APPLICATION

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Ensuring safety in chemical laboratories is essential, especially for students who may lack experience handling hazardous substances. Studies have shown that university laboratories often present higher risks of accidents than industrial settings, primarily because students have limited familiarity with safety protocols and equipment [1]. Common issues include misunderstandings of hazard symbols, improper waste disposal, and inadequate use of personal protective equipment (PPE). To address these challenges, we developed an augmented reality mobile application to help students learn safe practices in chemical laboratories (WorkSafetyAR). The application uses a scripted interface that allows students to scan work safety textual materials and laboratory items, providing instant access to laboratory safety guidelines, proper PPE usage, and important information from Safety Data Sheets (SDS). By integrating this technology, we aim to improve students' understanding of chemical hazards and increase safety and efficiency in chemical laboratories. We also conducted user experience surveys among students, as these surveys provide direct insights into users' needs, preferences, and problems. The results of a SUS (System Usability Score) questionnaire indicate that users found the system easy to use, intuitive, and consistent, with an overall average score of 94.44, which is in the acceptable range, at grade level A, and rated as an excellent digital system [2,3]. In their responses to the open-ended questions, users highlighted the visualizations and interactivity as the best aspects of the digital system. They also suggested improvements, such as adding a soundtrack to some videos and improving image resolution.

[1] H.R. Ayi, C.Y. Hon, J. Chem. Health Saf. 25(6) (2018) 6-12.
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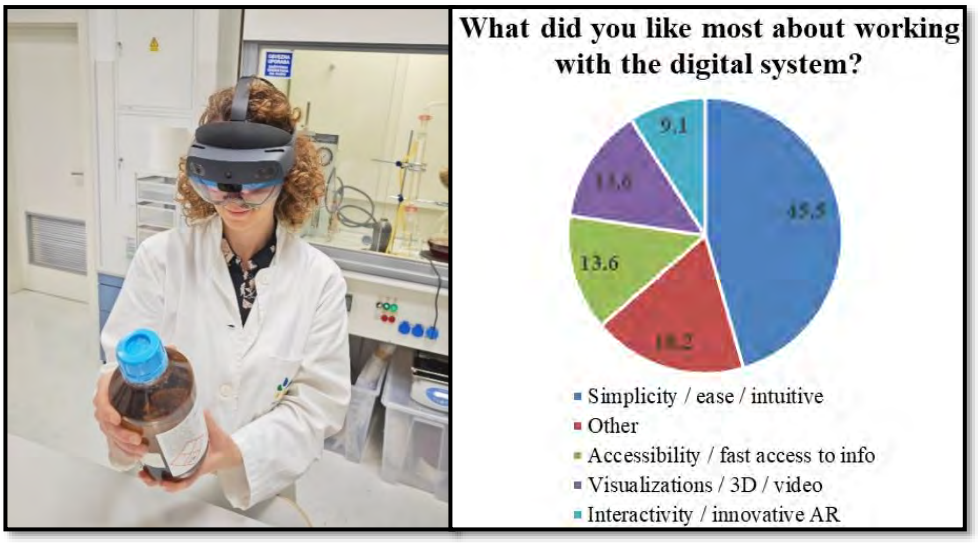

ISPITIVANJE UTJECAJA DODATKA BIOAKTIVNE KOMPONENTE NA SVOJSTVA NOVE FORMULACIJE DJELATNE TVARI

EVALUATING THE EFFECT OF BIOACTIVE COMPONENT ADDITION ON THE PROPERTIES OF A NEW ACTIVE INGREDIENT FORMULATION

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Mnoge djelatne tvari (API) posjeduju nepovoljna biofarmaceutska svojstva, poput slabe topljivosti u vodi i niske permeabilnosti, koja ograničavaju njihovu bioraspoloživost. Primjena niskotemperaturnih eutektičkih otapala (DES) predstavlja jedan od obećavajućih pristupa poboljšanju terapeutske učinkovitosti API-ja [1,2].
U ovome su radu pripremljena tri različita DES-a, dobivena miješanjem mliječne kiseline s netoksičnim komponentama (fruktoza, glicerol i glicin) u odabranim molarnim omjerima. Otapanjem API-ja ceritiniba (CRT) u tako pripremljenim otapalima ispitan je njihov utjecaj na topljivost i permeabilnost. Provedena je fizikalno-kemijska karakterizacija DES-ova određivanjem gustoće, viskoznosti i kiselosti, dok je infracrvenom spektrofotometrijom s Fourierovom transformacijom (FTIR) potvrđen nastanak vodikovih veza između komponenata DES-a i nastanak API-DES sustava. Topljivost čistog praškastog CRT-a i pripadajućih API-DES sustava ispitana je testom *in vitro* oslobađanja djelatne tvari. Također, ispitana je permeabilnost čistog praškastog CRT-a i CRT-a iz API-DES sustava. Prema Biofarmaceutskom klasifikacijskom sustavu (BCS), CRT pripada četvrtoj skupini, tvarima niske topljivosti i niske permeabilnosti [3]. S obzirom da je primjenom API-DES sustava postignuta viša koncentracija API-ja u vodenom mediju, dodatno je istražen potencijal povećanja permeabilnosti i difuzivnosti uvođenjem bioaktivnih komponenata u formulaciju. U sklopu rada određena je potrebna količina bioaktivne komponente koja poboljšava svojstva formulacije. Termodinamička svojstva i topljivost komponenata predviđeni su modelom COSMO-RS, kojim je procijenjen utjecaj dodatka različitih bioaktivnih komponenata na topljivost CRT-a u DES-u.

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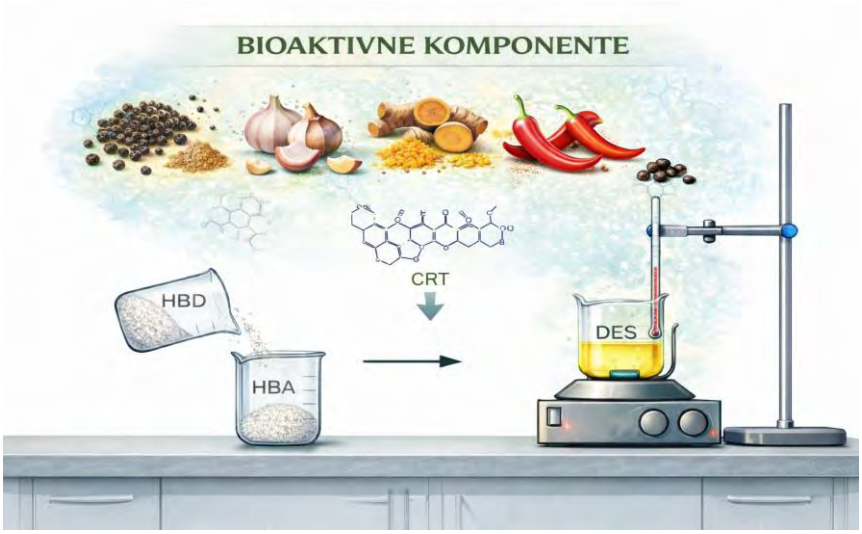
Ovo istraživanje provedeno je u okviru projekta LiBiDES financiranog od strane Europske unije - NextGenerationEU fonda iz izvora 581 - Mehanizam za oporavak i otpornost u okviru Programskog financiranja javnih visokih učilišta i javnih znanstvenih instituta u Republici Hrvatskoj.



BAND ALIGNMENT AND CHARGE TRANSFER IN g-C_3N_4/IN_2O_3 HETEROJUNCTIONS FOR EFFICIENT SOLAR-DRIVEN POLLUTANT DEGRADATION

Suresh Kumar Pandey,[1] Sandra Romac,[1] Josipa Papac Zjačić,[1] Hrvoje Kušić,[1] Marin Kovačić,[1] Marijana Kraljić Roković,[1] Ana Lončarić Božić,[1] Boštjan Žener,[2] Boštjan Genorio,[2] Urška Lavrenčič Štangar[2]

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Designing highly efficient photocatalysts for solar-driven pollutant degradation requires precise control over interfacial charge separation and light-harvesting capabilities. In this work, we engineer a g-C_3N_4/In_2O_3 heterojunction with tailored band alignment to enhance photocatalytic performance under visible-light irradiation. The heterostructure is synthesized through a facile thermal annealing and hydrothermal route, yielding intimate interfacial contact and improved crystallinity. Systematic band-structure analysis using UV-Vis spectroscopy, Mott-Schottky measurements, and photoluminescence reveals the formation of an efficient type-II (step-scheme/S-scheme) junction that promotes spatial charge separation, suppresses electron-hole recombination, and broadens the absorption range. Photocatalytic degradation tests using representative CECs demonstrate significantly accelerated reaction kinetics compared with pristine g-C_3N_4 and In_2O_3 alone. The enhanced activity is attributed to synergistic band alignment, increased carrier mobility, and extended lifetime of photogenerated charges at the heterointerface. This study highlights the potential of rational band-structure engineering in g-C_3N_4 based hybrid photocatalysts and offers a promising pathway toward efficient, sustainable solar-driven environmental remediation technologies.

This work has been supported by Croatian Science Foundation under project: Tailored solar-active materials for photocatalytic degradation of contaminants of emerging concern, SOL-MAT-CLEAN, IP-2025-02-8507.

MODELING OF BIOMASS PYROLYTIC REACTIONS IN THE GAS PHASE WITH H_2 NONTHERMAL PLASMA

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Pyrolysis of biomass is a promising technology for producing chemical and fuel feedstocks, in line with sustainable chemistry principles. However, conventional biomass pyrolysis yields oils with a high fraction of oxygenated compounds. These compounds adversely affect the stability of pyrolytic oils and lower their suitability as fuels. Post-pyrolysis upgrading of said pyrolytic oils, such as the technologically mature catalytic hydrogenation, requires significant capital investment and operating costs. Integrating the key upgrading process into the pyrolysis process itself could significantly reduce investment and operating costs. One such approach is the introduction of nonthermal hydrogen plasma into the pyrolysis unit, by means of a high-voltage corona discharge in the vicinity of the thermally treated biomass. Hydrogen radicals (H•) and other reactive species formed in the discharge zone can facilitate these upgrading reactions in situ. However, to size the pyrolysis unit appropriately, it is important to gain insights into the behaviour of radical species within and beyond the nonthermal plasma zone. To this end, the interplay between plasma chemistry and process variables, i.e., temperature, pressure, flow rate and electrode current, was modelled using Python. Specifically, H• and free electron (e^-) density plots were obtained, in order to assess areas where hydrogenation reactions occur and to assess potential tar formation. Furthermore, density functional theory (DFT) calculations were carried out to obtain relevant thermodynamic and activation energy parameters for gas phase reactions of the model compounds.

PRIPREMA pH-SENZORSKIH FILMOVA IMOBILIZACIJOM SMJESE INDIKATORA

PREPARATION OF pH-SENSITIVE FILMS BY IMMOBILIZATION OF AN INDICATOR MIXTURE

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Mikroreaktorski sustavi omogućuju provođenje kemijskih reakcija u sustavima malih dimenzija, uz intenzivan prijenos tvari i energije. pH-senzorski filmovi pripremljeni su imobilizacijom smjese indikatora u silanskom filmu, a njihova funkcionalnost najprije je ispitana na 3D-ispisanim pločicama izrađenim tehnologijom proizvodnje rastaljenim filamentom (engl. *fused filament fabrication*, FFF) od transparentnog filamenta poli(etilen-tereftalata) obogaćenog glikolom (PETG). Nakon navedenog, filmovi su naneseni na stijenke kanala 3D-ispisanih mikroreaktora. Za izradu tankih senzorskih filmova primijenjena je sol-gel metoda, koja omogućuje jednostavno nanošenje na podlogu, inkapsulaciju indikatora u stabilnu matricu te sintezu materijala pri niskim temperaturama. Kao prekursori sol-gel metode korišteni su tetraetoksisilan (TEOS) i feniltrimetoksisilan (FTMS). Pripremljeni filmovi karakterizirani su metodom kontaktnog kuta te infracrvenom spektroskopijom s Fourierovom transformacijom, dok je analiza RGB vrijednosti korištena za procjenu intenziteta promjene boje. Promjenom pH vrijednosti kapljevine u mikroreaktoru dolazi do vidljive promjene boje senzorskog filma unutar jedne minute. Potvrđena je mogućnost višekratne uporabe senzorskih filmova.

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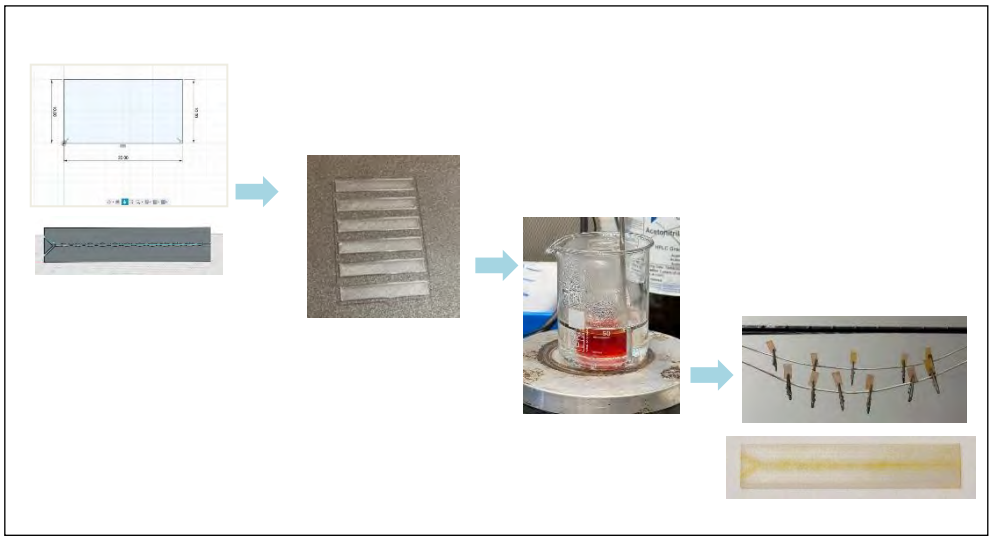

OPTIMIZACIJA POSTUPKA FORMIRANJA NEGATIVNE ELEKTRODE U LITIJ-IONSKIM BATERIJAMA

OPTIMIZATION OF THE NEGATIVE ELECTRODE FORMATION IN LI-ION BATTERIES

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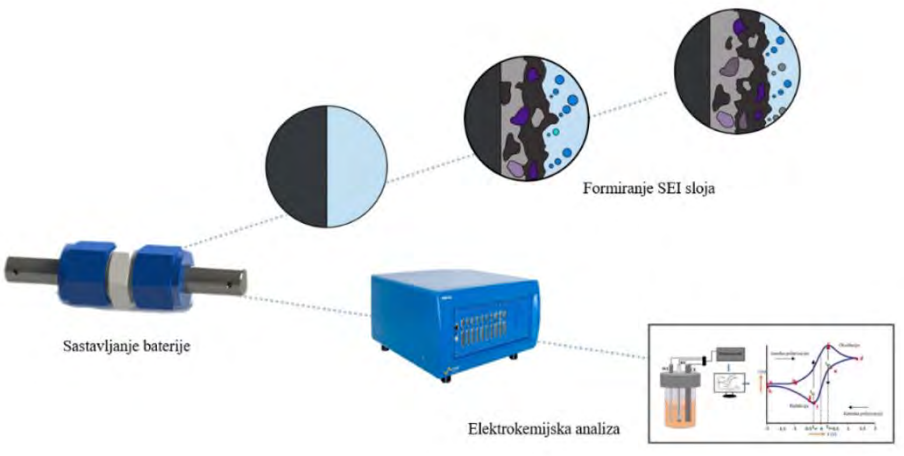
Sve veći zahtjevi za pouzdanim sustavima skladištenja obnovljive energije potaknuli su intenzivan razvoj litij-ionskih baterija. One predstavljaju jednu od najnaprednijih dostupnih tehnologija zahvaljujući visokoj gustoći energije i snage. Unatoč napretku u razvoju elektrodnih materijala, učinkovitost baterije uvelike ovisi o uvjetima tijekom prvih ciklusa, odnosno procesu formiranja. Formiranje predstavlja kontrolirano inicijalno punjenje tijekom kojeg se na negativnoj elektrodi stvara stabilan SEI (engl. *Solid Electrolyte Interphase*) sloj. Kvaliteta i homogenost SEI sloja izravno utječu na kapacitet, radni vijek i sigurnost baterije.

Proces formiranja baterija tradicionalno se provodi pri sporim, konstantnim strujama što osigurava stabilno formiranje SEI sloja. Sam proces je vremenski zahtjevan, stoga se istražuju brže metode koje uključuju brže ili pulsne struje. Novi načini formiranja omogućuju ubrzavanje postupka, utječu na debljinu i homogenost samog SEI sloja te poboljšanje samog rada baterije.

U ovom radu ispitan je utjecaj iznosa struja i oblika strujnog pulsa na formiranje negativne elektrode na bazi grafita. Elektrode su pripremljene u obliku suspenzija koje su sadržavale grafit, PVDF (poliviniliden fluorid) kao vezivo te NMP (*N*-metil pirolidon) kao otapalo. Nakon nanošenja na bakrene folije i sušenja, elektrode su sastavljene u Swagelok testne ćelije s litijevom elektrodom i litijevim heksafluorofosfatom u smjesi etilen-karbonata i dimetil-karbonata ($LiPF_6$ u EC/DMC) kao elektrolitom. Provedene su elektrokemijske analize, uključujući cikličku voltametriju, elektrokemijsku impedancijsku spektroskopiju te galvanostatsko punjenje i pražnjenje. Dobiveni rezultati omogućuju bolji uvid u utjecaj različitih postupaka formiranja na nastajanje SEI sloja te doprinose optimizaciji procesa s ciljem poboljšanja karakteristika litij-ionskih baterija.

Ovaj rad financiran je iz sredstava Europske unije u sklopu projekta NPOO.C3.2.R3-I1.04.0187: Napredni inovativni materijali i tehnologije za proizvodnju litij-ionskih baterija.



TAILORING THE MICROSTRUCTURE OF METAL–ORGANIC FRAMEWORKS FOR ENHANCED GAS SEPARATION AND STORAGE

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Post-combustion carbon capture requires adsorbents with high CO_2 capacity, strong CO_2/N_2 selectivity, and long-term stability. Metal–organic frameworks (MOFs) with tailored microstructures are promising adsorbents for CO_2 capture and separation due to their high porosity and tunable functionality [1]. In this work, we focus on post-combustion CO_2/N_2 separation using UiO-66 (Zr_6-benzenedicarboxylate MOF) and its amino-functionalized derivatives as model systems. Through modulator-induced defect engineering and crystal size control, we synthesized MOFs with hierarchical porosity and unsaturated metal sites [2,3]. Comprehensive characterization (BET surface area ~1200 m^2/g; PXRD, FTIR, SEM, TGA) confirms that defect creation and linker functionalization do not compromise the framework's crystallinity or thermal stability. Gas adsorption isotherms at 298 K indicate a remarkable increase in CO_2 uptake (~3.2 mmol/g at 1 bar) for the defect-engineered UiO-66-NH_2 compared to the non-defective analog, attributable to the introduction of extra porosity (open Zr^{4+} sites from missing-linker defects [4]) and CO_2-philic amine functionalities [5]. Ideal Adsorbed Solution Theory (IAST) calculations predict a high CO_2/N_2 selectivity of ~28 under flue gas conditions, highlighting the efficacy of amine-functionalized defects in preferential CO_2 binding. Breakthrough experiments using a 15% CO_2/85% N_2 mixture demonstrate that the optimized material effectively captures CO_2 with sharp separation fronts and maintains performance over 100 adsorption–desorption cycles. Our findings illustrate that microstructure tailoring—via deliberate defect introduction and linker functionalization—substantially enhances CO_2 adsorption capacity and selectivity in UiO-66-type MOFs. This study underpins the potential of defect-engineered MOFs as robust, high-performance sorbents for post-combustion carbon capture applications.

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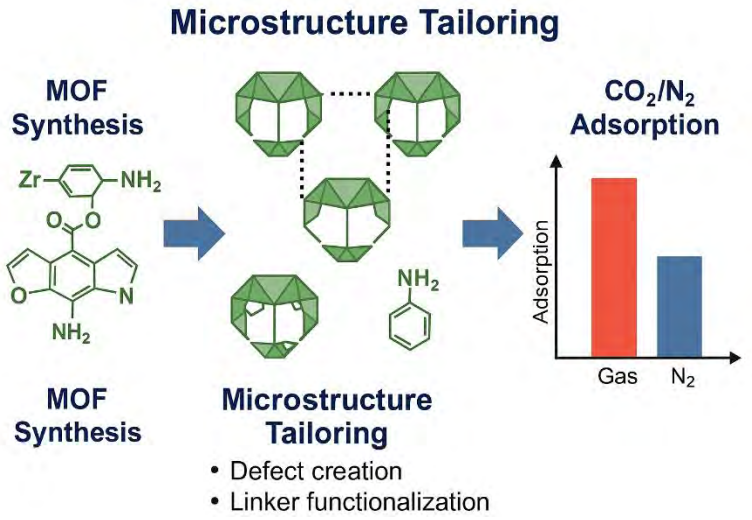

IN SILICO ISPITIVANJE NASTAJANJA KOKRISTALA U FARMACEUTSKOM RAZVOJU

IN SILICO STUDY OF COCRYSTAL FORMATION IN PHARMACEUTICAL DEVELOPMENT

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Kokristali su kristalične tvari koje nastaju međusobnim povezivanjem dviju ili više molekula putem nekovalentnih interakcija. Privlače veliku pozornost u industriji i znanstvenim istraživanjima jer poboljšavaju fizikalno-kemijska svojstva djelatnih tvari (engl. *active pharmaceutical ingredient*, API) kao što su topljivost, kemijska stabilnost, bioraspoloživost i dr. [1]. Međutim, eksperimentalno ispitivanje nastajanja kokristala u farmaceutskom razvoju, poznatije pod nazivom *cocrystal screening,* izrazito je dugotrajno, zahtjevno i skupo. Cilj tih ispitivanja je utvrditi mogućnost nastajanja kokristala između API-ja i koformera te ispitati stabilnost novonastalog kristalnog oblika. Primjenom računalnih metoda ispitivanja nastajanja kokristala (tzv. *in silico* metoda) znatno se smanjuju trajanje i troškovi *cocrystal screening*-a [2]. Osim toga, korištenjem računalnih metoda smanjuje se potrošnja kemikalija te proces ispitivanja postaje ekološki prihvatljiviji i održiviji. U ovom radu prikazan je pregled najčešće primjenjivanih računalnih metoda ispitivanja nastajanja kokristala u dostupnoj znanstvenoj literaturi. Računalne metode predstavljaju jedan od najnovijih pristupa u ovom području, a njihova primjena još je uvijek u fazi razvoja. Od računalnih metoda ističu se teorija gustoće funkcionala (DFT) i površinsko mapiranje, COSMO-RS (engl. *Conductor-like Screening Model for Real Solvents*) model, metoda molekularne dinamike, metoda Gibbsove slobodne energije, metoda izračuna energija kristalne rešetke i predikcija kristalne strukture te strojno učenje [3]. Rad obuhvaća i razvoj klasifikacijskog modela strojnog učenja za predviđanje nastajanja kokristala između API-ja i koformera za koje su ishodi eksperimenata dostupni u znanstvenoj literaturi. Modeli strojnog učenja razvijeni su koristeći platformu za analizu podataka KNIME i programski jezik *Python*. Pomoću SMILES (engl. *Simplified Molecular-Input-Line-Entry System*) zapisa API molekule i koformera generirani su njihovi molekularni deskriptori, poput *NumHDonors* (broj donora vodika), *MolWt* (molekulska masa) i dr., koji kvantitativno opisuju svojstva molekula i omogućuju njihovu daljnju obradu u softverskim proračunima. Molekularni deskriptori omogućuju podatkovno utemeljen (engl. *data-driven*) pristup predviđanju nastajanja kokristala. Modeli pružaju informaciju o tome hoće li određena kombinacija API-ja i koformera formirati kokristal ili neće, čime se dobivaju preliminarni rezultati koji mogu značajno ubrzati proces ispitivanja potencijalnih koformera.

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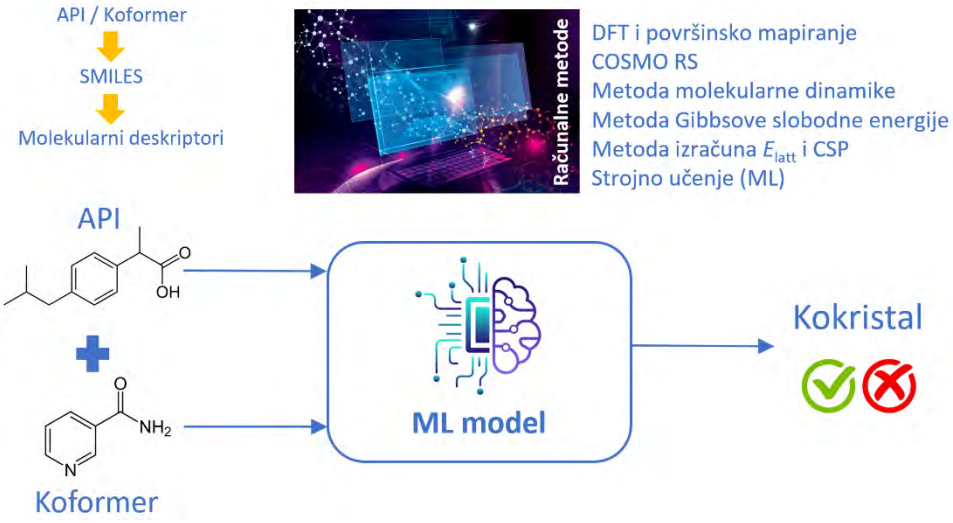

Primijenjena kemija
Applied chemistry

RAZGRADNJA BOJE PRIMJENOM VISOKOENTROPIJSKIH OKSIDA CERIJA

DYE DEGRADATION OVER CERIA-BASED HIGH-ENTROPY OXIDES

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Visokoentropijski oksidi (engl. *High entropy oxides*, HEOs) predstavljaju skupinu materijala sa širokim rasponom potencijalnih primjena zahvaljujući svojem jedinstvenom sastavu i kristalnoj strukturi. Ovi materijali su jednofazne čvrste otopine koje sadrže pet ili više glavnih metalnih kationa u ekvimolarnim omjerima te pokazuju iznimnu stabilnost zbog nasumične raspodjele kationa unutar kristalne rešetke [1]. U ovom radu sintetizirani su jedno- i dvofazni visokoentropijski oksidi polazeći od CeO_2 i/ili NiO kao matičnih oksida: $Ce_{0.2}La_{0.2}Pr_{0.2}Sm_{0.2}Eu_{0.2}O_2$ (CLPSE), $Ce_{0.2}La_{0.2}Pr_{0.2}Sm_{0.2}Eu_{0.2}O_2$/NiO (CLPSE-N) i $Ce_{0.2}La_{0.2}Pr_{0.2}Sm_{0.2}Eu_{0.2}O_2$/$Ni_{0.25}Cu_{0.25}Mg_{0.25}Zn_{0.25}O$ (CLPSE-NCMZ). Nitratne soli metala otopljene su u otopini limunske kiseline (w = 10 %), a vrijednost pH podešena je na 5 pomoću koncentrirane otopine amonijaka (w = 25 %). Otopina je zagrijavana na 95 °C do nastanka crne smole, koja je zatim sušena preko noći na 120 °C te kalcinirana na 600 °C tijekom 8 h uz brzinu zagrijavanja od 2 °C min^{-1}. Dobiveni materijali karakterizirani su rendgenskom difrakcijom na prahu (PXRD), Ramanovom spektroskopijom, UV-Vis spektroskopijom čvrstog stanja, termogravimetrijskom analizom (TGA), skenirajućom elektronskom mikroskopijom (SEM) i rendgenskom fotoelektronskom spektroskopijom (XPS). Vrijednosti energetskog razmaka valentne i vodljive vrpce izračunate su Taucovom metodom, dok je TGA analiza korištena za određivanje unosa kisika. Prije ispitivanja razgradnje bojila, suspenzije koje su sadržavale metilensko modrilo (engl. *Methylene blue*, MB) i katalizator miješane su u mraku 30 min. Razgradnja MB praćena je *in situ* UV/Vis spektroskopijom pod vidljivim svjetlom (halogena lampa, 20 W) 45 min u kinetičkom modu rada na 664 nm (maksimum apsorbancije MB, 10^{-5} mol L^{-1}). Rezultati pokazuju da sintetizirani HEO materijali značajno poboljšavaju razgradnju MB u usporedbi s njegovom samorazgradnjom.

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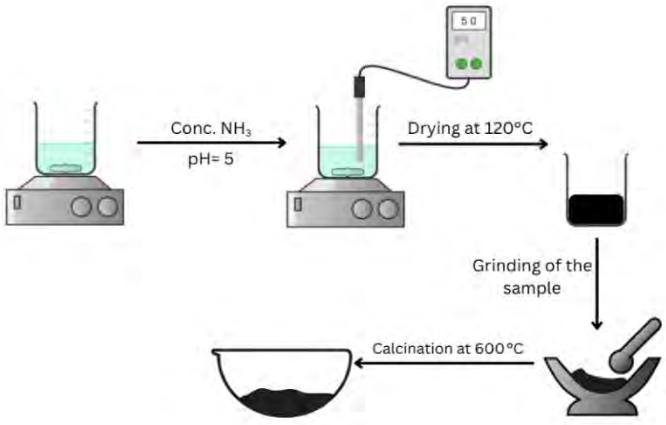

FROM SYSTEMIC TO TOPICAL: DEVELOPING A RELIABLE HPLC METHOD FOR QUANTIFYING MINOXIDIL AND RITLECITINIB IN INNOVATIVE PHARMACEUTICAL PRODUCTS

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Alopecia areata (AA) is a prevalent autoimmune condition characterized by hair loss, with the collapse of hair follicle immune privilege being a pivotal event in its pathogenesis. Minoxidil is an antihypertensive agent which decreases elevated blood pressure through vasodilation and is currently used in the treatment of AA due to its side effect of hirsutism. Minoxidil is an antihypertensive agent which decreases elevated blood pressure through vasodilation and causes hirsutism as a side effect. It is the most commonly used drug in the treatment of AA as it promotes hair follicle growth and prevents the progression of follicles to the telogen phase. As topical minoxidil is unable to alleviate the local inflammatory response, its use is limited in the treatment of moderate to severe AA.

The combination of minoxidil and a Janus Kinase (JAK) inhibitor, represents an increasingly utilized therapeutic strategy for the treatment of AA. This approach targets the complex pathology of AA using two distinct mechanisms. The JAK inhibitor primarily functions by inhibiting the JAK-STAT pathway, thereby suppressing the autoimmune inflammatory response. Minoxidil, as a potent vasodilator, extends the anagen phase of the hair cycle, thus improving blood flow to the affected scalp areas. Ritlecitinib is the latest orally applied JAK inhibitor approved by the FDA and EMA for the treatment of severe AA [1].

The aim of this research was to develop a reliable HPLC/DAD method for simultaneous determination of minoxidil and ritlecitinib as an analytical support for development of novel oral and topical pharmaceutical product.

Chromatography was performed using an Agilent 1260 Infinity II HPLC System. The chromatographic separation was performed in isocratic mode on Zorbax SB-C18 (4.6 x 100 mm, particle size 2.7 µm) column with flow rate 1 mL/min using mobile phase consisting of 10 mM ammonium acetate (pH 5.2) and methanol (65:35, v/v). Minoxidil and ritlecitinib were quantified at a fixed analytical wavelength of 280 nm (spectral bandwidth of 4 nm).

The observed retention time of minoxidil was 2.40 min and ritlecitinib 3.81 min with a total run time of 5 min, making the method both time- and cost-effective as well as eco-friendly. The peak purity of was determined to be above 999.5.

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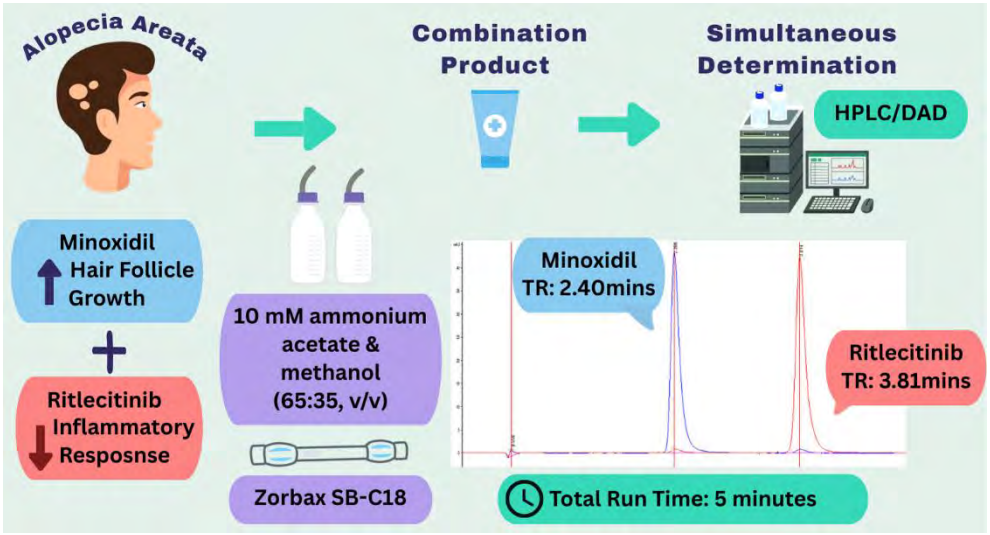
This research was funded by the Croatian Science Foundation, grant number: HRZZ-DOK-2021-02-7922.



INTERAKCIJA TERNARNIH KOORDINACIJSKIH SPOJEVA BAKRA(II) S DNA

INTERACTION OF TERNARY COORDINATION COMPOUNDS OF COPPER(II) WITH DNA

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Ternarni koordinacijski spojevi bakra(II) s aminokiselinama i *N*-heterocikličkim bazama privlače pozornost zbog svoje antiproliferativne aktivnosti. Navedeni spojevi pokazuju sposobnost interakcije s DNA tumorskih stanica, čime ometaju stanične procese tumorskih tkiva [1]. Cilj ovog istraživanja bio je ispitati utjecaj kombinacije različitih aminokiselina i *N*-heterocikličkih baza na interakciju s DNA, s namjerom da se odredi najpovoljniji strukturni dizajn ternarnog koordinacijskog spoja. Time se nastoji pridonijeti racionalnom dizajnu potencijalnih antitumorskih spojeva bakra(II). U ovom su radu sintetizirani spojevi bakra(II) s *N*-heterocikličkim bazama (2,2'-bipiridin (bpy), 1,10-fenantrolin (phen), pirazino[2,3-f][1,10]fenantrolin (pyphen) i aminokiselinama (glicin (HGly), L-homoserin (HhSer): $[Cu(Gly)(H_2O)(bpy)]_2SO_4 \cdot H_2O$ (**1**), $[Cu(L\text{-}hSer)(H_2O)(phen)]_2SO_4 \cdot 5H_2O$ (**2**), $[Cu(Gly)(H_2O)(pyphen)][Cu(SO_4)(Gly)(pyphen)] \cdot 6H_2O$ (**3**). Spojevi **1** i **3** pripravljeni su otopinskim sintezama i mehanokemijski, dok je spoj **2** dobiven isključivo mehanokemijskom sintezom. Spojevi **1** i **2** sintetizirani su prema poznatim protokolima te je njihova struktura već ranije opisana u literaturi [2,3]. Sinteza i strukturna karakterizacija spoja **3** u ovom radu određena je metodom difrakcije rendgenskog zračenja na jediničnom kristalu. Čistoća svih uzoraka potvrđena je difrakcijom rendgenskog zračenja na polikristalnom uzorku. Interakcije spojeva **1**, **2** i **3** s dvolančanom dodekamernom DNA (dlDNA, PDB kod: 1BNA)[4] ispitane su UV-VIS spektrofotometrijom i fluorimetrijom, čime su određene konstantne vezanja (slika 1). Pokazano je da heterocikliča baza značajno pridonosi jačini vezanja s dlDNA i slijedi trend K_b(1-dlDNA) < K_b(2-dlDNA) < K_b(3-dlDNA). Rezultati pokazuju da kombinacija različitih strukturnih motiva aminokiselina i heterocikličkih baza utječe na afinitet vezanja ternarnih koordinacijskih spojeva bakra(II) prema dlDNA, što naglašava važnost dizajna liganada u razvoju bioaktivnih koordinacijskih spojeva bakra(II).

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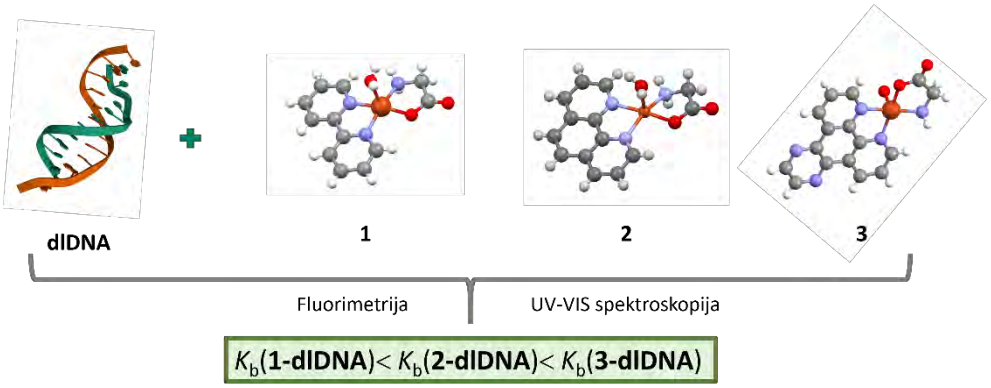

SINTEZA I KARAKTERIZACIJA TERNARNOG KOMPLEKSA BAKRA(II) S 1,10-FENANTROLINOM I L-FENILALANINOM TE ISPITIVANJE INTERAKCIJE S DNA

SYNTHESIS AND CHARACTERIZATION OF A TERNARY COPPER(II) COMPLEX WITH 1,10-PHENANTHROLINE AND L-PHENYLALANINE AND INVESTIGATION OF ITS INTERACTION WITH DNA

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Ternarni kompleksi bakra(II) su se pokazali kao spojevi s višestrukim biomedicinskim potencijalom, uključujući antibakterijsku i antitumorsku aktivnost [1]. Posebno se ističu ternarni kompleksi u kojima je ion bakra(II) koordiniran s *N*-heterocikličkom bazom i aminokiselinom[2]. U ovom radu prikazana je sinteza i strukturna karakterizacija novog ternarnog kompleksa bakra(II) koji sadrži 1,10-fenantrolin (phen) i aromatsku aminokiselinu L-fenilalanin (L–HPhe), $[Cu(Phe)(H_2O)(phen)][Cu(SO_4)(Phe)(phen)]\cdot 11H_2O$ (1). Odabir L-fenilalanina temelji se na njegovoj aromatskoj prirodi, koja može povećati sposobnost interakcije s DNA putem π–interakcija. Time se željelo ispitati postoji li razlika u afinitetu vezanja novopriređenog spoja 1 s DNA u odnosu na slične ternarne komplekse bakra(II) koji umjesto aromatske aminokiseline sadrže polarnu ili alifatsku aminokiselinu. Ternarni spoj 1 uspješno je pripremljen otopinskom sintezom te mu je određena kristalna struktura metodom difrakcije rendgenskog zračenja na jediničnom kristalu. U kompleksnom spoju 1 postoje dvije različite kompleksne vrste, kompleksni kation i anion. U obje kompleksne vrste su u ekvatorijalnoj ravnini na bakar(II) didentatno koordinirani 1,10-fenantrolin i fenilalaninatni ion, dok je u aksijalnom položaju u kompleksnom kationu vezana molekula vode, a u anionskoj vrsti sulfatni anion (slika 1). U kristalnoj strukturi kristalizacijske molekule vode zauzimaju 25 % volumena jedinične ćelije te se pakiraju u 2D slojeve. Čistoća spoja 1 potvrđena je metodom difrakcije rendgenskog zračenja na polikristalnom uzorku te je uočena njegova nestabilnost izvan matičnice. UV–VIS spektrofotometrijom i fluorimetrijom ispitana je interakcija spoja 1 s dvolančanom DNA (dlDNA) i pokazano je da se radi o vezanju u utor DNA. U tijeku je ispitivanje interakcija DNA sa sličnim ternarnim spojevima Cu(II) prema DNA, a koji ne sadrže aromatske aminokiseline te će se procijeniti utjecaj aminokiseline na afinitet vezanja.

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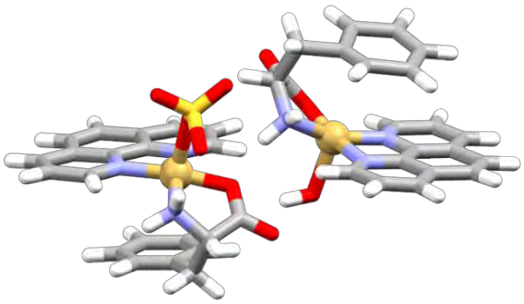

SINTEZA I STRUKTURNA KARAKTERIZACIJA NOVE METALOORGANSKE MREŽE BAKRA(II) S L-ASPARAGINOM I 4,4'-BIPIRIDINOM

SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF A NOVEL COPPER(II) METAL-ORGANIC FRAMEWORK WITH L-ASPARAGINE AND 4,4'-BIPYRIDINE

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Koordinacijski spojevi bakra (II) s aminokiselinama i heterocikličkim ligandima privlače značajnu pozornost zbog svoje raznolike strukturne kemije, sposobnosti samoorganizacije te potencijalnih primjena u području kristalnog inženjerstva i poroznih materijala [1]. Posebno su zanimljive metaloorganske mreže (engl. metal-organic framework, MOF), koje zbog svoje izrazite poroznosti pronalaze primjenu u skladištenju i razdvajanju plinova te u drugim područjima vezanim uz porozne materijale [2,3], pri čemu njihova struktura i stabilnost u čvrstom stanju ovise o vrsti i količini uključenog otapala [3]. Jedna od potencijalnih primjena jest i skladištenje vode. Nedostatak pitke vode te vode za navodnjavanje gorući je problem današnjice, a jedno potencijalno rješenje su metaloorganske mreže dizajnirane za kontrolirano vezanje vode [4]. U ovom radu provedena je sinteza nove višekomponentne meteloorganske mreže otopinskom sintezom. Strukturna karakterizacija spoja provedena je difrakcijom rendgenskog zračenja na jediničnom kristalu, čime je potvrđena da se radi o trodimenzijskoj metaloorganskoj mreži. Bakrovi(II) ioni premošćeni su asparaginatnim ionima i molekulama 4,4′-bipiridina, pri čemu nastaje metaloorganska mreža formule $\{[Cu_3(Asn)_2(bpy)_4](NO_3)_4 \cdot xL\}_n$ (MOF1), gdje L označava molekule otapala uključene u kristalnu strukturu. Dobivena struktura sadrži trodimenzijske kanale ispunjene molekulama otapala i nitratnim ionima, koji zauzimaju približno 61 % volumena jedinične ćelije, dok najveće dimenzije pora iznose približno 7×7 $Å^2$.

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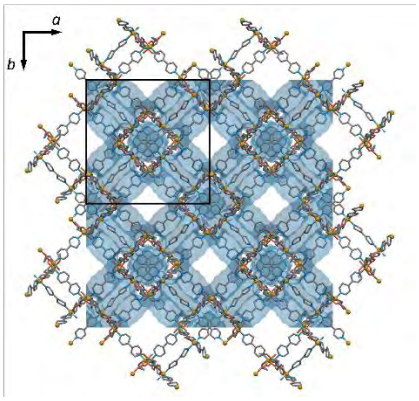

SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF NOVEL BENZAZOLE-BASED 1,2,3-TRIAZOLE AND HYDRAZONE DERIVATIVES

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Benzoxazole and benzothiazole derivatives have been widely studied due to their broad biological activities and importance in medicinal chemistry. These heterocycles exhibit diverse pharmacological properties, including anticancer, antiviral, antioxidant, anti-inflammatory, anticonvulsant, and antifungal effects [1]. Their rigid bicyclic structures and favourable electronic features make them versatile pharmacophores capable of interacting with multiple biological targets, and they are therefore considered privileged scaffolds in rational drug design. Furthermore, 1,2,3-triazoles and hydrazones have emerged as effective linker systems for tuning physicochemical properties, improving stability, and enhancing binding interactions in drug-like molecules. The 1,2,3-triazole ring is chemically robust and metabolically stable, while hydrazones provide tuneable electronic properties and intrinsic biological activity [2, 3]. Incorporation of these linkers into heterocyclic frameworks can significantly influence molecular conformation and strengthen interactions with biological targets [4].

Herein, we report the synthesis of novel benzoxazole derivatives bearing a 1,2,3-triazole moiety (I) *via* a Cu catalysed click reaction between the corresponding azides and prepared *O*-propargylated benzoxazoles in methanol. In addition, benzothiazole-based hydrazone derivatives (II) were synthesized through the reaction of 2-amino-5-substituted benzothiazoles with hydrazine hydrate, followed by a condensation reaction with appropriate 2-hydroxybenzaldehydes to afford the corresponding hydrazones. The structures of all synthesized compounds were confirmed by ^{1}H and ^{13}C NMR spectroscopy.

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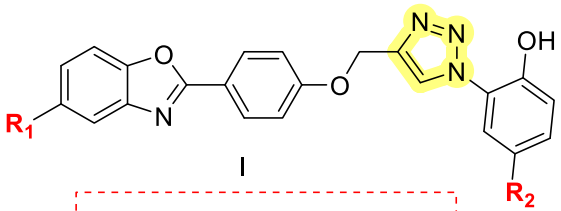
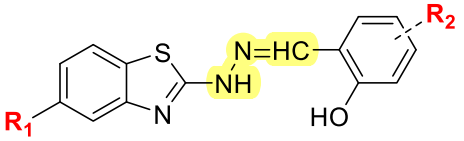
[4] Argirova, M. A. et al., RSC Adv. 11 (2021) 39848.

This work was supported by the Croatian Science Foundation under the project HRZZ-IP-2022-10-9420.



I

R_1 = H, Cl, F
R_2 = H, CH_3, OCH_3, F, Cl, Br



II

R_1 = H, Cl, F
R_2 = 4-OCH_3, 5-OCH_3, 4-NO_2, 4-F, 4-Br

SOLVOLYTIC REACTIVITY OF PHENYLSULPHINATE IN MIXTURES OF WATER AND APROTIC SOLVENTS

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The reactivity of organic compounds and the structural factors affecting it are key concepts in organic chemistry. The ability to predict solvolysis rates is particularly valuable when working with compounds during synthesis, purification, and storage. Since solvolysis is generally an undesirable process in organic synthesis, understanding the conditions that govern it is essential for controlling reaction conditions, improving stability, and preventing unwanted decomposition. The evaluation of solvolytic reactivity can be reliably achieved using the Mayr equation (1):

$$\log k\ (25\ °C) = s_f(E_f + N_f) \qquad (1)$$

In equation (1), k is a first-order rate constant, E_f represents the electrofugality parameter of reference benzhydryl electrofuges, while N_f and s_f define leaving-group–specific parameters describing the solvolytic ability of the nucleofuge. It should be noted the nucleofugality parameters N_f and s_f strongly depend on the physicochemical properties of the solvent in which the solvolysis occurs with more polar media generally favouring solvolysis of anionic leaving groups [1-3].

In order to determine and compare the nucleofugality parameters of the phenylsulfinate leaving group in 60 % aqueous acetone and acetonitrile, a series of benzhydryl phenylsulfinates were synthesized, and rate constants for solvolyses of substrates in 60 % acetone and 60 % acetonitrile (v/v) at 25 °C were measured using the conductometric method. From the log k/E_f plots, and using E_f values of the reference benzhydryl electrofuges, the nucleofuge-specific parameters N_f and s_f of phenylsulfinate were determined. The obtained N_f values expand the nucleofugality scale of phenylsulfinate to aprotic solvents-water mixtures and allow prediction of solvolysis rates and half-lives for a wide range of phenylsulfinate-containing substrates in aprotic solvent media.

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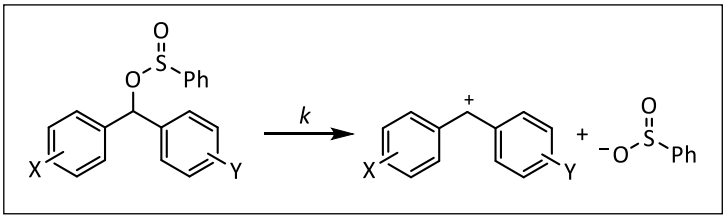

ASSESSMENT OF THE ANTIMICROBIAL ACTIVITY OF BISINDOLE SYSTEMS USING COMPUTATIONAL MOLECULAR DOCKING METHODS

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Computational chemistry represents a foundation of modern chemical science and plays a crucial role in understanding chemical processes at the molecular level [1]. It enables precise prediction of molecular properties and reactivity prior to experimental synthesis, thereby accelerating research and reducing the need for extensive laboratory testing. By integrating theoretical models with advanced computational algorithms, it is possible to investigate molecular interactions at atomic resolution, providing insights that often surpass the capabilities of traditional experimental methods [2].
A growing challenge in medicine is the decreasing effectiveness of antimicrobial drugs, caused by the evolution of microorganisms and their ability to acquire various resistance mechanisms. Therefore, the aim of this study was to apply computational methods to evaluate the antimicrobial activity and to investigate in detail the potential mechanism of action of bisindole systems. A key part of the research involved the use of molecular docking to model interactions between optimized bisindole structures and the selected target enzyme, DNA gyrase B. The obtained computational results provided insight into the affinity, stability, and possible binding modes of the bisindole derivatives, enabling assessment of binding energies and identification of key interactions within the enzyme's active site responsible for molecular recognition. Furthermore, these computational analyses allowed the identification of structural features that contribute to enhanced antimicrobial activity [3,4].

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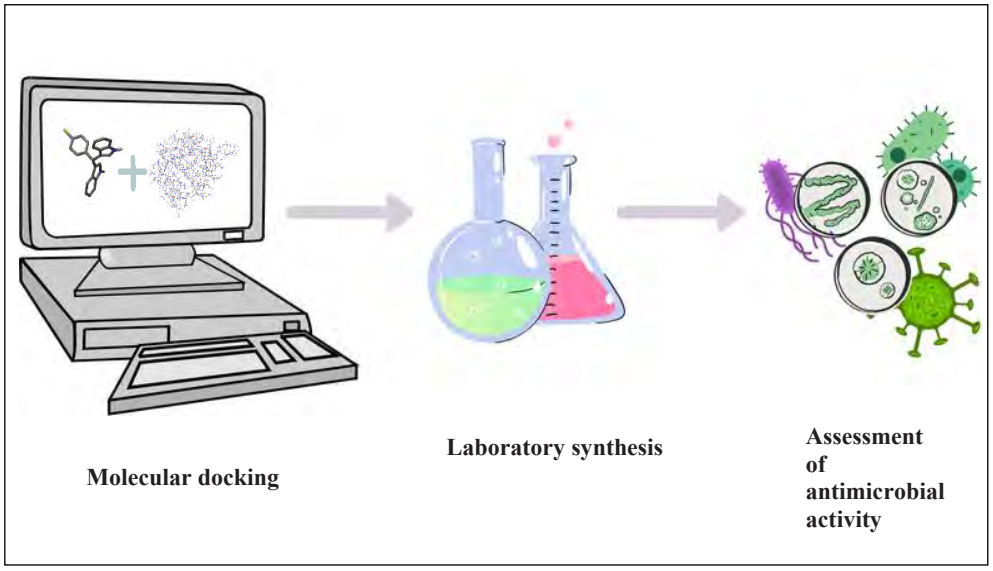

SYNTHESIS AND BIOLOGICAL ACTIVITY OF NOVEL BISINDOLE SYSTEMS

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Indole, as an important bioactive molecule, is a component of many natural products such as the plant growth hormone, serotonin, tryptophan and melatonin. Due to the widespread occurrence of indole derivatives in nature, they have often been investigated in the organic and medical industries. Numerous drugs containing an indole core are being explored for the treatment of pathological conditions such as bacterial, fungal, viral, tubercular, and HIV infections, as well as malaria [1].
Considering previous research and its significant findings, this work focuses on the synthesis of new bisindole derivatives to examine their biological activity. A practical and novel method for the synthesis of indole derivatives was used, employing $Cu(NO_3)_2 \cdot 3H_2O$ as a catalyst. The current protocol [2] offers several advantages: an easily accessible and inexpensive catalyst, mild reaction conditions (room temperature), good yields, high selectivity, and experimental simplicity. The synthesized indole derivatives were tested *in vitro* for antibacterial activity against the microbial species *Pseudomonas aeruginosa*, *Bacillus subtilis*, *Candida albicans* and *Aspergillus niger*, using the agar diffusion method. The plausible inhibitory mechanism by which these compounds could serve as antibacterial and antifungal drug candidates was elucidated through *in silico* molecular docking studies.

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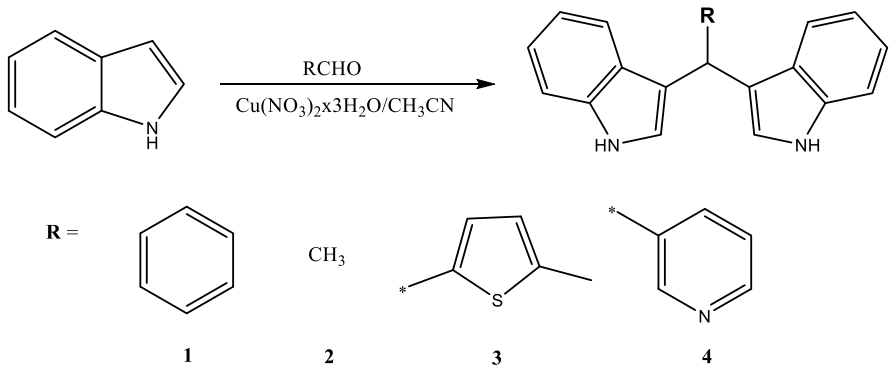

ISPITIVANJE KEMIJSKE STABILNOSTI INDOMETACINA: IDENTIFIKACIJA RAZGRADNIH PRODUKATA PRIMJENOM LC/MS I MS/MS TEHNIKE

INVESTIGATION OF INDOMETHACIN CHEMICAL STABILITY: IDENTIFICATION OF DEGRADATION PRODUCTS USING LC/MS AND MS/MS TECHNIQUE

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U okviru ove studije provedena je sveobuhvatna analiza kemijske stabilnosti indometacina primjenom forsiranih uvjeta razgradnje, s ciljem razumijevanja potencijalnih degradacijskih mehanizama i identifikacije nepoznatih produkata razgradnje. Ispitivana je osjetljivost indometacina na različite stresne uvjete, uključujući kiselo i lužnato okruženje, povišenu temperaturu, izloženost svjetlosti i prisutnost kisika.
Tijekom studije, primijenjene su kromatografske metode visoke rezolucije (HPLC, UPLC) u kombinaciji s masenom spektrometrijom (MS) za detekciju i identifikaciju degradacijskih produkata. Poseban fokus stavljen je na onečišćenja koja su se pojavila u značajnim udjelima, a prethodno nisu bila poznata. Korištenjem napredne MS/MS analize i interpretacije fragmentacijskih obrazaca, uspješno su identificirane strukture novih degradacijskih spojeva.
Dobiveni rezultati pružaju uvid u kemijsku stabilnost indometacina te omogućuju bolju procjenu rizika tijekom razvoja formulacija i skladištenja. Ova studija doprinosi razumijevanju degradacijskih puteva indometacina i može poslužiti kao temelj za izradu strategija stabilizacije u farmaceutskom razvoju.

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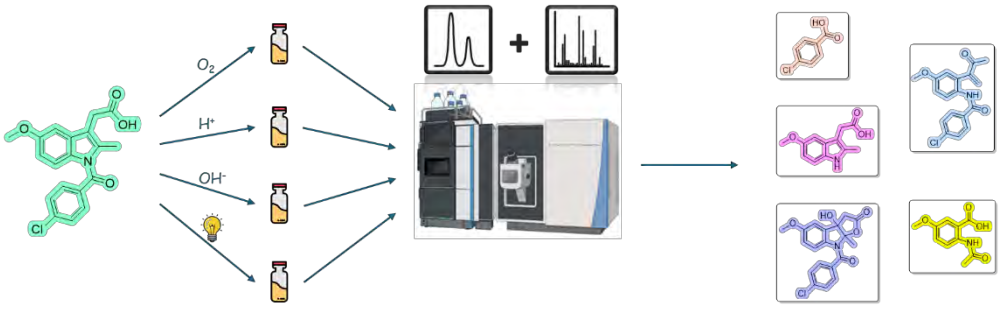

CONCENTRATION- AND TEMPERATURE-DEPENDENT INFRARED SPECTROSCOPY IN CONFORMATIONAL ANALYSIS OF FERROCENE PEPTIDOMIMMETICS

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IR spectroscopy, one of the most commonly used spectroscopic techniques, provides valuable information about the conformational space of peptides in solution. This method enables the assessment of protein structure based on the frequency values at which chemical bonds absorb infrared radiation, with absorption intensity increasing as the polarity of chemical bonds increases. IR spectroscopy measures the wavelength and intensity of infrared radiation absorption and identifies functional groups, while also providing reliable insight into the conformational space of the analyzed peptides. Stretching frequencies above 3400 cm^{-1} are attributed to free NH groups, while NH group frequencies below 3400 cm^{-1} indicate their involvement in hydrogen bonds. Furthermore, the absorption bands of carbonyl ester groups, present below 1730 cm^{-1}, also suggest their participation in hydrogen bonding.

By measuring concentration-dependent IR spectra, it is possible to determine whether the hydrogen bonds are intramolecular or intermolecular. Intermolecular hydrogen bonds are disrupted by progressively diluting the solution of the analysed sample, resulting in a significant weakening of the intensity of the associated NH group signals, while the intensity of free NH groups increases.

Temperature-dependent IR spectra are used to study changes in the vibrational properties of molecules at different temperatures. This technique provides valuable information about the thermodynamic and structural properties of molecules, as well as their behavior under varying temperature conditions. Temperature changes can significantly affect the stability of intermolecular hydrogen bonds. Furthermore, temperature changes can induce conformational changes in molecules, further contributing to the understanding of their structural dynamics. This method allows for the analysis of how molecular interactions and vibrational patterns adapt to temperature changes, making temperature-dependent IR spectroscopy a key tool in the study of complex molecular systems.

Therefore, we analysed peptides **I** and their analogues, depsipeptides **II** (**1**–**6**) to deduce the pattern of intramolecular hydrogen bonding using concentration- and temperature-dependent IR spectroscopy. As expected, replacing an amide bond with an ester group reduces the number of available hydrogen bond donors, which affects the conformational patterns.

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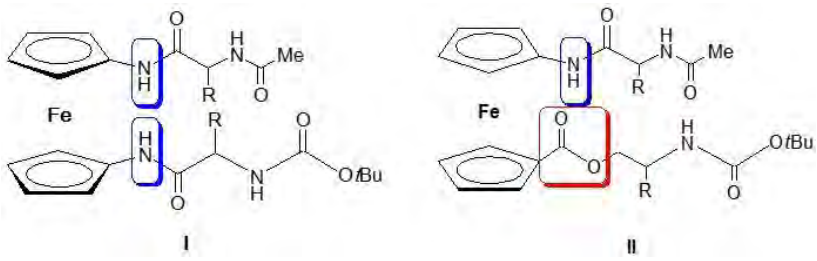

SYNTHESIS AND IN SILICO BIOAVAILABILITY ASSESSMENT OF NOVEL STEROIDAL HYDRAZONE DERIVATIVES

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Steroid hormones and related steroidal molecules remain a major focus of chemical and biomedical research due to their central roles in physiological processes and widespread clinical applications. Natural steroids can be structurally modified by introducing heteroatoms within core cyclopentaneperhydrophenanthrene framework or attaching additional heteroatom-containing substituents. These modifications can substantially affect physicochemical properties, modulate biological activity, and improve safety profiles. Increasing attention has been directed toward nitrogen-containing steroid derivatives, which exhibit a broad range of pharmacological activities, including antitumor, antimicrobial, anti-HIV, antimalarial, antitubercular, anti-Alzheimer, antidiabetic, and antiparasitic effects [1].

Several D-ring nitrogen-substituted steroid derivatives are either approved for clinical use or are in various stages of clinical trials. A notable example includes abiraterone, an established antitumor agent for prostate carcinoma. Although comprehensive biochemical and pharmacological assessments remain incomplete for many compounds in this class, recent literature indicates that D-ring nitrogen-substituted steroids constitute a promising area of research [2].

In light of these considerations, the present work involved the synthesis of three novel hydrazone derivatives of (16*E*)-3β-hydroxyandrost-5-en-16,17-dione 16-oxime, specifically those bearing 2-(hydroxybenzylidene)hydrazinylidene, (pyridin-2-ylmethylidene)hydrazinylidene, and (pyridin-3-ylmethylidene)hydrazinylidene moieties at the C-17 position.

Over recent decades, *in silico* ADME/T prediction has become a key component of modern drug design. These computational approaches streamline development by enabling early assessment of bioavailability, safety, and activity directly from molecular structure, allowing the identification of promising candidates before costly experimental and clinical studies [3].

The biological potential of the newly synthesized compounds was initially evaluated using *in silico* ADME/T analyses, performed with SwissADME and ProTox-3.0. The results indicate that these compounds generally satisfy the fundamental criteria for favorable oral bioavailability and exhibit low predictive toxicity. These findings underscore their promising pharmacokinetic profiles and warrant further comprehensive biological assessment.

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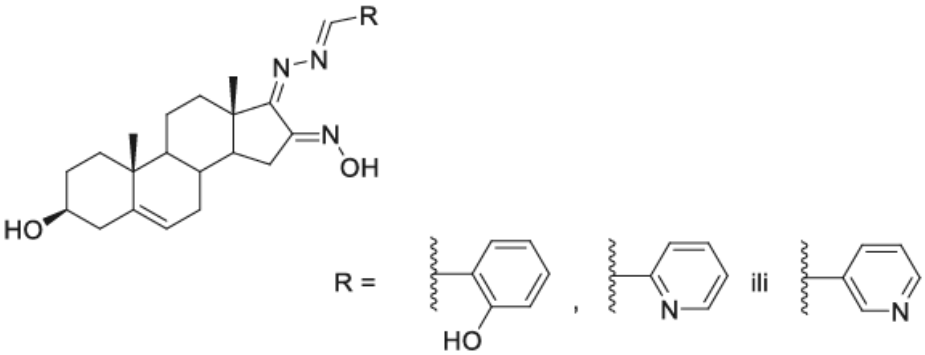

DESIGN AND SYNTHESIS OF ISOXAZOLE-BRIDGED PYRIDINE AND QUINOLINE CONJUGATES AND THEIR METAL COMPLEXES WITH POTENTIAL ANTITRYPANOSOMAL ACTIVITY

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Trypanosomatida protozoa include several medically important parasitic species, among which the *Trypanosoma brucei* species is responsible for human African trypanosomiasis (HAT), commonly known as sleeping sickness. This neglected tropical disease remains a major health burden in sub-Saharan Africa, highlighting the urgent need for new and selective chemotherapeutic agents [1-3]. New nitroheterocyclic derivatives bridged by an isoxazole moiety and linked to pyridine or quinoline fragments were designed and synthesized, with the aim to obtain potential antitrypanosomal agents. Nitroheterocycles were reacted with propargyl bromide to produce alkyne derivatives, which were subsequently coupled with chlorinated pyridine-carbaldehyde oxime and chlorinated quinoline-carbaldehyde oxime to form novel pyridine and quinoline conjugates. These conjugates were subsequently used as ligands in the preparation of metal complexes. The structures of all synthesized compounds were confirmed using NMR, UV-Vis, and FTIR spectroscopy. Antitrypanosomal evaluations of the newly prepared conjugates and their metal complexes are currently ongoing.

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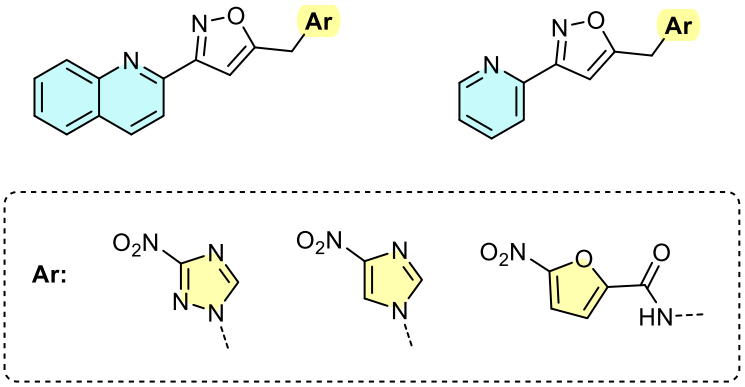

NOVI POTENCIJALNI BIOLOŠKI AKTIVNI REZVERATROL-BENZIMIDAZOLNI I REZVERATROL-OKSAZOLNI HIBRIDI

NEW POTENTIAL BIOLOGICALLY ACTIVE RESVERATROL-BENZIMIDAZOLE AND RESVERATROL-OXAZOLE HYBRIDS

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Cilj ovog rada je sinteza rezveratrolnih soli koje bi se potencijalno mogle koristiti u liječenju neurodegenerativnih poremećaja zbog sposobnosti inhibiranja enzima butirilkolinesteraze [1]. U prijašnjim istraživanjima, heterociklički analozi rezveratrola pokazali su iznimnu biološku aktivnost [2]. Uočeno je još slobodnog prostora u aktivnom mjestu enzima za potencijalno vezanje. Stoga, rezveratrolnu strukturu nadograđujemo dodatnim heterocikličkim jezgrama, poput benzimidazola i oksazola, za koje se predviđa pojačana inhibicijska aktivnost. Prevođenjem rezveratrolnih derivata u nabijene soli, čije strukture su označene s 1 i 2 u grafičkom sažetku, očekuje se višestruko poboljšanje njihovih bioloških svojstava, kako inhibicijskih, tako i antioksidacijskih. Sintetski put sastoji se od 6 koraka. Prvi korak je Wittigova reakcija u kojoj salicilni aldehid reagira s 2-tienilnom fosfonijevom soli pri čemu se povezuju *trans*-dvostrukom vezom. Nakon što se hidroksilna skupina na fenilnom prstenu zaštiti acetatnom skupinom, Vilsmeierovim formiliranjem se uvede aldehidna skupina na položaj 5 tiofenskog prstena. Time se omogućava vezanje nove heterocikličke strukture na taj položaj. Provedeno je i odštićivanje hidroksilne skupine. Posljednji korak sinteze je prevođenje derivata u nabijene soli alkiliranjem pomoću benzilnih bromida. Struktura dobivenih spojeva potvrđena je NMR i HRMS analizom. Spojevima će bit ispitana inhibicijska svojstva prema butirilkolinesterazi te će računalnom kemijom biti povedeno molekulsko pristajanje u aktivno mjesto enzima.

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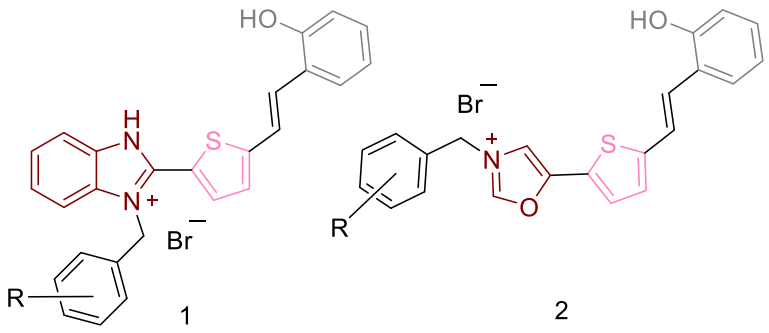

EVALUATION OF ANTIOXIDANT AND ANTIBACTERIAL ACTIVITY OF IMINES BASED ON SUBSTITUTED BENZALDEHYDES AND THIOSEMICARBAZIDES

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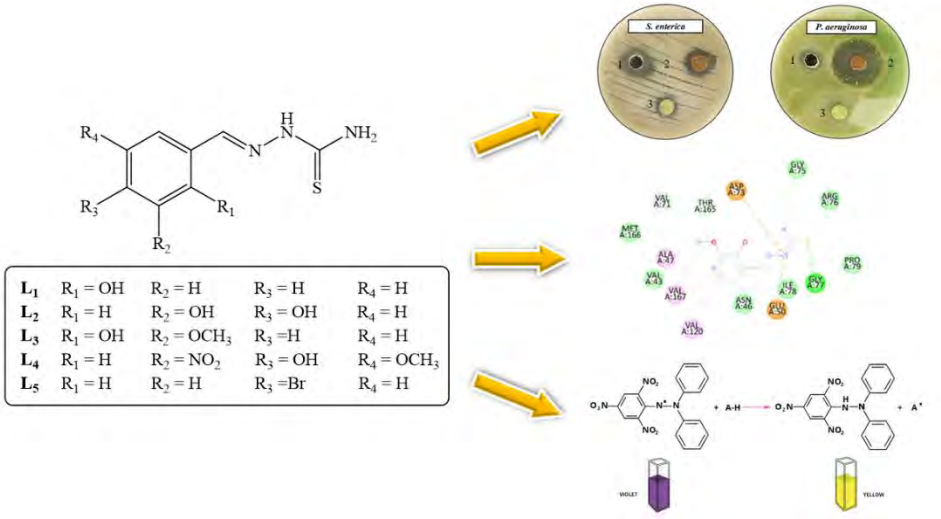
In this study, the antioxidant and antibacterial activity of substituted salicylaldehyde and thiosemicarbazide-based imines was analyzed. Five compounds were synthesized and characterized by mass spectrometry (MS), nuclear magnetic resonance spectrometry (NMR), infrared spectrometry (IR), and ultraviolet-visible absorption spectrometry (UV/VIS). The ability to inhibit free radicals was tested by the DPPH and ABTS methods, and the reduction potential by the FRAP method. In order to investigate the potential mechanism of antibacterial activity of the synthesized compounds, in silico molecular docking studies of bacterial DNA gyrase, a well-established antibacterial target present in most Gram-positive and Gram-negative bacteria, were performed. Molecular docking simulations were performed using AutoDock Vina. *In vitro* antibacterial activity was tested by the diffusion technique on reference bacterial strains from the WDCM collection. The antioxidant activity of the synthesized imines is extremely high. All tested compounds form an attractive charge interaction with Asp73, suggesting a similar binding mode and potential for comparable inhibitory activity. *In vitro* antibacterial potential testing confirmed that the imines exhibit moderate to strong antibacterial activity, which is in direct correlation with the structure of the compounds.



SINTEZA I KARAKTERIZACIJA PEPTIDOMIMETIKA S FENILALANINOM

SYNTHESIS AND CHARACTERIZATION OF PHENYLALANINE-BASED PEPTIDOMIMETICS

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Ugijevom višekomponentnom reakcijom dobiva se kondenzacijski produkt četiri polazna spoja u samo jednom koraku [1]. *α*-adicijom iminijevog iona, nastalog iz karbonilnog spoja i amino komponente, te kisele komponente na izocijanid nastaje *α*-međuprodukt koji se pregrađuje u produkt, *α*-acilamino amid, sličan peptidu [1, 2]. Zbog mogućnosti korištenja širokoga spektra polaznih spojeva u sintezi produkata koji su po strukturi peptidomimetici, reakcija se primjenjuje i u otkrivanju potencijalnih lijekova [3]. U ovom radu, koristeći *α*-aminokiselinu fenilalanin s *N*-*tert*-butiloksikarbonilnom skupinom, benzilamin, paraformaldehid i *tert*-butil-izocijanid, sintetiziran je Ugijev produkt. Sljedeći korak je uključivao skidanje zaštitne skupine pri čemu je dobivena slobodna amino skupina Ugijevog produkta. Hofmannovim iscrpnim metiliranjem dobivenog amina sintetiziran je treći spoj, kvarterna amonijeva sol, prema literaturnom postupku uz manje prilagodbe [4]. Struktura spojeva potvrđena je 1D te 2D ^{1}H i ^{13}C spektroskopijom nuklearne magnetne rezonancije te spektrometrijom masa visoke razlučivosti. Biološka aktivnost pripremljenih spojeva prema enzimu butirilkolinesterazi evaluirana je određivanjem IC_{50} vrijednosti, (koncentracija inhibitora koja je potrebna za inhibiciju 50% enzima).

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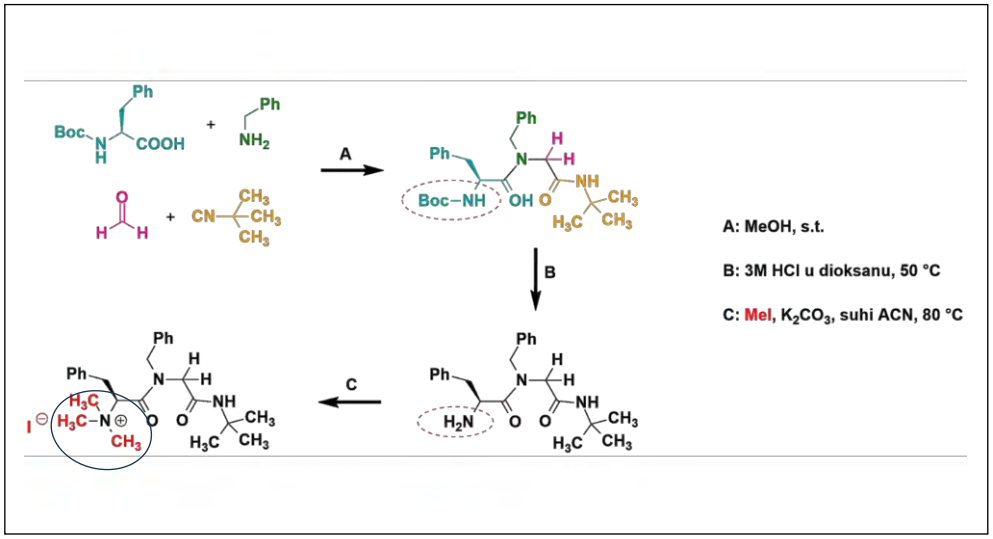

MECHANISTIC AND KINETIC INVESTIGATION OF DOPAMINE-GLUTATHIONE INTERACTION USING AN EC′ ELECTROCHEMICAL MODEL

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The interaction between dopamine (DA) and glutathione (GSH) plays a central role in maintaining cellular redox balance, particularly in neuronal environments where oxidative stress contributes to numerous pathological processes [1, 2]. When DA and GSH are present in the same medium, GSH can significantly influence the oxidative behavior of DA, modifying both its preferred reaction pathway and the resulting electrochemical response. These alterations are especially pronounced under mildly alkaline conditions, where the nucleophilic strength of GSH increases, intramolecular cyclization of DA and the nucleophilic addition of GSH to DA-*o*-quinone become kinetically favored [3]. The present study integrates comprehensive electrochemical experiments with mathematical voltammetric simulations to elucidate the mechanistic pathways involved and to quantitatively determine the relevant kinetic parameters governing this system. Voltammetric measurements were performed in acetate buffer at pH 5.02, conditions chosen to suppress spontaneous DA autoxidation, as well as in near-physiological (pH 7.12) and basic media (pH 8.55), where the intramolecular cyclization of DA and subsequent nucleophilic addition by GSH are markedly accelerated. Cyclic voltammetry (CV) and square-wave voltammetry (SWV), conducted using a glassy carbon electrode, revealed substantial changes in peak-current intensities, peak positions, peak separation, and peak morphology upon introduction of GSH.

To rationalize the experimental findings, mathematical simulations were performed assuming an EC′ mechanism, consisting of an initial electron-transfer (E) step followed by a catalytic (C′) step between oxidized DA and GSH. Systematic variation of the standard rate constant of electron transfer (ks), pseudo-first order catalytic rate constant (kc), and the chemical rate parameters enabled the construction of simulated voltammograms that closely reproduced the experimentally observed current-potential profiles. The optimized kinetic parameters provide quantitative evidence supporting the proposed EC′ model and reveal the extent to which GSH acts as a catalytic reagent.

Overall, this combined experimental-theoretical approach offers a deeper mechanistic understanding of how GSH modulates the oxidative chemistry of DA. The results highlight the value of mathematical simulation in validating complex electrochemical pathways and provide a foundation for interpreting DA-GSH reactivity in biological systems where redox homeostasis is critical.

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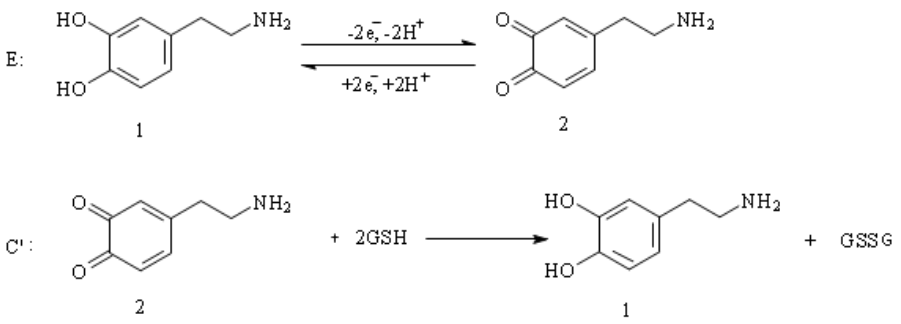

SYNTHESIS, STRUCTURAL CHARACTERIZATION AND ANTITRYPANOSOMAL ACTIVITY OF BENZIMIDAZOLE DERIVATIVES

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Human African trypanosomiasis (HAT) is a life-threatening neglected tropical disease caused by *Trypanosoma brucei* and transmitted by tsetse flies [1, 2]. Despite available therapies, current treatment options are limited by significant toxicity, challenging administration, and rising drug resistance, underscoring the urgent need for safer and more effective alternatives. Efforts to control HAT are further complicated by globalization, environmental change, coinfections, and the recent reallocation of global health resources. In this context, the benzimidazole scaffold has emerged as a valuable motif in antiparasitic drug discovery due to its purine-like character and its ability to interact with diverse biological targets. Previous work from our group and others has shown that benzimidazole derivatives display strong antiprotozoal activity, particularly when C-2 functionalization incorporates an amide linkage or bioisosteric groups such as 1,2,3-triazoles, often in combination with N-1 substitution [1-3].
As part of our ongoing research toward developing benzazole derivatives with antiprotozoal activity, we designed, synthesized, and evaluated a targeted series of benzimidazole amide and benzimidazole Schiff base analogues.

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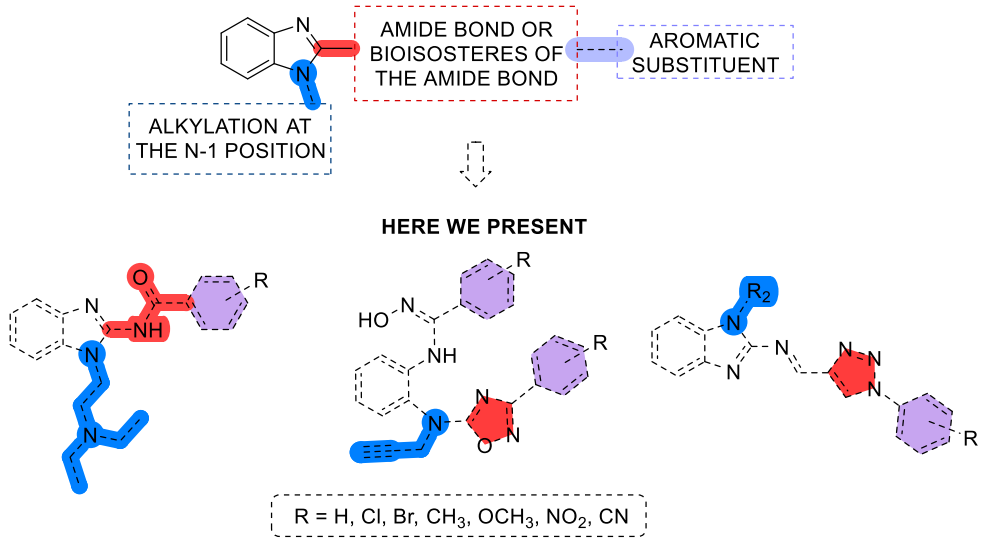

INDENE DERIVATIVES AS POTENTIONAL CANDIDATES FOR ANTIMICROBIAL DRUGS

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The problem of antibiotic resistance requires the development of new antimicrobial agents, among which indene derivatives occupy an important place due to their structural diversity and favorable biological profile [1].
In this work, the synthesis of new aryl-substituted indene derivatives is described. First step includes the reaction of indene with different aldehydes in ethanolic KOH solution under reflux, followed by reduction with lithium aluminium hydride in dry THF. The products were purified by column chromatography and characterized by spectroscopic methods. The antimicrobial activity of the synthesized compounds was evaluated by the disk diffusion method on *Bacillus subtilis* 3020, *Pseudomonas aeruginosa* 3011, *Candida lipolytica* 59 and *Aspergillus niger* 405 strains, while the plausible inhibitory mechanism by which these compounds could serve as antibacterial and antifungal drug candidates was elucidated through *in silico* molecular docking studies. Certain derivatives showed pronounced inhibition of the growth of Gram-positive bacteria and fungi, while no activity was observed against *Pseudomonas aeruginosa* 3011, confirming the possibility of indene scaffolds as starting structures for further development of antimicrobial candidates [2,3].

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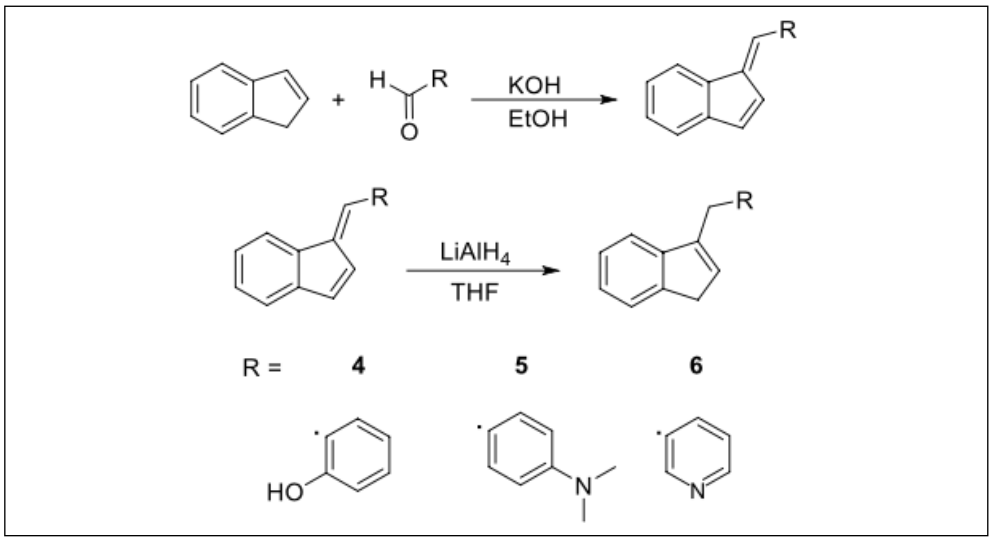

VALORIZATION OF EGGSHELLS INTO CaO FOR THE REMOVAL OF LEAD IONS FROM AQUEOUS SOLUTIONS: INVESTIGATION OF CHEMICAL PRECIPITATION CONDITIONS

Emina Kovačević, Aida Gogić, Aldijana Mustafić, Halid Junuzović, Sabina Begić, Husejin Keran, Amra Selimović, Indira Šestan, Melisa Ahmetović, Edina Ibrić

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Growing concerns regarding sustainability and environmental protection have led to increased interest in the production of calcium oxide (CaO) from waste eggshells. One of the effective methods for obtaining this material is the thermal decomposition of eggshells. In this study, waste chicken eggshells were thermally decomposed (calcination) at 800 °C for 7 hours [1], and the resulting CaO was subsequently utilized as a precipitating agent for the removal of lead ions from synthetic aqueous solutions. Chemical precipitation is considered a straightforward and economically viable water treatment technique, in which dissolved heavy metals are converted into insoluble forms and then separated by sedimentation and filtration processes [2]. The efficiency of the precipitation process was evaluated under various chemical precipitation conditions, including pH value, stirring speed and time, initial metal ion concentration, dosage of the precipitating agent, as well as the influence of coexisting nickel, iron, and cadmium ions. The obtained results demonstrated a high efficiency of lead ion removal exceeding 90 % even at a high initial lead concentration of 500 mg/L using CaO, indicating a strong precipitation capacity of the material. Enhanced removal efficiency was observed in the presence of other metal ions, reaching 92.50 % in the presence of cadmium ions and 99.99 % in the presence of iron ions. Fourier Transform Infrared (FTIR) analysis conducted before and after the precipitation process revealed characteristic bands and spectral shifts, confirming the occurrence of the precipitation mechanism. FTIR analysis performed prior to chemical precipitation revealed the presence of CO_3^{2-} vibration modes originating from the chemisorption of CO_2 on the catalyst surface, which are observed at absorption bands of 875.3, 1091.5, and 1416.45 cm^{-1}. In addition, a sharp absorption peak at 3640 cm^{-1} is attributed to the O–H stretching vibration in $Ca(OH)_2$, formed as a result of water adsorption from the atmosphere onto the CaO surface [3, 4]. These findings indicate that CaO derived from waste eggshells represents an effective, low-cost, and environmentally friendly material for the removal of lead ions from contaminated water.

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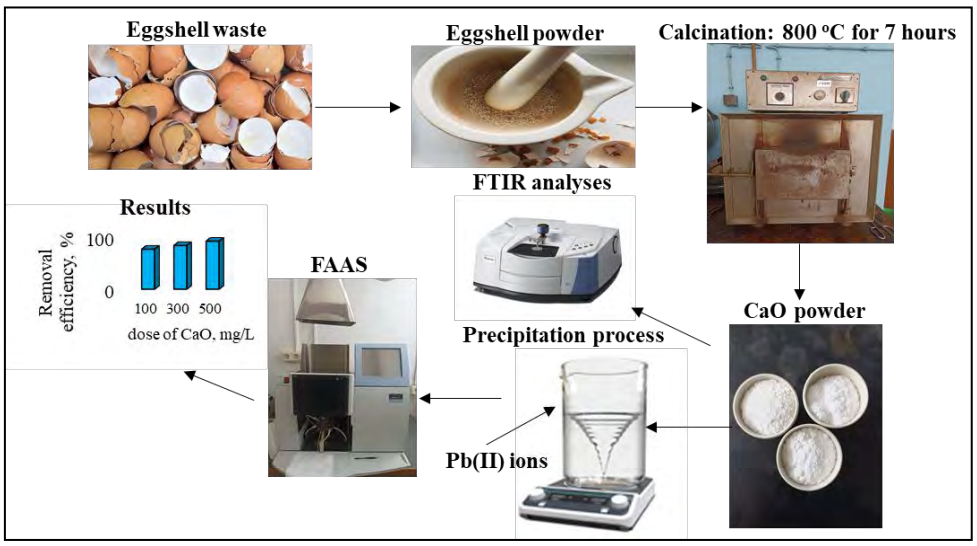

SYNTHESIS AND SPECTROSCOPIC CHARACTERIZATION OF COPPER(II) COMPLEXES WITH CHROMONE-2-CARBOXYLIC ACID

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Transition-metal complexes are of great interest due to their structural versatility and tuneable properties, making detailed characterization essential for elucidating structure-property relationships. Subtle changes in metal precursors or ligand environments can significantly affect coordination modes, stability and reactivity, which is particularly relevant for complexes derived from bioactive heterocyclic ligands [1, 2]. In this study, three Cu(II) complexes (1, 2 and 3) with chromone-2-carboxylic acid were synthesized in solution and characterized by thermogravimetric analysis (TGA), Fourier transform infrared (FTIR) and carbon-13 nuclear magnetic resonance (^{13}C NMR) spectroscopy. FTIR spectra confirm ligand deprotonation and bidentate O,O-coordination through shifts in ν(C=O) and ν(C–O), while variations in Δν(COO^-) indicate differences in coordination arising from the use of sulfate, nitrate, or acetate copper salts. TGA analyses show distinct thermal behavior: Complex 1 contains coordinated water and decomposes in multiple steps, whereas Complex 2 and Complex 3 display simpler profiles, indicating different hydration states and overall stabilities. In ^{13}C NMR spectra, strong broadening and hyperfine shifts near the metal center are consistent with Cu(II) paramagnetism, while detectable shifts of C-4 and C-9 confirm successful complexation.
Overall, the results demonstrate that even closely related synthetic conditions yield spectroscopically distinguishable complexes. Such findings provide valuable insight into how small synthetic variations influence coordination geometry and stability, contributing to a more systematic understanding of chromone-based Cu(II) chemistry.

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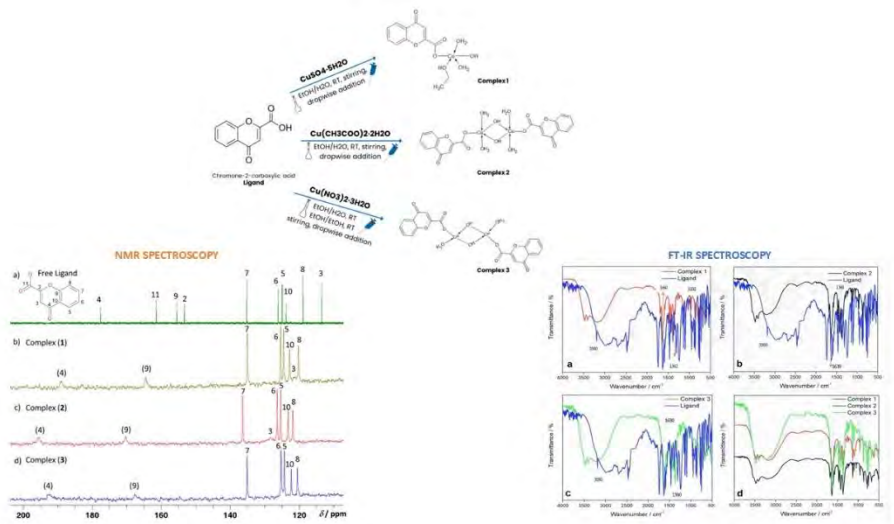

DEVELOPMENT AND VALIDATION OF AN UHPLC-MS/MS METHOD FOR THE DETERMINATION OF PHTHALATE ESTER METABOLITES IN HUMAN URINE SAMPLES

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Phthalate esters are among the most widely used plastic additives in consumer and industrial products. Within plastic materials, they are non-covalently bound to polymer chains and can therefore readily migrate into the environment [1]. Phthalates have been identified as chemicals of particular concern with respect to human health, as they may act as endocrine and metabolic disruptors. These compounds are rapidly absorbed and metabolized in the human body; consequently, the analysis of their urinary metabolites as biomarkers is considered a suitable approach for assessing internal exposure [1].

The aim of this study was to develop and validate a method for the quantitative determination of eight phthalate ester metabolites in human urine. A sample preparation procedure was developed and optimized, starting with enzymatic deconjugation of glucuronidated analytes, followed by solid-phase extraction. The prepared samples were analysed using an Agilent 1290 Infinity II UHPLC system coupled to a 6546 Q-TOF MS/MS. Successful chromatographic separation was achieved on a Kinetex phenyl-hexyl column (2.6 µm, 150 mm × 2.1 mm) using a linear solvent gradient from 90 % mobile phase A (0.1 % acetic acid in water) to 95 % mobile phase B (0.1 % acetic acid in acetonitrile).

Method performance parameters were evaluated within the concentration range of 1 to 100 ng/mL, in accordance with ICH Q2 guidelines [2], including linearity, accuracy, and precision. Limits of detection (LOD) ranged from 0.16 to 0.36 ng/mL, while limits of quantification (LOQ) ranged from 0.49 to 1.08 ng/mL. Method accuracy was improved through the use of isotopically labelled internal standards of the target analytes. To ensure reliable quantification, calibration was performed using matrix-matched standards in human urine that had been previously screened and confirmed to be free of the analytes of interest. Finally, the applicability of the method was demonstrated by analysing urine samples obtained from ten volunteer participants.

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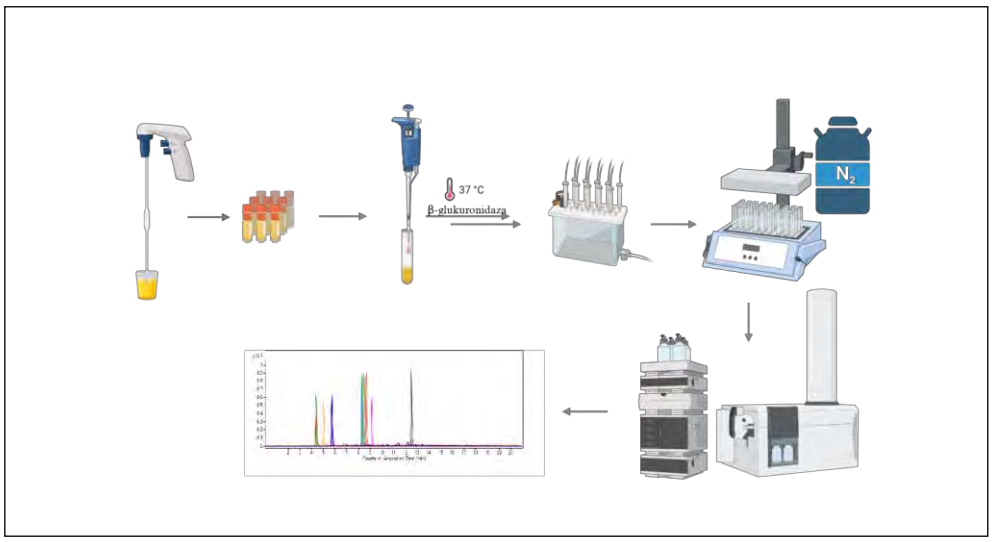

MECHANOCHEMICAL SYNTHESIS OF ZEOLITIC IMIDAZOLATE FRAMEWORKS USING STRUCTURE-DIRECTING LIQUID ADDITIVES AND THEIR ACTIVATION

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Zeolitic imidazolate frameworks (ZIFs) are a subclass of metal-organic frameworks (MOFs) [1], specific due to the fact that they are able to form numerous distinct topologies, all using tetrahedral metal atoms chained together via imidazolate linkers. The ZIF that is of interest to us is the simplest one, zinc imidazolate ($ZnIm_2$), for which at least 19 distinct topologies are known. The traditional approach to the synthesis of ZIFs using solvothermal methods often leads to polymorphic mixtures and is not preferred from the sustainable chemistry standpoint. We have therefore focused on mechanochemical methods, which show promise as a sustainable alternative for targeted preparation of desired topologies [2]. We demonstrated recently that the use of liquid additives can direct the synthetic outcome, and we showed using DFT (density functional theory) that the incorporation of additives provides a thermodynamic stabilization [3].
In this follow-up study our goal was to prepare the materials for which relative energies have been previously calculated using DFT and to attempt to activate them in order to experimentally determine the differences in enthalpy of ZIF containing and not containing solvent molecules. Synthesis was performed mechanochemically using liquid-assisted grinding (LAG), producing solvent-containing topologies. To obtain a solvent-free topology, we used vacuum-drying. The obtained products were analyzed using infrared spectroscopy (IR), powder X-ray diffraction (PXRD) and thermogravimetric analysis (TGA).

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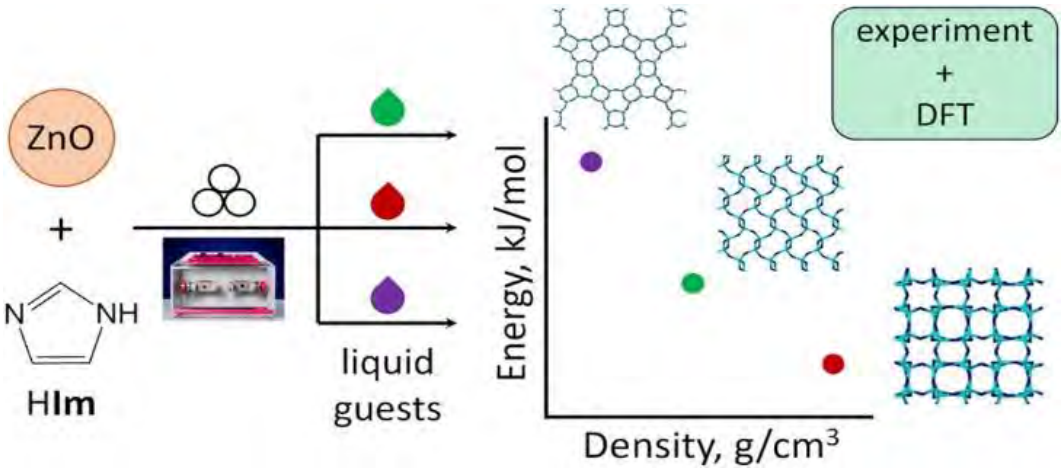

SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF NOVEL ACYLHYDRAZONE DERIVATIVES OF BENZOTHIAZOLE AND THEIR RHENIUM(I) CARBONYL COMPLEXES

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Benzothiazole and hydrazone derivatives represent important classes of heterocyclic compounds in medicinal chemistry due to their broad spectrum of biological activities and favorable structural properties [1, 2]. Benzothiazole scaffold is present in numerous bioactive molecules and marketed drugs, exhibiting antimicrobial, anti-inflammatory, antiviral, antioxidant, and antitumor effects. Hydrazones, characterized by simple synthesis and high structural versatility, show enhanced biological selectivity and reduced toxicity, and are widely applied in drug design and metal complex formation [3]. Organometallic and transition-metal complexes, particularly rhenium-based compounds, offer additional therapeutic potential owing to their structural diversity, kinetic stability, and novel mechanisms of action. The combination of heterocyclic ligands with metal centers represents a promising strategy for the development of innovative and more effective therapeutic agents.

This work describes a four-step synthesis of new acylhydrazone derivatives of benzothiazole and their rhenium(I) carbonyl complexes as potential biologically active agents, along with their structural characterization by ^{1}H and ^{13}C NMR spectroscopy and mass spectrometry. Acylhydrazone derivatives of 2-thiobenzothiazole (A) were synthesized *via* condensation reactions of prepared 2-thiobenzothiazole acetohydrazides with the corresponding benzaldehydes, yielding mixtures of *E* and *Z* isomers. Reactions of prepared benzothiazole-2-carbohydrazide with variously substituted benzaldehydes afforded 2-acylhydrazone derivatives of benzothiazole (B) as *E* isomers, whose stereochemical structures were further confirmed by NOESY experiments. The 2-acylhydrazone derivatives of benzothiazole (B) were used as ligands for the synthesis of rhenium(I) carbonyl complexes.

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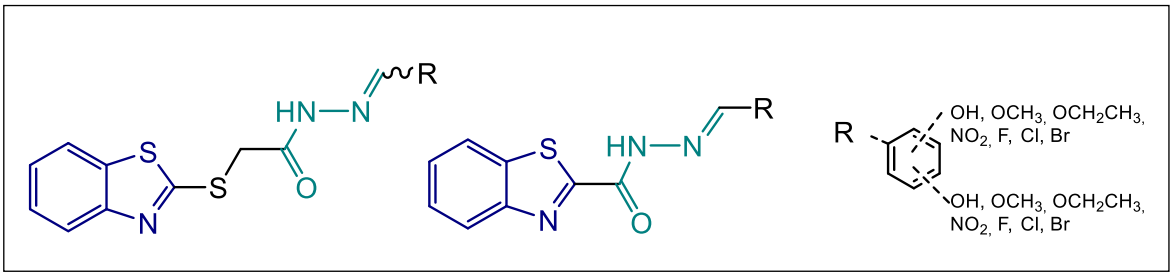
This work was supported by the institutional research project "Sustainable Synthesis, Characterization, and Complexation of Schiff Base and Hydrazone Ligands with Metals (OSKomLiMe)".



RAZGRADNJA FAVIPIRAVIRA NAPREDNIM OKSIDACIJSKIM PROCESIMA

DEGRADATION OF FAVIPIRAVIR USING ADVANCED OXIDATION PROCESSES

Ivana Mandir, Luka Večenaj, Dora Lastovčić, Viktorija Martinjak, Martina Miloloža Nikolić, Lidija Furač, Marinko Markić, Dajana Kučić Grgić, Matija Cvetnić, Tomislav Bolanča, Šime Ukić

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Onečišćenje vode predstavlja jedno od ključnih ekoloških i zdravstvenih pitanja 21. stoljeća. Među posebno zabrinjavajućim skupinama onečišćivala nalaze se farmaceutici, čija se prisutnost u površinskim i podzemnim vodama detektira u sve većem broju [1]. Favipiravir je antivirotik razvijen za liječenje gripe, a njegovo korištenje je značajno poraslo od početka pandemije COVID-19 jer je odobren od zdravstvenih institucija diljem svijeta u svrhu liječenja bolesti uzrokovane virusom SARS-CoV-2. Veliki dio ovog antivirotika završio je u sustavima otpadnih voda - bilo putem kanalizacije i uređaja za pročišćavanje, bilo direktnim ispuštanjem u površinske vode bez prethodnog tretmana [2]. S ciljem ublažavanja negativnog utjecaja farmaceutskih onečišćivala na okoliš, razvijaju se i primjenjuju napredne metode obrade voda. Među njima se posebno ističu napredni oksidacijski procesi (engl. *Advanced Oxidation Processes*, AOP), koji su visoko učinkoviti u razgradnji organskih onečišćivala [3]. Cilj ovog rada je odrediti djelotvornost naprednih oksidacijskih procesa na razgradnju favipiravira. Provedeni su procesi fotolize te fotoksidacije UV/H_2O_2 i UV/$S_2O_8^{2-}$ podešavanjem dvaju parametara, koncentracije oksidansa i početne pH-vrijednosti otopine favipiravira te se pratio njihov utjecaj na brzinu razgradnje. Metodom odzivnih površina razvijeni su matematički modeli koji opisuju i predviđaju utjecaj parametara na brzinu razgradnje favipiravira koja prati kinetiku prvog reda. ANOVA analiza potvrđuje značajnost razvijenih modela te rezultati pokazuju da se favipiravir razgrađuje pomoću sva tri procesa, no da je najveća brzina razgradnje prilikom UV/$S_2O_8^{2-}$ fotooksidacije.

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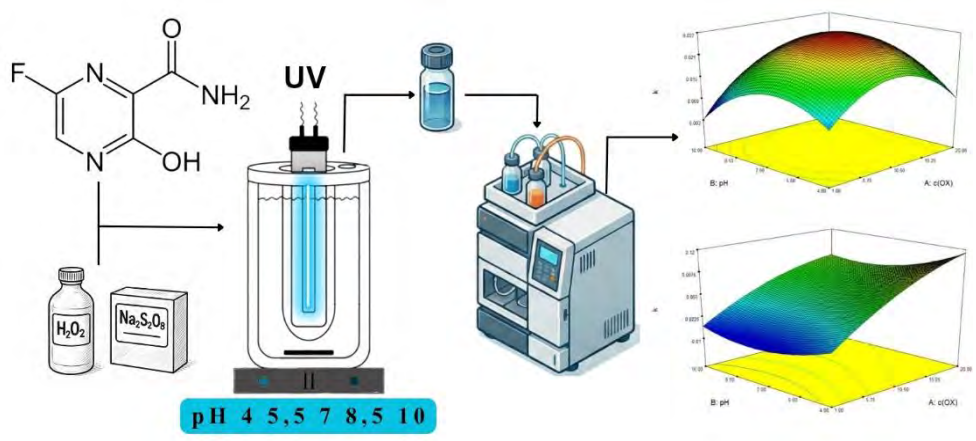
Ovo istraživanje provedeno je u sklopu projekta Okolišni aspekti SARS-CoV-2 antivirotika (EnA-SARS, IP-2022-10-2822) financiranog od strane Hrvatske zaklade za znanost.



MICROWAVE-ASSISTED SYNTHESIS OF QUATERNARY *N*-NICOTINOYLAMINO ACETAMIDE DERIVATIVES

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Alzheimer's disease (AD) is a progressive neurodegenerative disease and the leading cause of dementia worldwide. Acetylcholinesterase (AChE) and butyrylcholinesterase (BChE) inhibitors are commonly prescribed as symptomatic treatments for AD. Recently *N*-acylamino amides, more specifically nicotinamide derivatives, have been identified as cholinesterase inhibitors [1, 2]. Therefore, a *N*-nicotinoylamino acetamide was synthesised via the microwave-assisted Ugi multicomponent reaction [3] using paraformaldehyde, isobutylamine, nicotinic acid and *tert*-butyl isocyanide. The pyridine nitrogen of the nicotinamide moiety in the Ugi product was subsequently quaternized with benzyl and differently substituted benzyl bromides using microwave-assisted synthesis. The obtained products were characterised using standard analytical methods (^{1}H and ^{13}C NMR, FTIR, HRMS) and their purity was confirmed by HPLC. The inhibitory activity (IC_{50} values) of all products toward BChE isolated from horse serum was measured by Ellman method [4]. Interestingly, while the *N*-nicotinoylamino acetamide showed moderate BChE inhibition (IC_{50} = 2.1 mM), the quaternized products exhibited stronger inhibitory activity in the micromolar range and the submicromolar range.

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This work was supported by the Croatian Science Foundation under the project number HRZZ-IP 2022-10-9525.

BIOMIMETIC CHROMATOGRAPHIC INSIGHTS INTO THE PLASMA PROTEIN BINDING OF ETRASIMOD AND RITLECITINIB

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Biomimetic chromatography is an advanced analytical technique designed to simulate specific biological environments. This approach involves immobilizing key biological components, such as proteins (e.g., Human Serum Albumin, HSA), onto a stationary phase. The technique has been extensively applied in drug development to investigate the affinity, interaction mechanisms, and screening of numerous drugs and biologically active compounds [1-3]. Specifically, HSA-HPLC is a prominent example of biomimetic chromatography used to obtain crucial insights into plasma protein binding kinetics, which significantly influences drug distribution and elimination in the human body. These measurements became particularly relevant for etrasimod and ritlecitinib because both compounds represent novel oral therapies for autoimmune diseases [4, 5]. Their degree of HSA binding is critical for understanding their pharmacokinetics, potential for drug-drug interactions, and for ensuring safe and effective dosing in clinical practice.

The interaction of etrasimod and ritlecitinib with HSA was analysed using a column provided by ChromTech: Chiralpak-HSA, 50x4.6 mm, 5-µm particle size. The mobile phase consisted of 20 mM potassium phosphate buffer (pH 7.4) as phase A and i-propanol as phase B. A linear gradient from 0 to 30% i-propanol was applied from 0 to 6 min, and subsequently held at 30% i-propanol for 9 min. Detection was performed at a wavelength of 280 nm for both compounds. The HSA-HPLC method was verified using warfarin, a known HSA binder, demonstrating the successful separation of its racemate within 6 min. Retention time of etrasimod was 9.28 min (RSD = 0.81%), while ritlecitinib exhibited a retention time of 2.02 min (RSD = 0.33%). Following prior method calibration [1, 3], the HSA binding results demonstrated that etrasimod binds to HSA at a high level of 98.6%, and ritlecitinib binds at 81.4%. These high binding percentages underline the critical importance of HSA in governing the systemic exposure and free concentration of both etrasimod and ritlecitinib, which is essential for accurate clinical pharmacokinetic modeling.

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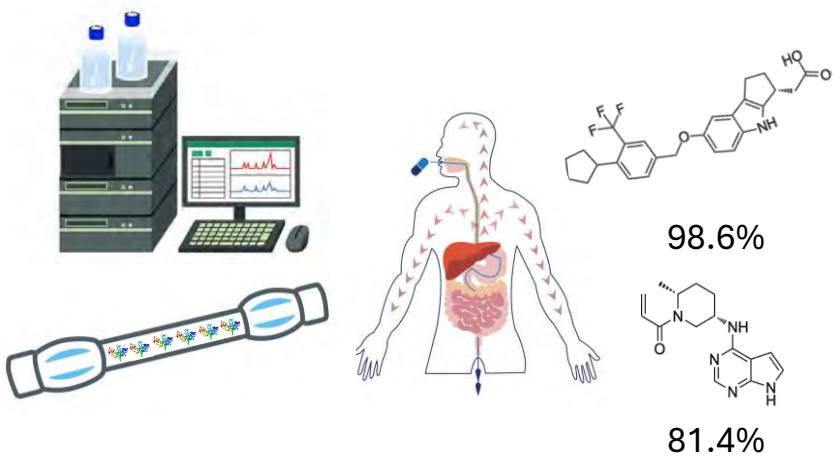

SYRINGIC ACID ADSORPTION ONTO β–GLUCAN: REACTION KINETICS AND ANTIOXIDANT ACTIVITY

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Syringic acid belongs to the group of polyphenols. It is abundant in many fruits and vegetables like olives, dates, grapes, pumpkin, but it is also present in honey and red wine. Since syringic acid showed many positive bioactivities like anti-inflammation, anticancer, antidiabetic, and antioxidant activity, its beneficial effects are important for human health [1]. Due to high bioavailability of syringic acid [1], its absorption is poor and bioactivity is low [2]. One way to increase the bioaccessibility of syringic acid is the adsorption onto dietary fiber like β-glucan from barley, where syringic acid adsorbs onto β-glucan and syringic acid–β-glucan complex occurs. β-glucan can carry syringic acid through gastrointestinal tract and possibly increase syringic acid bioacessibility. The aim of this work was to study interactions between syringic acid and β-glucan in the adsorption process in time. The kinetic models of pseudo-first and pseudo-second order were applied, and the half-reaction time was determined. Also, antioxidant activity of syringic acid and syringic acid–β-glucan complex was determined with DPPH$^{\cdot}$ method using the DPPH$^{\cdot}$ free radical. FTIR spectra were recorded for syringic acid, β-glucan and syringic acid–β-glucan complex. The results showed that syringic acid adsorbed onto β-glucan with adsorption capacity of 376 mg g^{-1}. The reaction rate constant k_1 was 2.14 h^{-1} and k_2 was 0.0074 g mg^{-1} h^{-1}. The half-reaction time for pseudo-first order was 0.32 h, and for pseudo-second order 0.54 h. Syringic acid–β-glucan complex showed higher antioxidant activity (88 % DPPH$^{\cdot}$ inhibition) than syringic acid (54 % DPPH$^{\cdot}$ inhibition). The FTIR spectrum showed that syringic acid adsorbed onto β-glucan. These results can be helpful for biomedical application of syringic acid and to increase its bioavailability.

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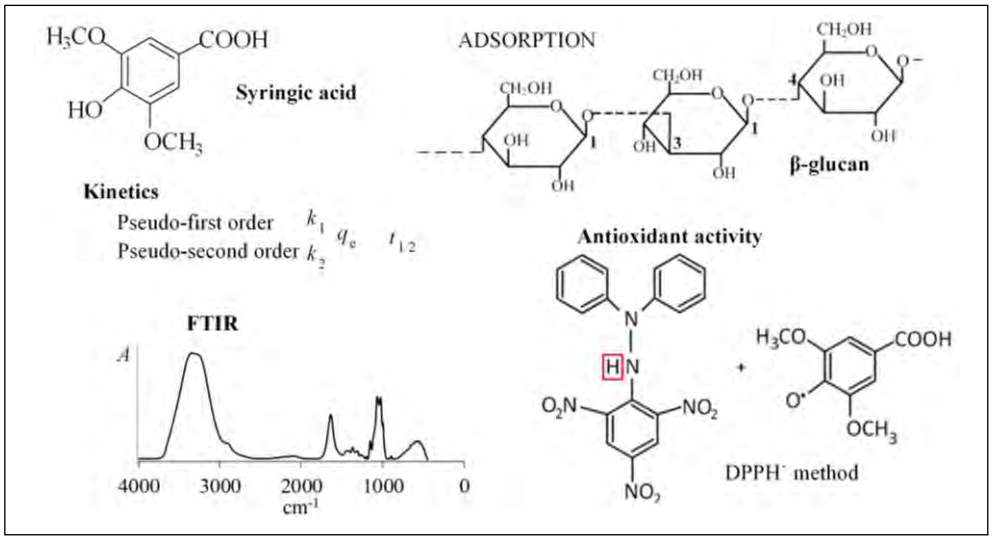

ADSORPCIJSKA SVOJSTVA DERIVATA POLI(4-VINILPIRIDINA) ADSORBIRANIH NA POVRŠINU NANOPLOČICA KVARCA

ADSORPTION PROPERTIES OF POLY(4-VINYLPYRIDINE) DERIVATIVES ADSORBED ON THE SURFACE OF QUARTZ NANOPLATES

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Polielektroliti, kao polimerni spojevi s ionizabilnim funkcijskim skupinama, pokazuju sposobnost adsorpcije na površine nanočestica putem elektrostatskih i neelektrostatskih interakcija [1]. U ovom su radu istražena adsorpcijska svojstva različitih derivata poli(4-vinilpiridina) adsorbiranih na površinu nanopločica kvarca s ciljem razumijevanja uloge strukture monomera u procesu adsorpcije. U te svrhe sintetizirana su tri *N*-alkilirana derivata poli(4-vinilpiridina) različitih duljina alkilnih lanaca kako bi se usporedila njihova adsorpcijska svojstva. Dobiveni spojevi okarakterizirani su spektroskopijom NMR, IR-spektroskopijom, termogravimetrijskom analizom te potenciometrijskom titracijom s bromidnom ion-selektivnom elektrodom. Nakon karakterizacije polielektrolita, nanopločice kvarca okarakterizirane su transmisijskom elektronskom mikroskopijom i elektroforetskim raspršenjem svjetlosti, a određena je i njihova specifična površina. Adsorpcijski eksperimenti provedeni su na kvarcnim nanopločicama pod kontroliranim uvjetima. Rezultati, analizirani UV–Vis spektroskopijom, obrađeni su korištenjem Hesselinkovog modela [2]. Pokazano je da derivati s kraćim alkilnim supstituentom na monomernoj jedinici pokazuju veću adsorpcijsku sposobnost u usporedbi s derivatima s duljim alkilnim supstituentom. Time je potvrđeno da hidrofobnost polimera i sterički učinci bočnih alkilnih lanaca imaju ključnu ulogu u procesu adsorpcije. Provedene su i molekulskodinamičke simulacije koje su pružile uvid u prostorne konfiguracije polielektrolita u blizini kvarcne površine te stabilnost adsorbiranih slojeva. Analiza simulacijskih trajektorija pokazala je da gustoća naboja i struktura polimernih lanaca izravno utječu na adsorpciju te na ravnotežu između elektrostatskih privlačnih sila i repulzije među segmentima lanca.

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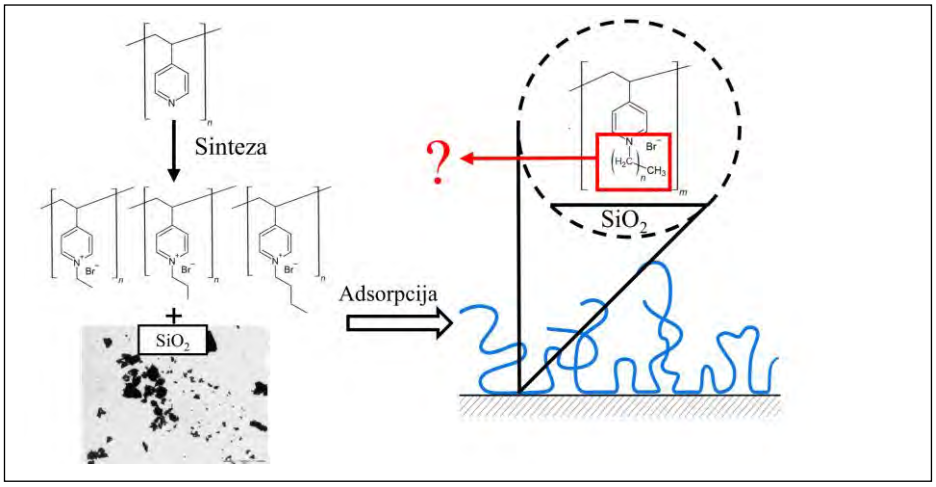
Ovo istraživanje financijski je podržala Hrvatska zaklada za znanost u okviru projekta POLYMIN2 (IP-2020-02-9571).



SYNTHESIS OF NEW 1,2,3-TRIAZOLE DERIVATIVES OF COUMARIN BY CONVENTIONAL AND SUSTAINABLE MECHANOCHEMICAL SYNTHESIS

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Coumarin represents a privileged scaffold within the benzopyrone class, consisting of a benzene ring fused to a pyrone ring, and serves as the structural core of many natural products. The synthesis of coumarin and its derivatives has attracted significant attention from both organic and medicinal chemists due to their versatile pharmacological activity, such as anti-inflammatory, antioxidant, antimicrobial, antiviral, and antiprolifrative effects [1]. Furthermore, 1,2,3-triazole ring has emerged as an important structural motif in medicinal chemistry due to its remarkable properties including moderate dipole character, hydrogen-bonding capability, resistance to metabolic degradation, and stability under *in vivo* conditions. Thus, the role of heterocyclic compounds has become increasingly important in the design of new biologically active structural entities [2]. In this study, 1,2,3-triazole derivatives of coumarin were prepared *via* a two-step reaction pathway using both conventional and mechanochemical approaches, with the aim of evaluating their antibacterial, antiviral, and antitumor activity. First, 4-*O*-propargylcoumarin and 7-*O*-propargylcoumarin were prepared using propargyl bromide as the alkylation reagent under basic conditions. These intermediates were then converted, both conventionally and mechanochemically, into the corresponding 1,2,3-triazole-substituted coumarins *via* a copper-catalyzed click-reaction with previously prepared azides. The mechanochemical method proved to be more effective than the conventional approach in the synthesis of 7-(1,2,3-triazolyl)coumarin derivatives compared to the 4-(1,2,3-triazolyl)coumarin derivatives. Due to its reduced solvent requirements and shorter reaction times, mechanochemical approach can be extended to the synthesis of related compound classes and can be regarded as a greener alternative to traditional solution-based protocols. Structural characterization of all synthesized compounds was carried out by ^{1}H- and ^{13}C-NMR spectroscopy, and the compounds were subjected to antibacterial, antiviral and antitumor evaluations.

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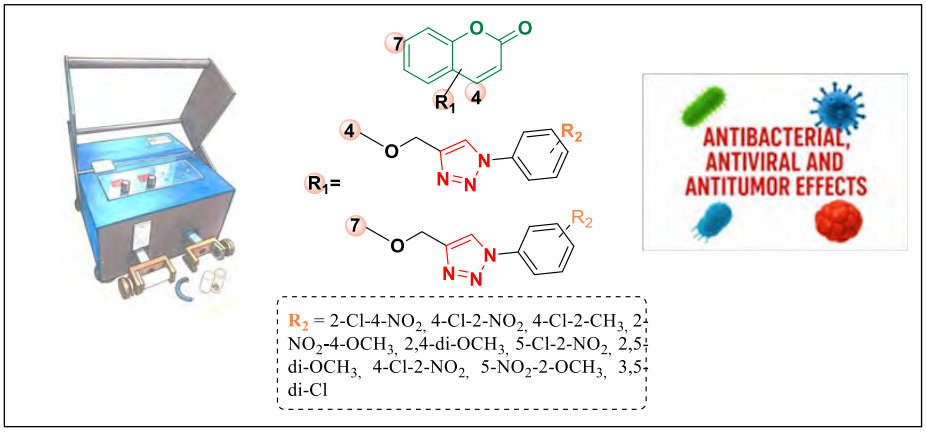
This work was supported by the Croatian Science Foundation under the project HRZZ-IP-2022-10-9420.



MORFOLINSKI I PIROLIDINSKI KARBAMATI U BORBI PROTIV NEURODEGENERATIVNIH POREMEĆAJA

MORPHOLINE AND PYRROLIDINE CARBAMATES IN THE FIGHT AGAINST NEURODEGENERATIVE DISORDERS

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Alzheimerova bolest najčešći je oblik demencije, obilježena progresivnim gubitkom kognitivnih funkcija te patološkim procesima kao što su nakupljanje β-amiloidnih plakova, hiperfosforilacija τ-proteina, oksidativni stres i neuroinflamacija [1]. Ključnu ulogu u razvoju simptoma ima i narušena kolinergička neurotransmisija, pri čemu porast aktivnosti butirilkolinesteraze u kasnijim stadijima bolesti čini taj enzim važnom terapijskom metom [2]. Karbamati su pritom posebno zanimljivi jer ostvaruju reverzibilnu kovalentnu inhibiciju putem karbamilacije katalitičke serinske skupine, omogućujući produljeno i kontrolirano farmakološko djelovanje [3]. Prethodna istraživanja u našem laboratoriju pokazala su da morfolinski karbamatni derivati ostvaruju najselektivniju inhibiciju butirilkolinesteraze zahvaljujući snažnim interakcijama unutar aktivnog mjesta, osobito s aromatskim i hidrofobnim ostacima [4]. Cilj ovog istraživanja jest nadogradnja najaktivnijih morfolinskih derivata uvođenjem dodatnih nabijenih heterocikličkih fragmenata koji sadrže dušik, pri čemu se dodatno razmatraju i pirolidinski karbamati zbog općenito povoljnijeg inhibicijskog profila heterocikličkih u odnosu na acikličke karbamate. Time se nastoji povećati broj mogućih elektrostatskih, vodikovih, π–π i dipolnih interakcija unutar aktivnog mjesta butirilkolinesteraze te potencijalno ojačati i sama kovalentna karbamilacija. Poseban je naglasak stavljen na dizajn derivata koji omogućuju dublje vezanje u katalitičkoj šupljini i povoljnije interakcije s perifernim anionskim mjestom, čime se može povećati afinitet i produljiti inhibicija. Dodatna funkcionalizacija ovih derivata u obliku soli razmatra se radi povećanja njihove hidrofilnosti i farmakokinetičke stabilnosti, čime bi se mogla unaprijediti apsorpcija i ukupna bioraspoloživost u biološkom sustavu. Sinteza i spektroskopska karakterizacija novih derivata nadopunit će se molekulskim modeliranjem radi identifikacije ključnih strukturnih elemenata koji određuju selektivnost i potentnost. Očekuje se da će ovako dizajnirani spojevi predstavljati perspektivne kandidate za daljnji razvoj selektivnih inhibitora butirilkolinesteraze u terapijskom pristupu Alzheimerovoj bolesti.

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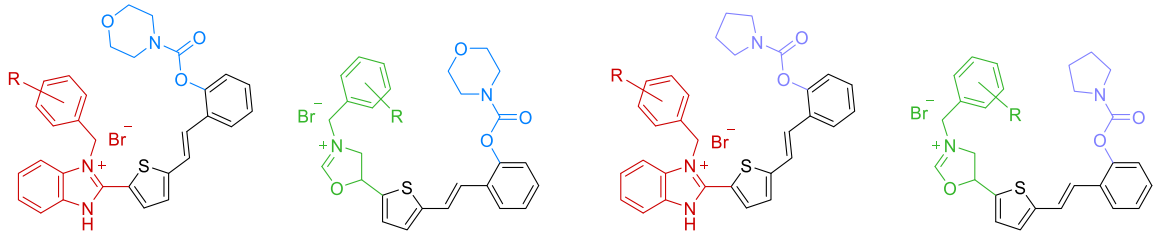

PROCJENA ZELENOSTI I PRAKTIČNOSTI NOVE KAPILARNOELEKTROFORETSKE METODE ZA ODREĐIVANJE TALAZOPARIBA U LJEKOVITOM OBLIKU I USPOREDBA S HPLC METODOM

GREENNESS AND PRACTICALITY ASSESSMENT OF A NEW CAPILLARY ELECTROPHORESIS METHOD FOR THE DETERMINATION OF TALAZOPARIB IN A DOSAGE FORM AND COMPARISON WITH HPLC METHOD

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Talazoparib je inhibitor enzima poli (ADP-riboza) polimeraze (PARP). Indiciran je u liječenju uznapredovalog ili metastatskog HER2-negativnog karcinoma dojke kod odraslih pacijenata s mutacijama *BRCA1/2* gena. U nedostatku farmakopejskih monografija, važno je razvijati praktične i održive metode za određivanje novih lijekova u farmaceutskim oblicima. Razvijena je i validirana nova kapilarnoelektroforetska (CE) metoda za određivanje talazopariba u kapsulama. Dodatno je razvijena i HPLC metoda radi usporedbe s CE metodom. U ovom su istraživanju pomoću metrika AGREE [1], BAGI [2] i RGB-12 [3] procijenjeni zelenost, praktičnost i bjelina (cjelokupna izvedba) ranije razvijenih CE i HPLC metoda. Zelenost je procijenjena AGREE softverom uzimajući u obzir 12 principa zelene analitičke kemije. U usporedbi s HPLC-om, CE metoda stvara manje količine analitičkog otpada, ima manju potrošnju energije te smanjuje uporabu toksičnih reagensa. Samim time, ostvarila je bolji AGREE rezultat u odnosu na HPLC metodu (0,72 naspram 0,52). Praktičnost koja je povezana s jednostavnošću te vremenskom i troškovnom učinkovitošću, procijenjena je BAGI softverom. Obje metode pokazale su sličnu praktičnost, s tim da je CE metoda ostvarila za nijansu bolji BAGI rezultat (65,0 naspram 62,5) s obzirom na kraće trajanje analize. RGB-12 indeks korišten je za cjelokupnu procjenu metoda, uzimajući u obzir analitičke i ekološke parametre te praktičnost. U skladu s ranijim procjenama, CE metoda pokazala je bolje ekološke karakteristike te sličnu praktičnost. Analitički parametri poput linearnosti, točnosti i preciznosti bili su usporedivi za obje metode. Ukupni RGB-12 indeks bio je veći za CE metodu (87,1 naspram 82,9 za HPLC metodu) primarno zbog njezinih boljih ekoloških svojstava u odnosu na HPLC. Rezultati provedenog istraživanja ukazuju na potencijal razvijene CE metode kao zelene i održive opcije za određivanje talazopariba u ljekovitom obliku.

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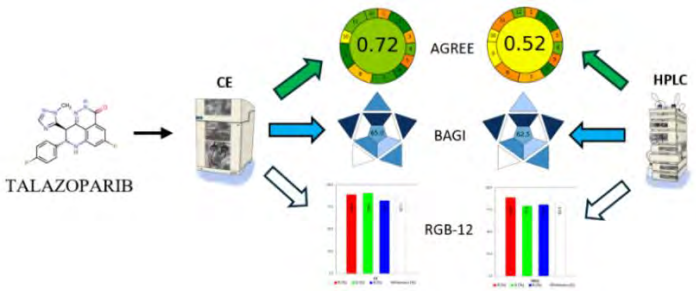
Ovo istraživanje je financirano sredstvima projekata Nova bioanalitička rješenja za personalizaciju terapije raka dojke (UIP-2019-04-8461) i Razvoj zelenih analitičkih metoda za otkrivanje čimbenika interindividualne farmakokinetičke varijabilnosti ciljanih antitumorskih lijekova (IP-2025-02-1882) Hrvatske zaklade za znanost i sufinanciran sredstvima Europske unije iz Europskog fonda za regionalni razvoj projektom FarmInova (KK.01.1.1.02.0021).



UTJECAJ MEMBRANSKIH PROCESA NA SMANJENJE EKOTOKSIČNOSTI KSENOBIOTIKA

THE INFUENCE OF MEMBRANE PROCESSES ON REDUCING THE ECOTOXICITY OF XENOBIOTICS

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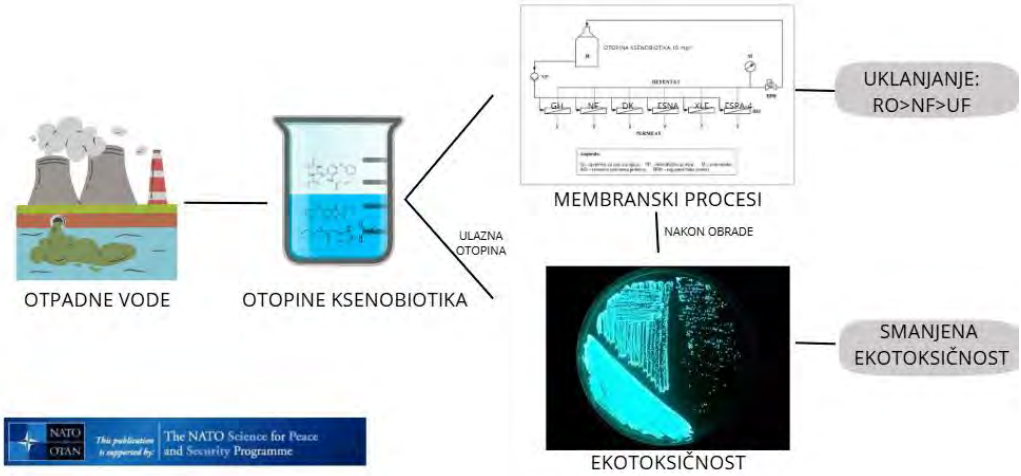
Antiparazitski lijekovi sve se češće detektiraju u vodnom okolišu zbog svoje postojanosti, slabe topljivosti i potencijala za bioakumulaciju. Njihova široka primjena u humanoj i veterinarskoj medicini rezultira dospijevanjem u otpadne vode, gdje konvencionalni sustavi obrade često ne osiguravaju učinkovito uklanjanje. U ovom radu ispitana je učinkovitost membranskih procesa, ultrafiltracije (UF), nanofiltracije (NF) i reverzne osmoze (RO), u uklanjanju triju odabranih antiparazitika: albendazola, mebendazola i febantela. Učinkovitost zadržavanja određena je u demineraliziranoj i modelnoj vodi, dok je ekotoksičnost prije i nakon tretmana procijenjena pomoću bakterije *Vibrio fischeri*. Dobiveni rezultati pokazuju da RO i NF membrane postižu najviša zadržavanja ispitivanih spojeva te značajno smanjuju ekotoksičnost uzoraka. Nadalje, rezultati daju uvid u mogućnost uklanjanja tvari membranskim tehnologijama i pružaju informacije o mogućim rizicima za okoliš i prirodne vodne sustave prilikom njihovog ispuštanja.

This research was funded by the NATO Science for Peace and Security Programme under grant id. G6087.



VIŠEKOMPONENTNI 1D KOORDINACIJSKI POLIMER BAKRA(II) SA SARKOZINOM I DERIVATOM BIPIRIDINA: STRUKTURA, TERMIČKA I SPEKTROSKOPSKA ANALIZA

MULTICOMPONENT 1D COPPER(II) COORDINATION POLYMER WITH SARCOSINE AND BIPYRIDINE DERIVATIVE: STRUCTURAL, THERMAL AND SPECTROSCOPIC ANALYSIS

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Porozni metaloorganski spojevi se intenzivno istražuju i postaju sve značajniji zbog svoje raznolike primjene u adsorpciji, katalizi, kiralnoj separaciji i sakupljanju vode [1,2]. Ovogodišnja Nobelova nagrada dodijeljena je upravo za istraživanje poroznih metaloorganskih mreža [3]. Višekomponentni metaloorganski polimeri sastavljeni su od dva ili više različitih organskih linkera, što omogućuje veću strukturnu složenost i širi raspon funkcionalnih svojstava. Cilj našeg istraživanja je priprema koordinacijskih spojeva koji se potencijalno mogu koristiti kao sakupljači atmosferske vode. Sakupljači vode su obećavajuće rješenje globalnog problema nedostatka pitke vode, koji trenutno pogađa jednu četvrtinu ljudi diljem svijeta [4]. Višekomponentni 1D koordinacijski polimer bakra(II) sa sarkozinom (HSar) i 1,2-bis(piridin-4-il)etanom (bpa) pripremljen je otopinskom sintezom i mehanokemijskim putem: $\{[Cu_4(NO_3)_2(Sar)_4(bpa)_4](NO_3)_2{\cdot}xH_2O\}_n$. Analiziran je rendgenskom difrakcijom na jediničnom kristalu i polikristalnom uzorku, FTIR spektroskopijom i termogravimetrijskom analizom. Kristalna struktura otkriva da je spoj 1D polimer te da sadrži molekule vode u džepovima. Spoj je pokazao stabilnost na sobnoj temperaturi i sobnoj vlažnosti zraka, ali se razgradio u suhom okruženju, što pokazuje njegov potencijal za kontroliranu adsorpciju i desorpciju vode.

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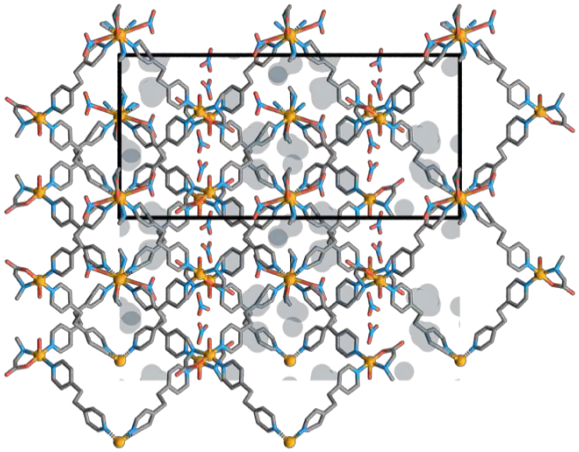

SYNTHESIS AND PHOTOCHEMISTRY OF CYANO-AMINOBIPHENYL PHOTOCAGES

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Photoremovable protecting groups (PPGs) represent a special class of protecting groups that can be removed in photochemical reactions. [1] The primary advantage of PPGs is the use of light as a reagent, which enables precise spatial and temporal control, thereby allowing selective activation of target molecules. Consequently, PPGs are widely employed across various research fields, for instance in studies investigating the roles of biologically active molecules in physiological processes. [2] In such applications, bioactive molecules are temporarily rendered inactive by the attachment of a PPG, and their activity is restored upon photochemical removal of the protecting group.
In our research group, the synthesis and photoreactivity of aminonaphthalene [3-5] and aminobiphenyl [6] photocages have been systematically investigated. These PPGs demonstrated excellent performance in the decaging of carboxylic acids, with aminobiphenyl derivatives exhibiting higher release efficiencies (Φ_R = 0.04 – 0.37) than aminonaphthalenes (Φ_R = 0.01 – 0.22). In an effort to extend the absorption wavelength range, we developed novel cyano-substituted aminobiphenyl derivatives as potential photocages for carboxylic acids and alcohols. The cyano-substituted aminobiphenyl derivatives were synthesized using standard organic synthetic methodologies through multistep sequences involving reactions such as bromination, alkylation, Suzuki-Miyaura cross-coupling, acetylation and Williamson ether synthesis. Following the synthesis, the photochemical reactivity of the resulting photocages (ethers and esters) was examined in an aqueous medium.

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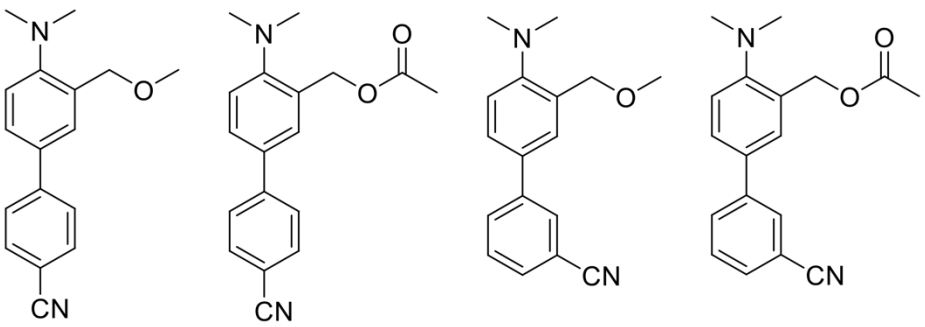

VOLTAMMETRY OF CAFFEINE

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Caffeine is a purine alkaloid and one of the most widely distributed biologically active compounds globally, with applications in the food, pharmaceutical, and cosmetic industries. Due to its significant psychoactive, diuretic, and stimulative effects, caffeine has been the subject of numerous studies aiming to understand its activity and reaction mechanisms in different environments. [1,2] One approach that has recently attracted increasing attention is electrochemical analysis using voltammetric techniques, which enable precise monitoring of redox processes and investigation of reaction kinetics and mechanisms.

In this study, the electrochemical oxidation of caffeine was investigated using cyclic voltammetry (CV) and square-wave voltammetry (SWV). The experiments were performed in acetate and phosphate buffer solutions across a broad pH range (acidic, neutral, and alkaline media), in order to examine the influence of the medium on the oxidative properties of caffeine. Moreover, the oxidation potential was found to shift systematically with changes in pH, indicating a clear dependence on the proton availability in the medium. The pH-dependent behavior suggests the involvement of proton-coupled electron transfer mechanisms. Both CV and SWV demonstrated high sensitivity and reproducibility for caffeine detection, highlighting their suitability as analytical tools. These findings contribute valuable insights into the redox kinetics of caffeine and enhance the understanding its electrochemical response under different environmental conditions. [3]

This work, complemented by a review of relevant scientific literature, provides a foundation for further research and opens possibilities for the application of electrochemical methods in the qualitative and quantitative analysis of caffeine.

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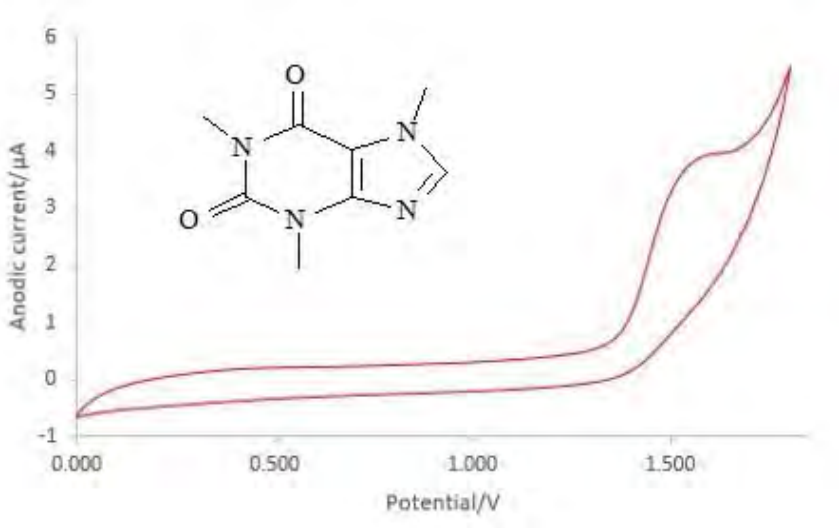

SPECTROPHOTOMETRIC ANALYSIS OF DEUCRAVACITINIB CONTENT IN TABLETS: A VALIDATED AND REPRODUCIBLE METHOD FOR ROUTINE QUALITY CONTROL

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Deucravacitinib, a selective oral allosteric inhibitor of tyrosine kinase 2 (TYK2), has been approved for the treatment of moderate to severe plaque psoriasis in adults. In Croatia, it was registered in April 2025 as a 6 mg tablet with once a day administration. Owing to its therapeutic relevance and the need for reliable quantification in pharmaceutical products, the aim of this study was to develop and validate a UV–Vis spectrophotometric method for the determination of deucravacitinib in tablet dosage form.

The analysis was carried out using a Lambda 25 UV–Vis spectrophotometer. A full spectral scan from 200 to 800 nm was obtained, and quantification was performed at 250 nm. Method validation followed International Council for Harmonisation guidelines (ICH Q2(R2)). [1]

The calibration curve demonstrated excellent linearity across the concentration range of 1–14 µg/mL (r = 0.9996). The limit of detection (LOD) and the limit of quantification (LOQ) were 0.30 µg/mL and 0.92 µg/mL, respectively. Accuracy, evaluated via recovery studies at 1, 8 and 14 µg/mL, yielded recoveries of 101.91%, 101.86% and 100.52%, with relative standard deviations (RSDs) below 0.5%. Precision was confirmed through intraday and interday analyses (n = 6) at the same concentration levels, producing RSD values between 0.03% and 0.05%. Interday reproducibility assessed over three consecutive days resulted in RSDs of 1.13%, 1.07% and 1.35%. Robustness was established by introducing small variations in analytical conditions, including wavelength adjustments (±2 nm; RSD < 0.03%), pH changes (4.5 and 8.5; RSD < 0.02%) and cuvette volume modification (0.75 mL; RSD < 0.04%). Assay of the tablet extract yielded a content of 101.24% (RSD = 0.15%, *n* = 3).

In conclusion, the developed UV–Vis spectrophotometric method is accurate, precise, and robust, and is therefore suitable for routine quality control analysis of deucravacitinib in tablet dosage form.

[1] ICH Q2(R2) Guideline on Validation of Analytical Procedures, Current Step 5 version, June 2024

Deucravacitinib

UV–Vis spectrophotometer

Parameter	Concentration / Condition	Result	RSD (%)
Linearity	1–14 µg/mL	r = 0.9996	
LOD		0.30 µg/mL	
LOQ		0.92 µg/mL	
Accuracy (Recovery)	1 µg/mL	101.91%	<0.5
	8 µg/mL	101.86%	
	14 µg/mL	100.52%	
Precision	Intraday (n=6)		0.03–0.05
	Interday (n=6)		
Robustness	Wavelength ±2 nm		<0.03
	pH 4.5 & 8.5		<0.02
	Cuvette volume 0.75 mL		<0.04

MICROWAVE-ASSISTED SOLUTION-PHASE SYNTHESIS OF DESMURAMYL PEPTIDES

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Desmuramyl-peptide (DMP) is an analogue of muramyl dipeptide (MDP, *N*-acetylmuramyl-L-alanyl-D-*iso*glutamine) without the *N*-acetylmuramyl group. MDP is a peptidoglycan fragment which acts as an immunomodulator or adjuvant by activating the innate immune system through the NOD2 receptor. Since the muramyl group isn't essential for inducing this response, structurally simplified DMP analogues can be designed with improved immunostimulating properties [1]. Thus, it has been shown that lipophilic, as well as mannosylated DMP analogues showed improved immunostimulant properties when tested *in vivo* [1, 2]. Solution-phase peptide synthesis is usually method of choice for the preparation of peptide part, with coupling reaction times ranging from 24 to 48 h. Microwave (MW) irradiation has shown to be incredibly useful in solid-phase peptide synthesis (SPPS) and can significantly cut down on reaction time and increase coupling efficiency, however, there aren't many examples of MW solution-phase peptide synthesis protocols [3]. Herein, a method for MW solution-phase synthesis of DMP analogues has been developed. Standard solution-phase peptide coupling methods have been explored in MW conditions. The MW method was optimized with respect to quantities of reagents used and choice of solvent, reaction time, temperature and power. The protocol outlined in the graphical abstract resulted in an excellent yield and purity of **5**. Additionally, methods for MW synthesis of DMP precursor D-Glu(OBn)-OH, as well as Val and Ile DMP analogues have also been developed here with good yield. A MW Boc deprotection method has also been attempted with very good yield [4]. Therefore, the coupling time and efficiency for synthesis of dipeptide **5**, as well as its precursor **2**, and deprotection of **5** has been improved significantly over the classical solution-phase peptide coupling methods [2]. A method for MW coupling of **5** with Boc-Phe-OH to yield tripeptide **7** is currently in development.

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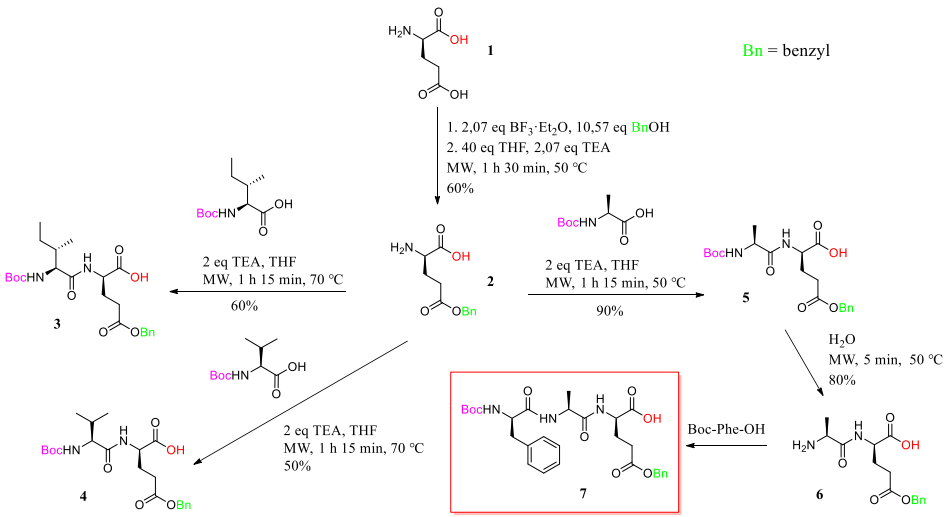
This work has been fully supported by Croatian Science Foundation under the project IP-2025-02-5568.



RAZGRADNJA OSELTAMIVIRA NAPREDNIM OKSIDACIJSKIM PROCESIMA

DEGRADATION OF OSELTAMIVIR BY ADVANCED OXIDATION PROCESSES

Dunja Pavlović, Luka Večenaj, Dora Lastovčić, Viktorija Martinjak, Martina Miloloža Nikolić, Lidija Furač, Marinko Markić, Dajana Kučić Grgić, Matija Cvetnić, Tomislav Bolanča, Šime Ukić

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Antivirusni lijekovi, kao i drugi farmaceutski aktivni spojevi, sve su prisutniji u vodenom okolišu te predstavljaju rastući ekotoksikološki problem. Antivirotici i njihovi metaboliti kontinuirano dospijevaju u vodene sustave putem ispusta uređaja za pročišćavanje otpadnih voda, koji često ne omogućuju njihovo potpuno uklanjanje. Među njima se posebno izdvaja oseltamivir, aktivni metabolit lijeka Tamiflu®, široko korištenog inhibitora neuraminidaze za liječenje infekcija virusom influence A. Tijekom pandemije COVID-19 Tamiflu® se primjenjivao u kombinaciji s drugim lijekovima u nizu kliničkih ispitivanja provedenih na bolesnicima zaraženima SARS-CoV-2 virusom. Istraživanja su pokazala kako oseltamivir pospješuje brži oporavaka kod pacijenata zaraženih ovim virusom. Zbog povećane primjene tijekom pandemije i njegove stabilnosti u okolišu, oseltamivir se sve više detektira u površinskim vodama.[1,2] Konvencionalni sustavi obrade, poput filtracije u kombinaciji s biološkim procesima, često nisu dovoljni za uklanjanje farmaceutskih onečišćujućih tvari te mogu pridonijeti razvoju mikrobne rezistencije. Stoga se sve više pozornosti usmjerava na napredne oksidacijske procese, koji se izdvajaju kao izrazito učinkovite metode za razgradnju toksičnih i teško razgradivih spojeva u vodenim matricama. [3] Cilj ovog istraživanja bio je procijeniti učinkovitost različitih naprednih oksidacijskih procesa u uklanjanju oseltamivira iz vodenih otopina. Provedeni su pokusi UV-fotolize te fotooksidacije u sustavima UV/H_2O_2 i UV/$S_2O_8^{2-}$, pri čemu su sustavno mijenjani početna pH-vrijednost i koncentracija oksidansa. Dobiveni kinetički podaci upućuju na to da svi ispitivani procesi rezultiraju razgradnjom oseltamivira te da slijede kinetiku pseudo-prvog reda. Metodom odzivnih površina razvijeni su prediktivni modeli koji opisuju utjecaj operativnih parametara na brzinu razgradnje, a njihova je statistička značajnost potvrđena ANOVA analizom.

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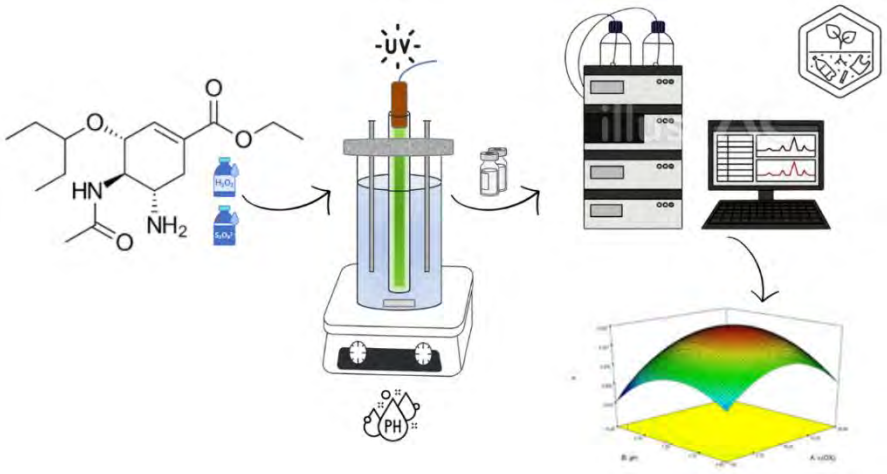
Ovo istraživanje provedeno je u sklopu projekta Okolišni aspekti SARS-CoV-2 antivirotika (EnA-SARS, IP-2022-10-2822) financiranog od strane Hrvatske zaklade za znanost.



SYNTHESIS AND SPECTROSCOPIC CHARACTERIZATION OF NEW BENZOXAZOLE DERIVATIVES AS POTENTIAL pH SENSORS IN SOLUTIONS

Iva Pinušić[1], Ela Gašparić[1], Marina Galić[1], Robert Vianello[2], Marijana Hranjec[1]

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Heterocyclic compounds with pronounced spectroscopic characteristics occupy an important place in modern research in organic chemistry. The development of small functional structures is particularly important for (chemo)sensor and optoelectronic systems, so their synthesis and rational design is at the centre of many current researches [1]. The benzoxazole core represents a highly relevant structural motif in medicinal chemistry, largely due to the broad spectrum of biological and pharmacological activities exhibited by its derivatives. Moreover, benzoxazole serves as a versatile synthetic platform for accessing structurally diverse bioactive compounds [2]. Since pH represents an essential biomarker for assessing mitochondrial function and the cellular microenvironment, its precise determination is important in a wide range of biological, technological and environmental processes, including living cell viability, industrial production, environmental monitoring and safety control of water, food and air [3]. Iminocoumarine and benzamide derivatives are known for their interesting spectroscopic properties as well as their application as fluorescent sensors [4,5].
This work presents the synthesis and spectroscopic characterization of iminocoumarine and benzamide derived benzoxazoles. The structures of newly prepared compounds were confirmed by means of ^{1}H and ^{13}C NMR spectroscopy as well as 2D NOESY NMR spectroscopy. Additionally, spectroscopic characterization and pH spectroscopic titrations were performed in order to determine possible application of chosen compounds as pH sensors in solutions followed by determination of p*K*a values.

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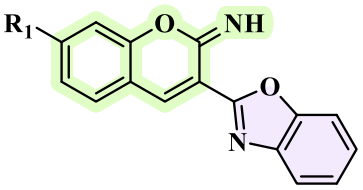
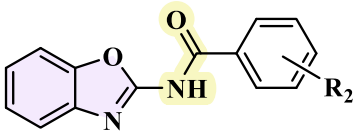
The Croatian Science Foundation funded this work (projects BenzpHSens HRZZ-IP-2020-02-8090 and BenzHetPot IP-2024-05-7208).



R_1= H, OH, -*N*,*N*-$(CHCH_3)_2$



R_2= H, NH_2, -*N*,*N*-$(CH_3)_2$, 2,4-diOCH_3, 2-OCH_3-4-OH

SYNTHESIS AND SPECTROSCOPIC CHARACTERIZATION OF BIOLOGICALLY ACTIVE BENZOXAZOLE DERIVATIVES

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Heterocycles represent one of the most significant classes of compounds within organic and medicinal chemistry. Owing to their structural flexibility and ability to participate in diverse biological interactions, benzoxazole frameworks are considered highly valuable motifs in drug discovery [1]. As a structural analog of the nucleobases adenine and guanine, benzoxazole stands out as an important nitrogen-containing heterocycle. Namely, benzoxazole interactions with macromolecules such as DNA, RNA or proteins are commonly attributed to the bioisosterism with the naturally occurring nucleotides [2,3]. The present heteroatoms enable the realization of non-covalent interactions important in rational drug design. Benzoxazole-based derivatives display a broad range of biological effects, including antitumor, antimicrobial, antiviral, and antioxidant activities [1,2].

This work presents the synthesis, spectroscopic characterization and biological evaluation of novel benzoxazole compounds. The synthesis of the main precursors of 2-arylbenzoxazoles was carried out by microwave-assisted cyclocondensation from differently substituted *ortho*-aminophenols and benzoyl chlorides. The 2-arylbenzoxazoles were used as precursors in organometallic Suzuki-Miyaura cross-coupling reactions, with the aim of obtaining more complex conjugates. They were also used as precursors in microwave-assisted amination reactions with various amines. The structures of the newly prepared compounds were confirmed by means of ^{1}H and ^{13}C NMR spectroscopy and well as MS spectrometry. Antiproliferative activity *in vitro* of prepared compounds was tested against several human cancer cells.

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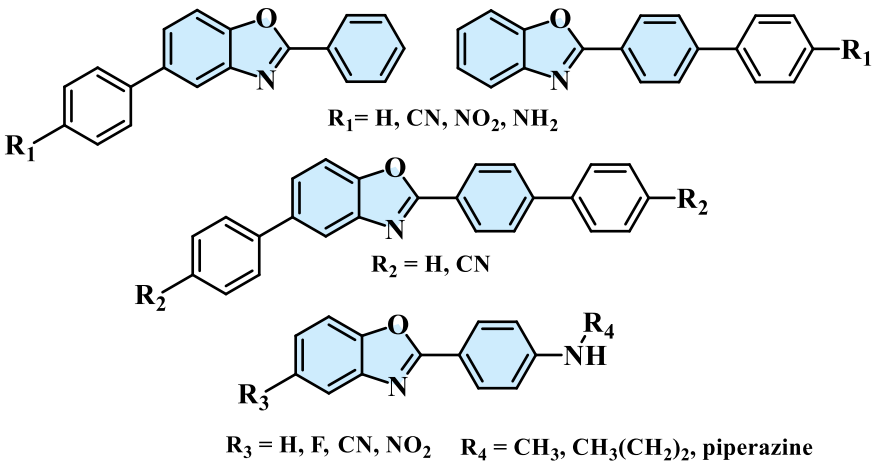
[2] S. Di Martino et al., Top. Curr. Chem. 382 (2024) 33.
[3] Galić et al., ChemMedChem 20 (2025) e202500429.

The Croatian Science Foundation funded this work (project BenzHetPot IP-2024-05-7208).



DESIGN AND SYNTHESIS OF NOVEL TRIAZOLE-SUBSTITUTED PHENANTHRO[9,10-*d*]IMIDAZOLE DERIVATIVES AND THEIR Ru(II) METAL COMPLEXES WITH POTENTIAL ANTITUMOR ACTIVITY

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Phenanthro[9,10-*d*]imidazole derivatives are an important class of heterocyclic compounds widely investigated for their diverse biological activities, including potential antitumor and antimicrobial effects. These compounds are known to exhibit antitumor activity through DNA intercalation or groove binding [1-3]. In this study, novel 1,2,3-triazole phenanthro[9,10-*d*]imidazole derivatives bearing various *p*-substituted phenyl groups were designed and synthesized. The synthetic strategy involved the initial preparation of aromatic azides, followed by a copper-catalyzed "click" reaction with propargyl alcohol to form 1,2,3-triazole intermediates. These intermediates were then oxidized to the corresponding aldehydes using Swern oxidation, which were subsequently condensed with phenanthrene-9,10-dione to construct the imidazole core. The resulting ligands were further used in the formation of ruthenium(II) *p*-cymene metal complexes to explore the effects of metal coordination on their physicochemical properties and biological activity. The structures of synthesized compounds and their metal complexes were characterized using NMR, UV-Vis spectroscopy and X-ray crystallographic analysis. The synthesized compounds will be further evaluated for their antiproliferative activity against human malignant tumor cell lines.

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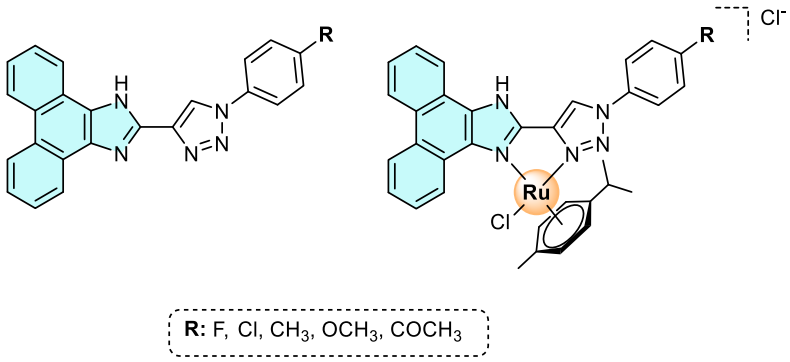

RAZVOJ 3D-ISPISANIH PROTOČNIH MIKROREAKTORA ZA INTENZIFIKACIJU FOTOKEMIJSKIH REAKCIJA

DEVELOPMENT OF 3D PRINTED FLOW MICROREACTORS FOR PHOTOCHEMICAL REACTION INTENSIFICATION

Karla Stražičić, Marijan-Pere Marković, Domagoj Vrsaljko, Petar Kassal, Irena Škorić

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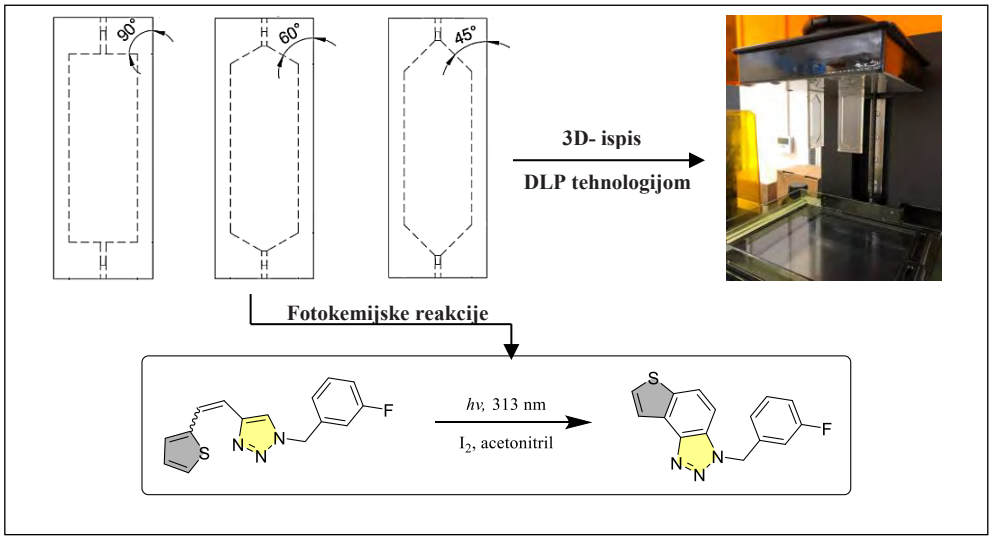
U ovom istraživanju su ispitani 3D-ispisani mikroreaktori za fotokemijske reakcije u kontinuiranom protočnom sustavu. Mikroreaktori jednakog unutarnjeg volumena izrađeni su DLP tehnologijom s tri različita kuta unutarnje geometrije (90°, 60° i 45°), a svaki tip imao je dva pokrova – polimerni i stakleni. Fotokemijske reakcije provedene su pod UV zračenjem (313 nm), koristeći smjese *cis*- i *trans*-izomera dobivene iz triazolnih aldehida i tiofenske fosfonijeve soli za sintezu fluorofenil-supstituiranih triazolnih derivata. Tijek reakcije praćen je elektrokemijskim senzorima te potvrđen UHPLC analizom. Polimerni pokrovi pokazali su bolju učinkovitost od staklenih zbog veće propusnosti UV zračenja, što je rezultiralo većim stupnjem konverzije. Najveći stupanj konverzije i najveći udio fotoprodukta postignut je u mikroreaktoru s kutom unutarnje geometrije od 45° i polimernim pokrovom. Diferencijalna pulsna voltametrija primijenjena je za praćenje konverzije reaktanta u stvarnom vremenu, pružajući brzu, ekonomičnu i osjetljivu alternativu UHPLC metodi, uz visoku osjetljivost, izvrsnu linearnost i vrlo dobru podudarnost s UHPLC analizom. Ovi rezultati potvrđuju potencijal 3D-ispisanih mikroreaktora za učinkovitu, ponovljivu i održivu primjenu u fotokemijskim procesima.



SYNTHESIS, STRUCTURAL CHARACTERIZATION AND DYEING PROPERTIES OF NOVEL AZO BENZOTHIAZOLE DERIVATIVES

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Azo dyes are among the most significant and versatile classes of chromophores, with broad applications across scientific, industrial, and pharmaceutical sectors. The incorporation of heterocyclic groups, such as benzothiazole, into azo dye structures enhances their coloring properties, tinctorial strength, and thermal stability, while also improving their solvatochromic behavior. Benzothiazolyl azo derivatives, in particular, are of growing interest due to their ability to form strong, vivid color shades ranging from red to blue, depending on the nature of the substituents. Furthermore, these dyes exhibit enhanced photophysical properties, nonlinear optical behavior, and biological activities, making them ideal for multifunctional applications [1,2].
In this work, the synthesis of novel 2-substituted-6-azobenzothiazole derivatives was carried out by diazotation reaction of 6-aminobenzothiazole and copulation with commercially available anilines. The described methods effectively prepared bis-disulfide derivatives, which served as a reagent for condensation reactions in NMP with ariously substituted aromatic aldehydes in order to introduce phenyl groups with different substituents at the C-2 position of the benzothiazole core. Spectroscopic characterization of dyes was performed using UV/Vis spectroscopy in 6 solvents of different polarities. pH titrations of dyes were performed in 13 buffer solutions of different pH values for the purpose of potential application as optical pH sensors. The dyeing properties of the new dyes were tested on polyamide textile material and the dye fastness to washing was also tested. Substituent variations on the benzothiazole ring significantly influenced both chromophoric behavior and colour-fastness.

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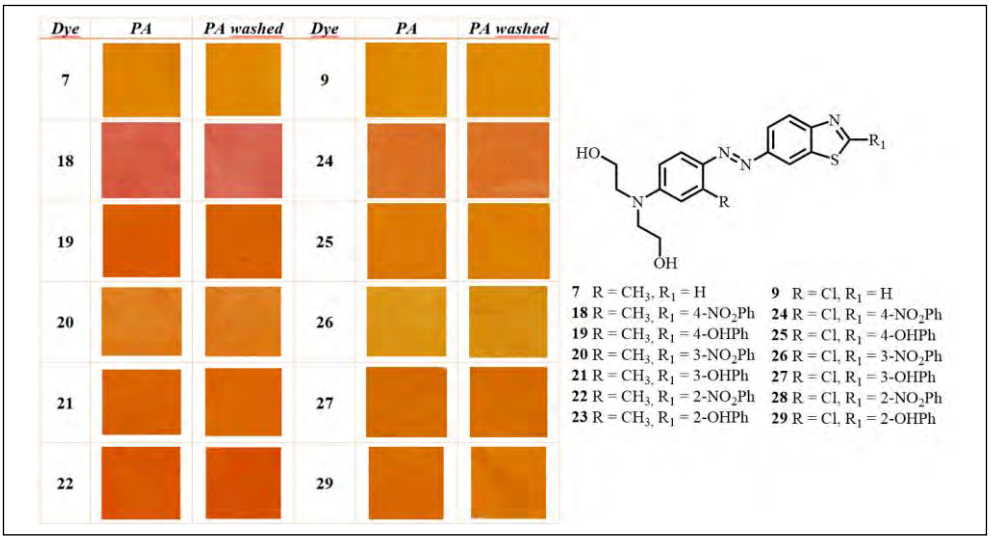

COMPUTATIONAL API FINGERPRINTING VIA THE *COFFEE RING* EFFECT

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The *coffee ring* effect, a ubiquitous phenomenon driven by capillary flow that forces suspended particles toward the pinned contact line of an evaporating droplet, has evolved from a simple physical curiosity into a sophisticated diagnostic tool for material science. While historically regarded as a nuisance in printing and coating technologies, this self-assembly mechanism offers a unique, high-fidelity "fingerprint" of molecular identity. This study leverages the complex hydrodynamics of the *coffee ring* effect to characterize and differentiate a diverse set of active pharmaceutical ingredients (APIs) based solely on their drying patterns.

Solutions of various undisclosed APIs were deposited onto glass substrates and allowed to dry under controlled conditions to mitigate variability arising from anisotropy or inconsistent settings. The resulting dried stains were digitized using optical microscopy to generate high-resolution photomicrographs. These images were subjected to a comprehensive computational pipeline comprising low-level analysis and parallel machine learning workflows. Initial preprocessing involved grayscale conversion, leading to image processing steps focused on contour detection, radial profiling, and area quantification to extract fundamental morphometric data. In an unsupervised learning stream, these raw metrics underwent feature engineering to produce tabular data, which was subsequently analyzed using clustering techniques to identify inherent morphological classes indicative of specific API properties. Parallel to this, a high-level supervised learning workflow was established to move towards a fully automated solution. Annotated and labeled photomicrographs are utilized to train visual deep learning models, generating embeddings competent for advanced tasks including object detection, localization, and robust classification or regression. Ultimately, this integrated framework illustrates that the computational analysis of simple evaporating droplets provides a scalable, non-destructive methodology for high-throughput API screening.

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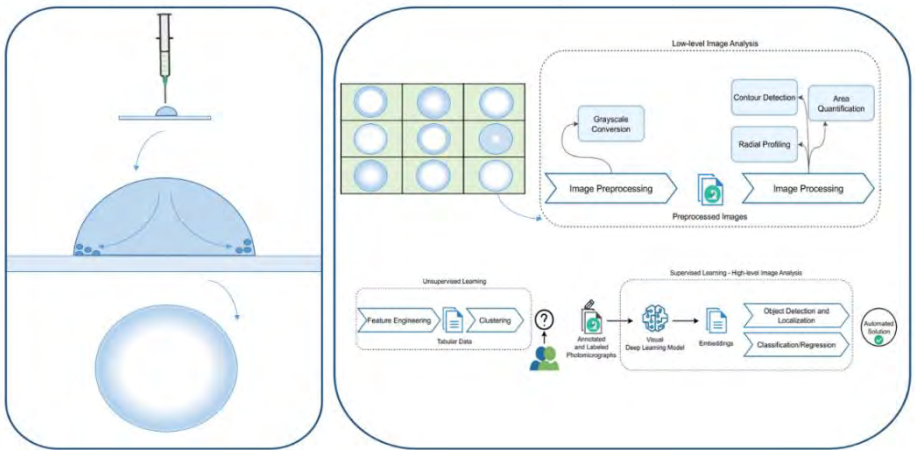
This paper was funded by the Croatian Science Foundation through the project IP-2024-05-4339 entitled " Coffee ring' effect in 'Lab on a Chip' environments in the development of new drug formulations", leader prof. Ernest Meštrović.



NOVEL SPIROOXETANE CONTAINING NAPHTOQUINONES – SYNTHESIS AND BIOLOGICAL ACTIVITIES

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Small molecules containing the naphtoquinone moiety, often discovered as natural products, have long been known to exhibit a number of different biological activites [1]. Naphtoquinone derivatives have been especially useful as anticancer agents, with drugs such as Doxorubicin and Daunorubicin in wide use since the 1970s. While working on the development of a synthetic route towards the naphtoquinone natural product Enceleaymcin A, we discovered that proline catalyses the condensation of 2-hydroxynaphtoquinone (Lawsone) **1** and 2-(oxetan-3-ylidene)propanal **2**, with the formation of *ortho*- and *para*- naphtoquinone products **3** and **4** containing a spriocyclic oxetane through a Knoevenagel condensation - 6π electrocyclization cascade [2]. The structures of **3** and **4** were confirmed using single crystal diffraction and NMR experiments. These compounds have shown interesting cytotoxic and antimicrobial activities which prompted the synthesis of substituted derivatives to further study the structure-activity relationship of these compounds.

[1] L Itzel López-López et al., Pharmaceuticals 16 (2023) 496.
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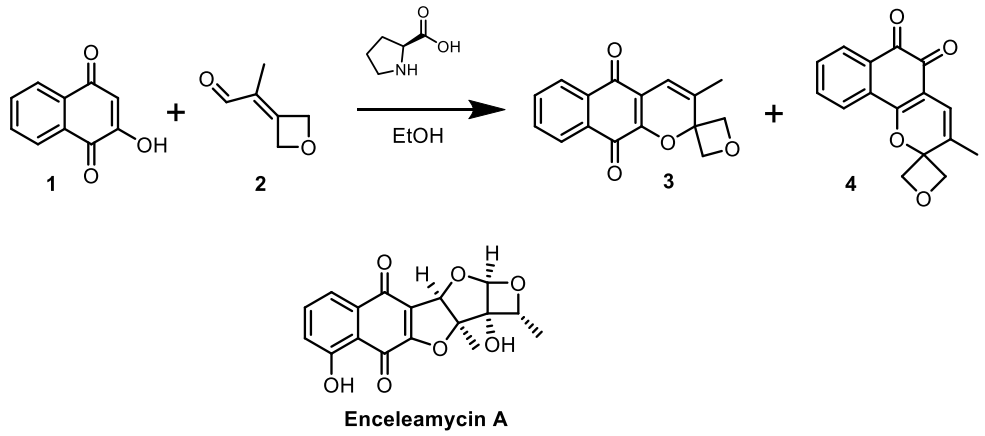
This work has been supported by The European Union – NextGenerationEU project ToSiAn NPOO.C3.2.R2-I1.06.0043 and by the Croatian Science Foundation project MicroSynTotal IP-2024-05-5352.



SELF-SENSITIZED PHOTOOXYGENATION OF DEHYDRO-α-LAPACHONE

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Dehydro-α-lapachone (**1**) is a naphtoquinone natural product that has shown interesting antivascular and cytotoxic activities [1]. The naphtoquinone moiety in **1** acts as a chromophore and enables absorption in the visible part of the spectrum. During preliminary studies towards the total synthesis of enceleamycin A, we were interested in the feasibility of a retro 6π electrocyclization reaction from the excited state in compounds similar to **1** [2]. We thus performed a series of light irradiation experiments. Upon irradiation with blue light in the presence of oxygen, **1** undergoes a self-sensitized photooxygenation. The endoperoxide **2** obtained by the addition of singlet oxygen to **1** rearranges, giving rise to compounds **3** and **4**. The structures of **3** and **4** were determined by single crystal diffraction experiments and were confirmed using NMR spectroscopy.
While compounds **3** and **4** were not previously reported in the literature, the reactivity of **1** described here raises the question whether compounds **3** and **4** could also be found in nature as *in vivo* oxygenation products.

[1] I. Garkavtsev et al., Proc. Natl. Acad. Sci. U.S.A. 108 (2011) 11596-11601.
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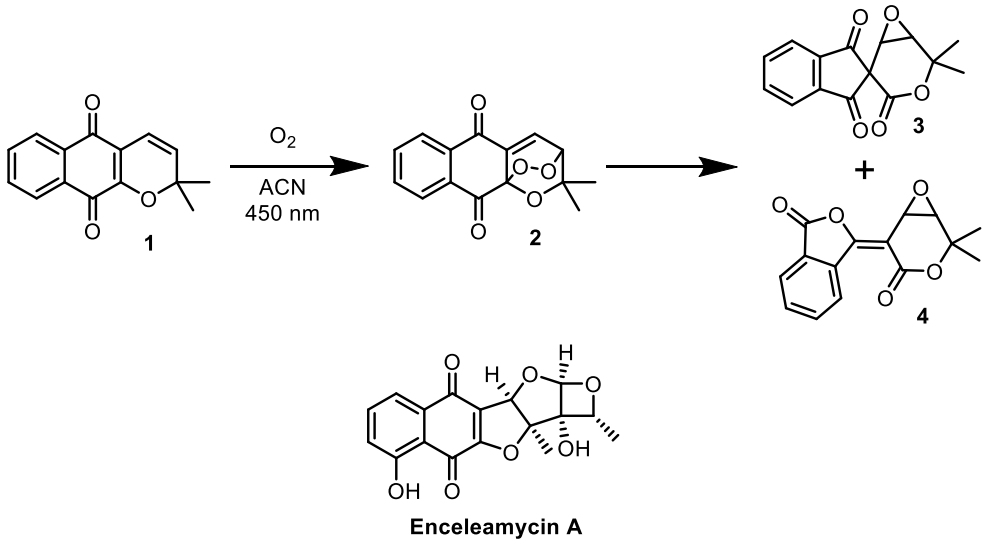
This work has been supported by The European Union – NextGenerationEU project ToSiAn NPOO.C3.2.R2-I1.06.0043 and by the Croatian Science Foundation project MicroSynTotal IP-2024-05-5352.



ANTIMICROBIAL ACTIVITY OF ARYL-INDENES: EXPERIMENTAL AND COMPUTATIONAL STUDIES

Dragana Vuk[1], Vilma Lovrinčević,[1] Nikica Baričević,[1] Monika Šabić Runjavec,[1] Marija Vuković Domanovac[1], Ines Despotović[2]

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The increasing incidence of antibiotic-resistant bacteria has become a major global health problem that requires the search for new and effective antimicrobial agents [1]. Indenes are an important group of organic compounds found in many natural and synthetic products that have shown promise in the fight against bacterial infections due to their diverse chemical structure and unique pharmacological properties [2,3].
In this work, the substituted indene derivatives is presented and its antimicrobial activities against different microbial species, *Bacillus subtilis* 3020, *Pseudomonas aeruginosa* 3011, *Candida lipolytica* 59 and *Aspergillus niger* 405, are evaluated. In an effort to elucidate the plausible inhibitory mechanism by which these compounds could be used as antibacterial and antifungal drug candidates, the *in silico* molecular docking study [4] was performed for selected molecules against the active site of DNA gyrase B (GyrB) and 14α-sterol demethylase (CYP51). The structures of the complexes formed between the potential inhibitor and the target enzyme were predicted, allowing the identification of the main interactions responsible for the inhibitory activity and the estimation of the binding affinity of the active molecule to the target enzyme.

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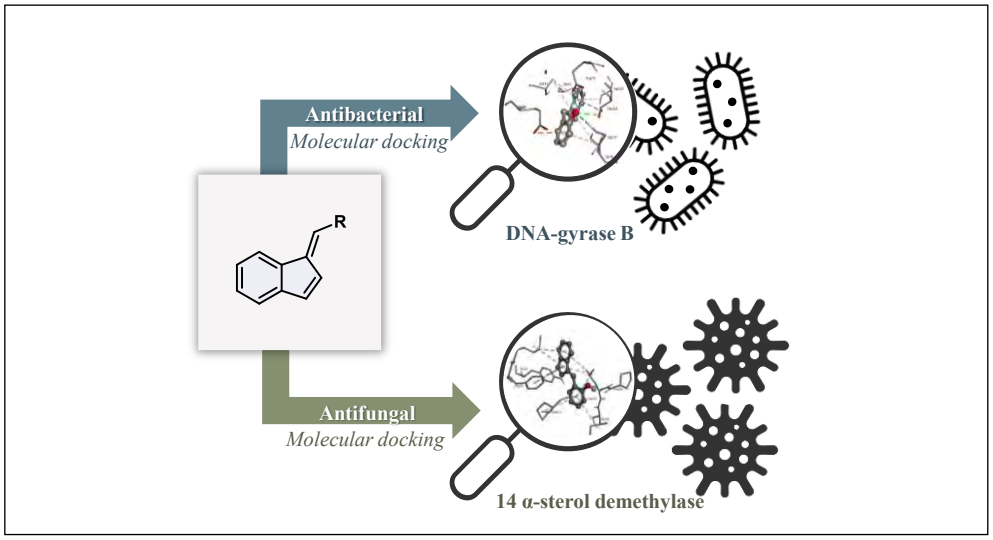

GC-MS KAO ANALITIČKI ALAT U PROCJENI UTJECAJA *TERROIRA* NA HLAPLJIVE SPOJEVE VINA SORTE ´PLAVAC MALI´

EVALUTION OF *TERROIR* INFLUENCE ON VOLATILE COMPOUNDS IN ´PLAVAC MALI´ BY GC-MS

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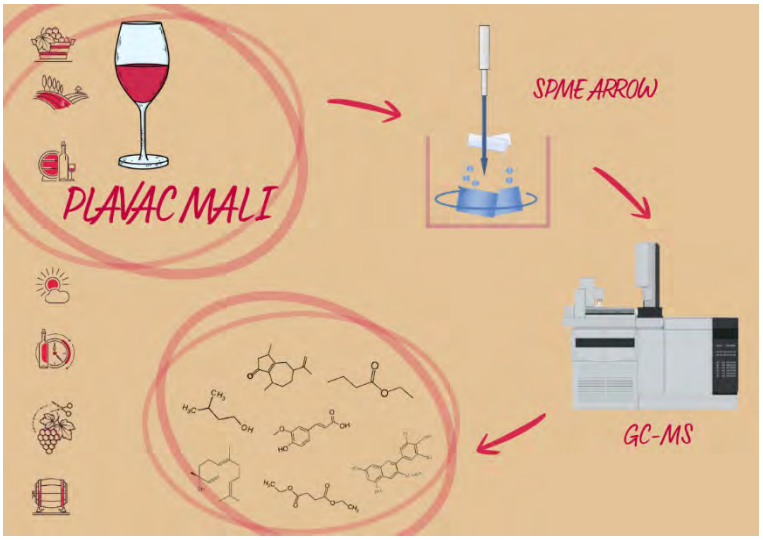
Razumijevanje utjecaja *terroira*, tj. skupa prirodnih i antropogenih čimbenika koji uključuju tlo, klimu, topografiju i vinogradarske prakse, a zajedno oblikuju kemijski i senzorni profil vina, na nastanak hlapljivih spojeva ključno je za optimiranje enoloških procesa i definiranje tipičnosti autohtonih sorata [1]. U ovom radu primijenjena je plinska kromatografija–masena spektrometrija (GC-MS) u kombinaciji s tehnikom mikroekstrakcije SPME-Arrow za detaljnu karakterizaciju hlapljivih sastavnica vina sorte ´Plavac mali´ dobivenih s različitih vinogradarskih mikrolokacija. SPME-*Arrow* metoda, zahvaljujući povećanoj apsorpcijskoj površini i poboljšanoj osjetljivosti, omogućila je pouzdano određivanje širokog spektra hlapljivih spojeva, uključujući estere, više alkohole, terpene, fenole te hlapljive masne kiseline, ključne za organoleptička svojstva vina [2]. Dobiveni kemijski profili integrirani su s pedoklimatskim parametrima položaja. Multivarijatna analiza ukazala je na jasno razdvajanje uzoraka prema *terroiru* te izdvojila markere odgovorne za razlikovanje aromatskih profila. Rezultati potvrđuju kako kombinacija SPME-*Arrow* i GC-MS predstavlja robusnu analitičku platformu za istraživanje okolišnih i tehnoloških utjecaja na aromatski profil vina ´Plavca malog´.

[1] D. Ivan Žeravica et al., Beverages 11 (2025) 87.
[2] Tomaz et al., OENO One 58 (2024) 1-13.



Razvoj materijala i proizvoda
Materials and products development

NAPREDNA KARAKTERIZACIJA NELINEARNIH PLGA KOPOLIMERA: ANALIZA RAZGRANATOSTI

ADVANCED CHARACTERIZATION OF NON-LINEAR PLGA COPOLYMERS: BRANCHING ANALYSIS

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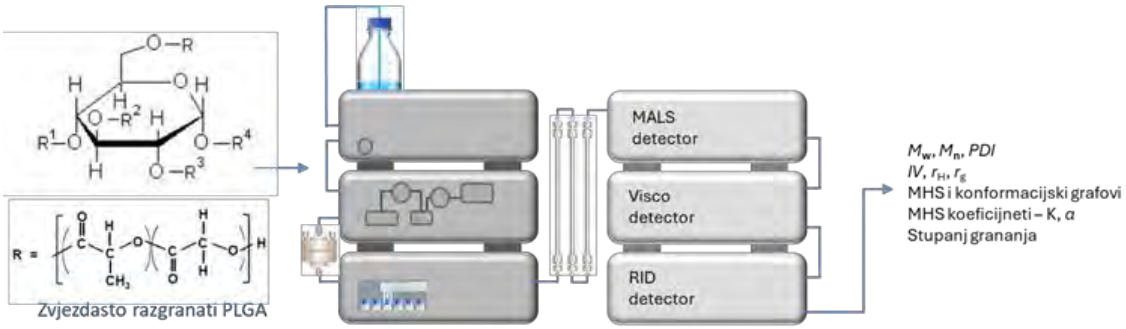
Poli(laktid-*ko*-glikolid) (PLGA) kopolimeri predstavljaju ključne materijale u području kontroliranog otpuštanja lijekova i regenerativne medicine zbog svoje biorazgradivosti i mogućnosti prilagodbe fizikalno-kemijskih svojstava. Dok su linearni PLGA sustavi temeljito istraženi, zvjezdasto razgranate građe nude dodatne prednosti poput modificirane kinetike razgradnje, povećane sposobnosti enkapsulacije i promijenjenih reoloških svojstava [1,2].
U ovom radu provedena je usporedna karakterizacija linearnih i zvjezdasto razgranatih PLGA kopolimera korištenjem kromatografije na propusnom gelu (GPC) s višestrukom detekcijom – refraktometrijom (RI), višekutnom laserskom raspršenošću (MALS) i viskozimetrijom. Ova metoda omogućuje apsolutno određivanje molekulske mase, intrinzične viskoznosti te uvid u konformaciju polimera u otopini.
Zvjezdasto razgranati PLGA uzorci pokazali su niže intrinzične viskoznosti i hidrodinamičke volumene u usporedbi s linearnim analogima slične molekulske mase, što ukazuje na kompaktniju strukturu. Korištenjem kombiniranih podataka iz MALS i viskozimetrijskih detektora, određeni su omjer razgranatosti i broj krakova kod zvjezdasto razgranatih kopolimera, čime se kvantificira stupanj razgranatosti i strukturna kompleksnost [2].
Rezultati naglašavaju ograničenja konvencionalne RI detekcije u analizi razgranatih polimera te potvrđuju važnost višedetektorskih sustava za pouzdanu karakterizaciju. Ovaj rad doprinosi razumijevanju odnosa strukture i svojstava PLGA sustava te pruža temelje za razvoj kompleksnih polimernih materijala za specifične terapijske primjene. Predložena metodologija primjenjiva je i na druge razgranate ili strukturno kompleksne polimere.

[1] Wang X. et al., Int. J. Pharm. 639 (2023) 122948.
[2] Hadar J. et. al., J. Control. Release 304 (2019) 75-89.



DEVELOPMENT AND CHARACTERIZATION OF SMART POLYMER BASED MULTIFUNCTIONAL COATINGS FOR PHOTOVOLTAIC SOLAR PANELS

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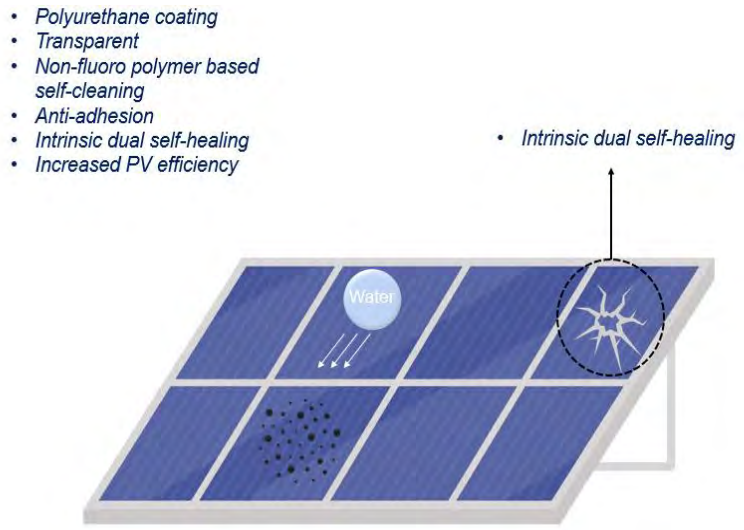
Solar energy, as an abundant and clean energy source, holds immense potential for ensuring a sustainable energy supply. However, to fully exploit this potential, it is critical to overcome key challenges that impair the efficiency and longevity of photovoltaic (PV) panels – most notably, surface contamination and physical degradation. Dust accumulation on panel surfaces can significantly obstruct incident sunlight, leading to efficiency losses of up to 60% [1]. This issue is particularly observed in large-scale solar farms and rooftop systems with limited accessibility, where conventional cleaning methods are labor-intensive and incur high operational costs. Furthermore, surface scratches and abrasion occurring over time degrade the optical and mechanical properties of the panels, ultimately shortening their operational lifespan [2]. This study aims to develop polyurethane-based functional coatings with self-cleaning and self-healing capabilities to address these limitations. By mitigating contamination and surface damage, the proposed coatings are expected to enhance energy conversion efficiency, reduce maintenance costs, and extend the service life of solar panels. To achieve these objectives, we employ a methodology based on the synthesis of polyurethane coatings that incorporate disulfide bonds and hindered urea bonds to enable intrinsic dual self-healing functionality, along with the integration of an inherently hydrophobic non-fluoro polymer to impart hydrophobic characteristics for self-cleaning performance. In contrast to prior studies that focus on either self-cleaning or self-healing functions in isolation, this study adopts a synergistic design approach to achieve both functionalities simultaneously within a single, durable, and optically transparent coating system, offering a more practical solution for real-world photovoltaic applications.

[1] H. K. Elminir et al., Energy Convers. Manag. 47 (2006) 3192–3203.
[2] A. Khan et al., J. Colloid Interface Sci. 577 (2020) 311–318.



UTJECAJ DISPERZANATA NA PROIZVODNJU LITIJ-IONSKIH BATERIJA

EFFECTS OF DISPERSANTS ON LITHIUM-ION BATTERIES PRODUCTION

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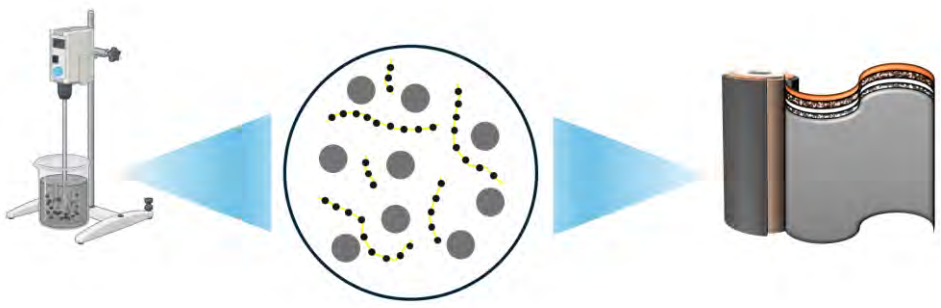
Lithium-ion batteries are currently the dominant energy storage technology due to their high energy density, long cycle life, and overall efficiency. Battery performance is strongly influenced by manufacturing parameters, especially the solid loading of the cathode and anode materials, which directly determines achievable energy density of electrode. However, increasing solid loading while preserving adequate processability remains a key challenge in electrode production.
In this study, we investigate the use of polyvinylpyrrolidone (PVP 30K) as a dispersant to increase solid loading in lithium-ion batteries while maintaining optimal rheological properties for electrode fabrication. The NMC cathode slurries were prepared using standard slurry process route, with PVP 30K added at concentration of up to 1%. The effect of dispersant concentration on slurry rheological properties was systematically studied to identify the highest achievable solid content that maintains processability. The prepared electrodes were evaluated through a combination of electrochemical and physical characterization to assess the impact of PVP 30K. Electrochemical testing, including electrochemical impedance spectroscopy (EIS) and galvanostatic cycling with potential limitation (GCPL), was employed to examine the impact on charge transfer and cycling stability. Additionally, scanning electron microscopy (SEM) was used to analyze the microstructure of the electrodes before and after cycling, while contact angle and adhesion tests provided insights into the dispersant's influence on coating quality and resulting interfacial properties. Overall, the results show that the addition of PVP 30K dispersant enables higher solid content without negatively affecting electrochemical performance, offering valuable insights for scaling up lithium-ion production processes.

This work was funded by the European Union within the project NPOO.C3.2.R3-I1.04.0187: Development of new materials and advanced innovative technologies for the production of lithium-ion batteries.



UTICAJ KLINKERA, GIPSA, TROSKE I PEPELA NA KVALITET CEMENTA

THE IMPACT OF CLINKER, GYPSUM, SLAG AND ASH ADDITIVES ON CEMENT QUALITY

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The cement industry plays a vital role in the construction sector, where cement is used as a basic material for infrastructure, residential, and industrial facilities. Cement production is an energy-intensive process accompanied by the emission of harmful substances that pose significant environmental concerns. Therefore, optimizing cement composition and incorporating mineral additives represent effective approaches to improving product quality while reducing environmental impact. This paper investigates the influence of clinker, gypsum, slag, and ash on the physicochemical properties and overall quality of Portland cement. Both chemical composition and physical properties, including compressive strength, are analyzed. Particular attention is given to parameters such as setting time, hydration kinetics, and strength development, as well as changes in the microstructure formed due to the addition of these materials. The main objective of this research is to evaluate the possibility of producing a new type of cement with improved performance and reduced environmental footprint. The theoretical part presents a review of recent studies concerning the role of mineral additives in cement systems and their industrial applications. The experimental part is based on laboratory testing of different cement compositions in order to determine optimal additive ratios. The results highlight the importance of mineral additives in modern cement production and confirm their contribution to sustainable industrial development by reducing resource consumption and environmental risk.

PRIPRAVA HETEROSPOJEVA CeO_2 I NATRIJEVOG BIRNESITA

PREPARATION OF CeO_2/SODIUM BIRNESSITE HETEROJUNCTIONS

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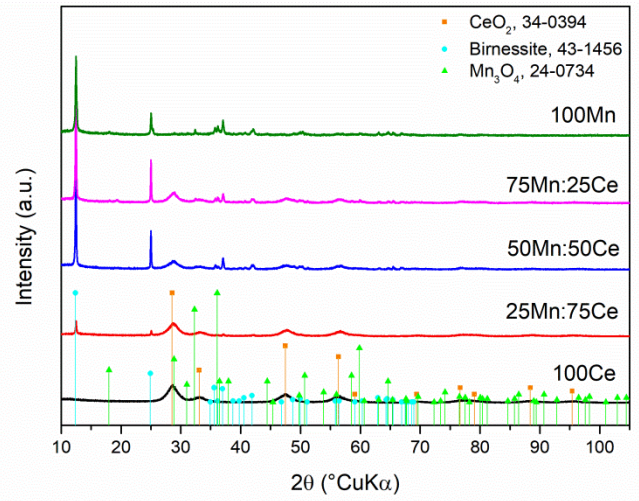
Rastuća razina industrijskog zagađenja predstavlja ozbiljnu ugrozu okoliša, pri čemu su naročit problem industrijske otpadne vode. Fotokatalitički procesi ističu se kao učinkovita metoda razgradnje zagađivala u otpadnim vodama budući da se temelje na primjeni poluvodičkih materijala aktiviranih svjetlosnim zračenjem. Ograničenja većine konvencionalnih fotokatalizatora, poput potrebe za aktivacijom UV zračenjem i sklonosti rekombinaciji fotogeneriranih nositelja naboja, potiču intenzivna istraživanja usmjerena razvoju novih materijala s poboljšanim svojstvima. Zbog svojih jedinstvenih elektroničkih svojstava, heterospojni materijali posljednjih godina pobuđuju sve veću pozornost i smatraju se značajanim materijalima za primjenu u fotokatalizi i katalizi općenito. Kombiniranjem poluvodiča različitih struktura i energetskih razina omogućuje se učinkovitiji prijenos nositelja naboja te smanjenje njihove rekombinacije [1]. U tom kontekstu, heterospoj cerijeva(IV) oksida (CeO_2) i manganovih oksida birnesitne strukture predstavlja atraktivan katalitički materijal.

U ovom radu heterospojevi cerijeva(IV) oksida i natrijevog birnesita pripravljeni su *in-situ* hidrotermalnom sintezom uz različite omjere cerija i mangana. Pripravljeni uzorci ispitani su primjenom rendgenske difrakcije na prahu (XRD), infracrvene spektroskopije s Fourierovom transformacijom (FTIR), UV-Vis difuzne refleksijske spektroskopije (UV-Vis DRS), pretražne elektronske mikroskopije (SEM) i energijski razlučujuće rendgenske spektroskopije (EDS) s ciljem određivanja njihove strukture, mikrostrukture i morfologije čestica.

[1] A. Balapure et al., RSC Appl. Interfaces 1 (2024) 43-69.



TOPLINSKA SVOJSTVA I RAZGRADNJA PLGA ČESTICA PRIREĐENIH PRECIPITACIJOM

THERMAL PROPERTIES AND DEGRADATION OF PLGA PARTICLES PREPARED BY PRECIPITATION

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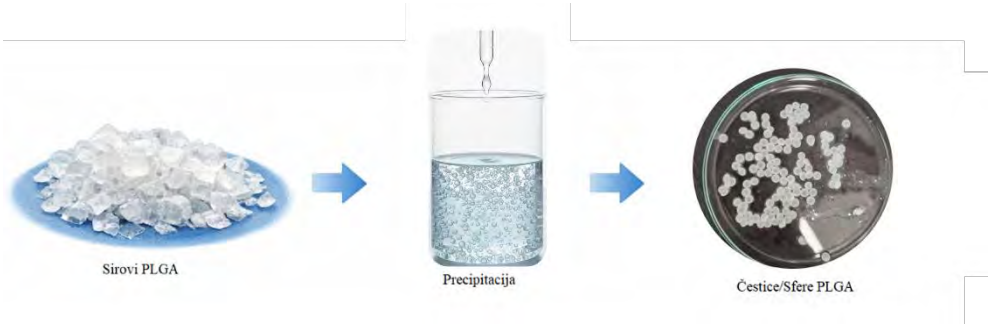
Poli(laktid-*ko*-glikolid) (PLGA) je biokompatibilan i biorazgradiv polimer koji se može lako prerađivati. Jedinstvena fizikalno-kemijska svojstva ovog materijala čine ga pogodnim za širok spektar primjena u biomedicinskom području. PLGA kopolimeri primijenjeni su u nosačima za regeneraciju tkiva te sustavima za isporuku lijekova. PLGA se hidrolizom razlaže na mliječnu i glikolnu kiselinu. Tijekom biorazgradnje PLGA mijenjaju se ključna fizikalno kemijska svojstva uključujući molekulsku masu, sadržaj vlage i temperaturu staklastog prijelaza [1]. U ovom radu pripremljene su PLGA sfere/čestice metodom precipitacije. Uzorci su otopljeni u prigodnom otapalu u masenom udjelu 20 % te nakon potpunog otapanja precipitirani su u neotapalu. Pripremljene su kuglice promjera oko 0,2 cm. Korišteni su polimeri molarnog udjela laktida od 100 do 50 mol% te inherentne viskoznosti 0,2 dL g^{-1} sa kiselinskom ili esterskom krajnjom skupinom. Priređenim uzorcima termogravimetrijskom analizom (TGA) praćeno je bubrenje polimera kroz gubitak mase uzrokovan uklanjanjem vode. Praćen je i porast temperaturne vrijednosti pri kojoj dolazi do maksimuma razgradnje. Diferencijalnom pretražnom kalorimetrijom (DSC) praćena je promjena udjela vode, kao i promjena temperature staklastog prijelaza. Uzorcima je praćena kinetika razgradnje u fosfatnom puferu (pH = 7,4) pri sobnoj temperaturi, a molekulska masa određivala se kromatografijom na propusnom gelu.

[1] C. Martins et al., Adv. Healthc. Mater. 7 (2018) 1701035.



RHEOLOGICAL BEHAVIOR, BARRIER PERFORMANCE, AND BIODEGRADATION OF PHBV/TIO$_2$ BIONANOCOMPOSITES

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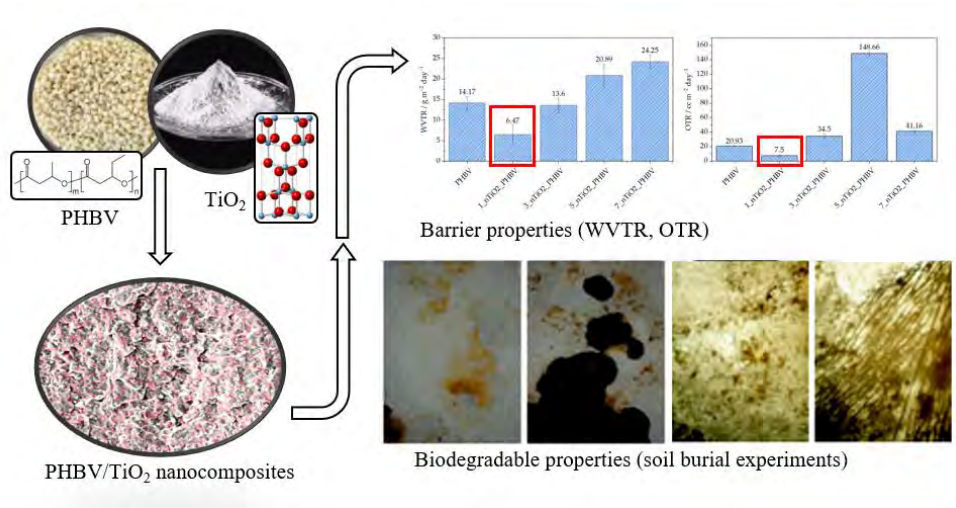
Biodegradable polymer nanocomposites have gained considerable interest as sustainable alternatives to conventional petroleum-based plastics, particularly for packaging applications where balanced barrier properties, melt processability, and environmental compatibility are required. In this study, poly(3-hydroxybutyrate-*co*-3-hydroxyvalerate) (PHBV) bionanocomposites reinforced with titanium dioxide (TiO_2) nanoparticles were developed to examine the influence of filler content on rheological behavior, barrier performance, and soil biodegradation. PHBV/TiO_2 nanocomposites containing 1, 3, 5, and 7 wt.% TiO_2 were prepared by melt mixing and subsequently molded into films suitable for characterization. Barrier properties were assessed through water vapour transmission rate (WVTR) and oxygen transmission rate (OTR) measurements, while rheological behavior was investigated by oscillatory shear tests at melt-processing temperatures. Biodegradation behavior was evaluated through controlled soil burial experiments over 56 days, supported by morphological and spectroscopic analyses. The results indicate that the incorporation of low TiO_2 contents, particularly 1 wt.%, leads to an improvement in barrier performance, reflected by reduced WVTR and OTR values. This behavior is generally associated with modifications in the internal structure of the polymer matrix caused by the presence of dispersed inorganic particles, which can influence diffusion pathways for permeating molecules. Rheological measurements show that TiO_2 addition affects the viscoelastic response of PHBV melts, resulting in lower complex viscosity and a diminished elastic contribution, suggesting changes in the melt structure and reduced formation of an interconnected elastic network. These effects contribute to improved melt flow behavior, especially at higher filler loadings. Soil burial tests confirm that all investigated nanocomposites retain their biodegradable character. An increase in TiO_2 content is accompanied by an accelerated degradation rate, which can be related to changes in material morphology and higher amorphous phase accessibility.

Financira Europska unija NextGenerationEU *This research was carried out 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-I1.04.0059) financed by the National Recovery and Resilience Plan (financed by the European Union, NextGenerationEU).*



TERNARNE ČVRSTE DISPERZIJE: PRIPRAVA I POTENCIJAL ZA KONTROLIRANO OSLOBAĐANJE DJELATNE TVARI

TERNARY SOLID DISPERSIONS: PREPARATION AND POTENTIAL FOR CONTROLLED DRUG RELEASE

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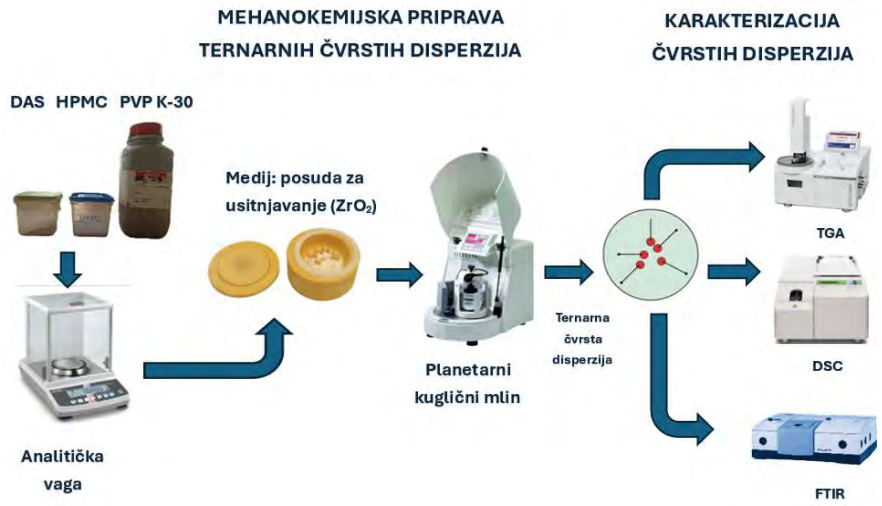
Dasatinib je antikancerogeni lijek koji se koristi u liječenju kronične mijeloične i akutne limfoblastične leukemije. Njegova slaba topljivost u vodi i izraženi metabolizam prvog prolaska rezultiraju ograničenom oralnom bioraspoloživošću i potencijalno teškim nuspojavama, poput kardiotoksičnosti, hepatotoksičnosti i plućnih komplikacija, koje su popraćene neželjenim profilom koncentracije djelatne tvari u krvotoku [1].
S ciljem povećanja njegove topljivosti i poboljašanja svojstva lijeka pripravljene su ternarne čvrste dispezije s poli(vinil-pirolidon)om i hidroksipropil-metil-celulozom mljevenjem u planetarnom kugličnom mlinu. Mehanokemijska aktivacija omogućuje pripravu bez primjene otapala poštujući načela zelene kemije, a istovremeno poboljšavaju topljivost i bioraspoloživost dasatiniba [2].
Pripravljene trokomponentne čvrste disperzije karakterizirane su diferencijalnom pretražnom kalorimetrijom, termogravimetrijskom analizom i infracrvenom spektroskopijom s Fourierovim transformacijama. Detaljna analiza ukazuje na stabilnost formulacije i potencijal ternarnih čvrstih disperzija u poboljšanju primjenskih svojstava lijeka.

[1] K. Sokač et al., Int. J. Pharm. 675 (2025) 125552.
[2] Martínez et al., Pharmaceutics. 14 (2022) 2003.



UTJECAJ PROCESA VALJANJA NA SVOJSTVA NMC ELEKTRODA U LITIJ-IONSKIM BATERIJAMA

INFLUENCE OF THE CALENDARING PROCESS ON THE PROPERTIES OF NMC ELECTRODES IN LITHIUM-ION BATTERIES

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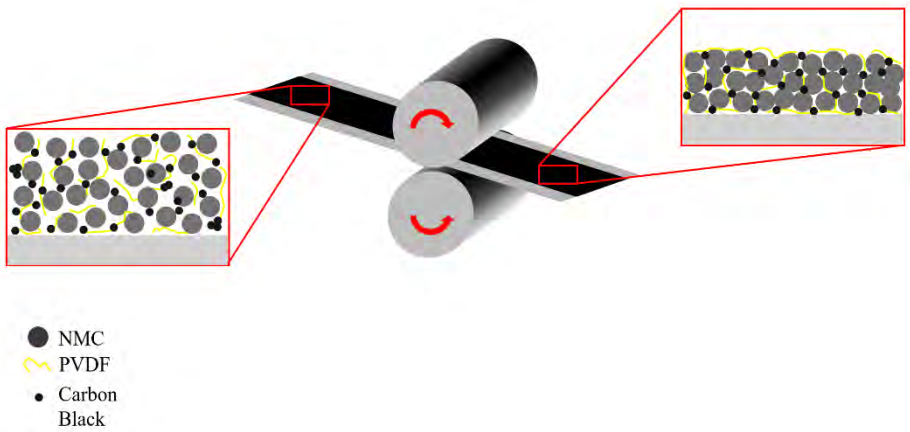
Baterijski sustavi temelj su današnje energetskih sustava, s primjenom u prijenosnoj elektronici i električnim vozilima. Među njima, litij-ionske baterije predstavljaju vrhunac dosadašnjeg razvoja baterijske tehnologije. Litij-ionske baterije ističu se visokim kapacitetom i učinkovitosti, niskim samopražnjenjem i dugim životnim vijekom što čini razlog njihovog kontinuiranog razvoja. Unatoč iznimnim performansama litij-ionskih baterija, njihove konačne performanse će uvelike ovisiti o načinu izrade. Posebno su kritične pojedine faze proizvodnje elektroda koje izravno utječu na mikrostrukturu materijala. Jedan od takvih koraka je proces valjanja (eng. *calendaring*) tijekom kojeg se elektrode mehanički komprimiraju prolaskom kroz valjke, pri čemu se mijenja debljina i poroznost polazne elektrode. U ovom radu pripremljene su elektrode s NMC-om kao aktivnim materijalom, vodljivim aditivom te polivinilden fluoridom (PVDF) kao vezivom pri čemu je kao otapalo korišten N-metil pirolidon (NMP). Dobivene elektrode su komprimirane na valjčanoj preši do različitih stupnjeva kompresije (12,5-50%) u odnosu na početnu debljinu. U svrhu procjene učinka različitih stupnjeva valjanja, provedena su elektrokemijska testiranja primjenom elektrokemijskom impedancijskom spektroskopijom (EIS) te galvanostatskim punjenjem i pražnjenjem (GCPL) dok je fizikalna karakterizacija odrađena uz pomoć pretražne elektronske mikroskopije (SEM), mjerenje kontaktnog kuta i adhezijske testove.
Dobiveni rezultati pokazuju kako povećanje stupnja kompresije dovodi do promjena mikrostrukture i površinskih svojstava elektrode što se u konačnici odražava na dobivenim vrijednostima kapaciteta i otpora prijelaza naboja. Provedeno istraživanje potvrđuje važnost kontrole stupnja valjanja u procesu proizvodnje litij-ionskih baterija i njegov utjecaj na konačne performanse baterije.

Ovaj rad financiran je iz sredstava Europske unije u sklopu projekta NPOO.C3.2.R3-I1.04.0187: Napredni inovativni materijali i tehnologije za proizvodnju litij-ionskih baterija.



PRIPRAVA I KARAKTERIZACIJA BIORAZGRADIVIH KOMPOZITA POLILAKTID/KONOPLJA

PREPARATION AND CHARACTERIZATION OF BIODEGRADABLE COMPOSITE POLYLACTIDE/HEMP

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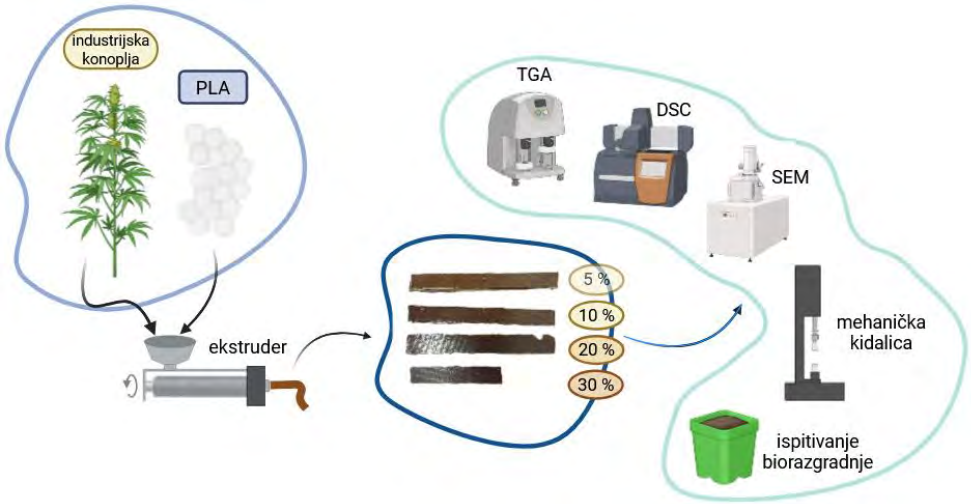
Rastuća ekološka osviještenost dovodi do sve veće potražnje za održivim materijalima, čime izravno utječe na razvoj biorazgradivih kompozita. Takvi kompoziti temelje se na polimerima dobivenih iz obnovljivih izvora i prirodnim punilima [1]. Polilaktid (PLA) jedan je od najčešće korištenih biorazgradivih polimera, dok se industrijska konoplja primjenjuje kao ojačavalo prirodnog podrijetla s ciljem poboljšanja svojstava i ubrzanja razgradnje materijala [2]. Međutim, dodatak prirodnih punila može značajno utjecati na toplinska, mehanička i strukturna svojstva kompozita, zbog čega je nužno ispitati optimalan udio punila u PLA matici. Kompoziti s udjelima konoplje od 5, 10, 20 i 30 mas. % pripravljeni su ekstrudiranjem, te okarakterizirani primjenom termogravimetrijske analize (TGA), diferencijalne pretražne kalorimetrije (DSC), pretražne elektronske mikroskopije (SEM), mehaničkim ispitivanjima te ispitivanjem biorazgradnje ukopavanjem kompozita u tlo tijekom 60 dana. Rezultati su pokazali ravnotežu toplinskih i mehaničkih svojstava uz umjereno poboljšanu razgradnju kompozita pri udjelima konoplje ≤ 10 %. Suprotno tome, viši udjeli punila dovode do slabe disperzije i separacije faza, što uzrokuje pad svojstava kompozita.

[1] K. Satyanarayana et al., Prog. Polym. Sci. 9 (2009) 982-1021.
[2] K. Madhavan Nampoothiri et al., Bioresource Technology 22 (2010) 8493-8501.



ELEKTROKEMIJSKA SINTEZA WO_3 FOTOANODE DOPIRANE Co

PREPARATION OF Co-DOPED WO_3PHOTOANODE VIA ELECTROCHEMICAL METHOD

Tadea Lažeta[1], Marija Labudović[1], Mustapha EL Cadiri[2], Suresh Kumar Pandey[1], Sandra Romac[1], Hrvoje Kušić[1], Marijana Kraljić Roković[1]

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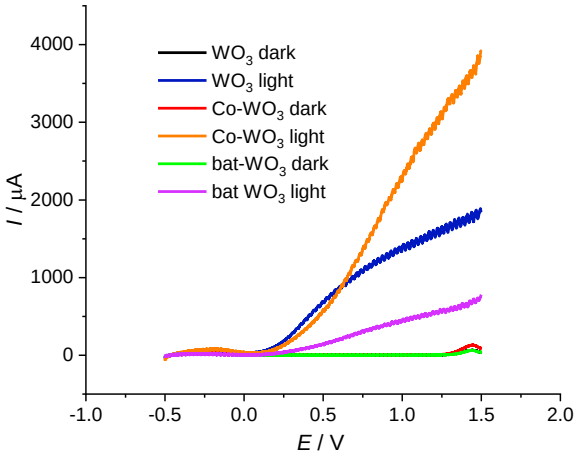
Photoelectrochemical processes (PEC) attract increasing attention because they find application in degradation of target pollutants, hydrogen generation and synthesis of organic molecules. Various semiconductor materials, such as UV-responsive TiO_2 and ZnO_2, or visible light-responsive SnS_2, BiVO4, Fe_2O_3, and WO_3, have been used for this purpose. WO_3 is an n-type semiconductor characterized by a band gap of 2.5–2.8 eV, excellent electron mobility, an appropriate hole diffusion length, and good stability in acidic media [1]. However, poor visible light response and rapid recombination of charge carriers limit the practical application of WO_3 as an effective photocatalyst. Structural modifications with transition metals can be used to adjust the band gap and enhance the photocatalytic efficiency of WO_3.
The aim of this study was to synthesize WO_3 layers at fluorine-doped tin oxide (FTO) glass, by cathodic electrodeposition, using a peroxotungstic acid precursor. In addition to WO_3, Co-dopedWO_3 layer and layer modified by spent battery materials (black mass)were prepared by adding Co-salts or black mass solution (black mass /deep eutectic solvent)to the peroxotungstic acid precursor. The Co-doping process is usually conducted during synthesis by hydrotermal/solvotermal, co-precipitation or sol-gel methods. In this work, electrochemical method was used due to the simplicity of synthesis, possibility to conduct process at low temperatures and possibility to apply photoactive material directly on the conductive surface. The direct application avoids subsequent steps and ensures good adhesion at conductive support, which is necessary for good electrochemical response of active material. Therefore, it was expected for materials prepared in this work to show high photoelectrochemical activity. The photoelectrochemical response of the obtain materials was characterized by linear sweep voltammetry (Fig. 1), electrochemical impedance spectroscopy, chronoamperometry, open circuit potential monitoring and UV/Vis spectroscopy.

[1] L. Bu et al., Catalysts (2025) 1061.

The authors acknowledge the support through project HORIZON-MSCA-2024-SE-01 (WAVEE, Number: 101236518) and project Tailored solar-active materials for photocatalytic degradation of contaminants of emerging concern (SOL-MAT-CLEAN) (IP-2025-02-8507)



PRIPREMA I KARAKTERIZACIJA POLIMERNIH HIDROGELOVA S PČELINJOM PELUDI

PREPARATION AND CHARACTERIZATION OF POLYMER HYDROGELS WITH BEE POLLEN

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Hidrogelovi su trodimenzionalni umreženi hidrofilni polimeri čija je karakteristika sposobnost upijanja i zadržavanja velike količine vode. Zbog toga nalaze sve veću primjenu u medicini, farmaciji, za pripremu kontaktnih leća, kozmetičkih i higijenskih proizvoda, senzora i ambalaže te u poljoprivredi.
U ovom su radu pripremljeni hidrogelovi na bazi polimera poli(vinil-alkohola) i natrijevog alginata uz dodatak pčelinje peludi. Sve su upotrijebljene komponente za pripremu hidrogelova u ovom istraživanju biorazgradljive, biokompatibilne, netoksične i sigurne za rukovanje i primjenu, a imaju i nisku cijenu. Hidrogelovi su pripremljeni iz otopina polimera u destiliranoj vodi, metodom zamrzavanje/odmrzavanje. Ovo je vrlo prikladan i poželjan postupak pripreme hidrogelova jer do umreživanja dolazi bez upotrebe kemijskih sredstava koja mogu biti toksična i nagrizajuća. Pčelinja pelud vrijedan je pčelinji proizvod i primjenjuje se kao dodatak prehrani. To je pelud navlažena pčelinjom slinom i nektarom koju pčele donose u košnicu, ima antibakterijsko, antivirusno, antifungalno i protuupalno djelovanje. Vanjski dio stijenke peludnog zrnca građen je od biopolimera sporopolenina [1] koji je otporan na kemijsku i enzimsku razgradnju. Prisutnost pčelinje peludi u hidrogelovima može doprinijeti produljenju trajnosti hidrogelova i njihove otpornosti na mikroorganizme tijekom skladištenja i upotrebe, primjerice tijekom primjene u obliku obloga za rane [2].
Pripremljenim je hidrogelovima određen sadržaj vode i stupanj bubrenja u destiliranoj vodi i u fiziološkoj otopini. Karakterizacija hidrogelova provedena je infracrvenom spektroskopijom s Fourierovom transformacijom (FTIR), a određena su im mehanička svojstva i ispitana je mogućnost njihovog samozacjeljivanja. Rezultati FTIR spektroskopije ukazuju na sličnost u strukturi poli(vinil-alkohola) i pčelinje peludi, tj. na kompatibilnost komponenti u pripremljenim hidrogelovima. Hidrogelovi s pčelinjom peludi pokazuju poboljšana mehanička svojstva u odnosu na hidrogel pripremljen bez peludi, tj. pelud djeluje kao ojačalo u ovim materijalima. Hidrogelovi pokazuju i mogućnost samozacjeljivanja što im, s mogućnošću bubrenja u tekućinama, daje potencijal za primjenu kao obloga za rane.

[1] F.-S. Li et al., Nat. Plants. 5 (2019) 41–46.
[2] B.Tyliszczak et al., J. Appl. Pharm. Sci. 5 (2015) 10–14.

Istraživanja u ovom radu provedena su u sklopu projekta „Funkcionalni polimerni kompozitni hidrogelovi“ (Institucionalni istraživački projekt SUZG FKIT financiran iz izvora 581 – mehanizam za oporavak i otpornost).

OBRADA I PRIMJENA POLIMERNE FRAKCIJE KAO PUNILA U ASFALTNOJ INDUSTRIJI

PROCESSING AND INCORPORATION OF POLYMERIC FRACTION AS A FILLER IN ASPHALT MIXTURES

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This study examines the application of circular economy principles in the processing of polymeric fractions generated during solvent regeneration processes, with a specific focus on their use as a filler material in asphalt mixtures. The scientific objective is to assess whether such waste-derived material can be processed into a stable and homogeneous form suitable for partial substitution of conventional mineral filler, while reducing environmental burden and dependence on virgin raw materials [1].

A multi-stage experimental approach was adopted. Following an analysis of current asphalt production practices and regulatory requirements, laboratory characterisation of polymeric fractions was performed to identify key parameters influencing processability and performance, including particle size distribution, viscosity, volatile content and homogeneity [2]. Based on these findings, the material was subjected to filtration and controlled dehydration to obtain poylmeric fractions suitable for incorporation into asphalt mixtures. Laboratory-scale mixing trials demonstrated that fully dehydrated polymeric fractions exhibit improved handling characteristics and more reliable incorporation into asphalt mixtures when used as a filler, compared to less processed material. The reduced volatile content and increased dimensional stability of dehydrated polymeric fractions enabled more consistent dosing, improved homogenisation and better compatibility with the bitumen–aggregate system. These characteristics are particularly relevant given the operational constraints and process sensitivity of asphalt plants, where stable filler behaviour is essential for maintaining mixture quality and production continuity [3].

Preliminary industrial trials confirmed the technical feasibility of using the processed polymeric fractions as a filler component. The results obtained so far indicate that polymeric fractions can be effectively valorised as a functional filler in asphalt production, providing a viable pathway for waste reduction, resource efficiency and implementation of circular economy principles in the construction sector.

[1] F. L. Roberts et al., HMA (1996) 286–304.
[2] Y. Xue et al., Constr. Build. Mater. 56 (2014) 7–15.
[3] Brown et al., NCAT Report Series (2009)

Istraživanje je provedeno u okviru projekta koji financira Europska unija – NextGenerationEU (šifra projekta: NPOO.C3.2.R2-I1.04.0038).

KARAKTERIZACIJA PLGA DOZIRNOG SUSTAVA ZA PRODULJENO OSLOBAĐANJE INDOMETACINA: UVID U MEHANIZAM OSLOBAĐANJA LIJEKA

CHARACTERIZATION OF A PLGA-BASED DRUG DELIVERY SYSTEM FOR SUSTAINED RELEASE OF INDOMETHACIN: ELUCIDATION OF DRUG RELEASE MECHANISM

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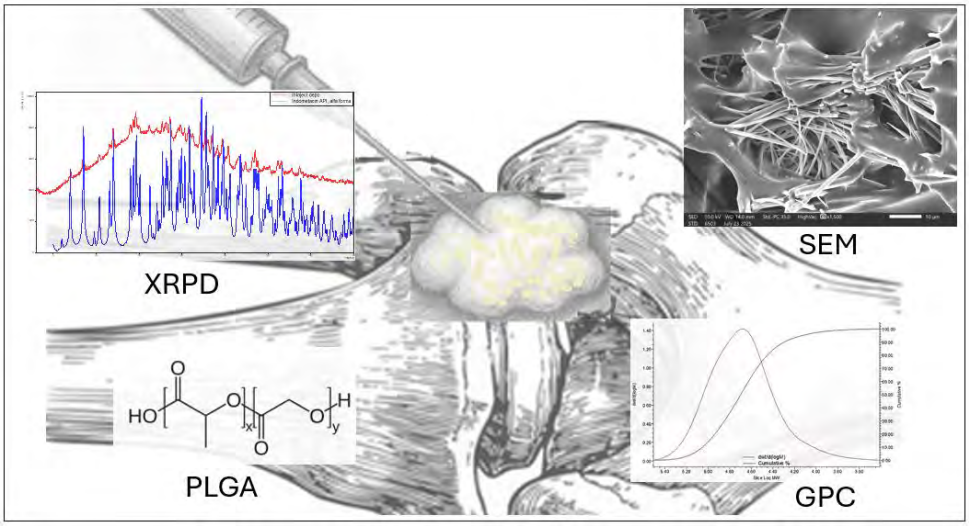
U ovom radu provedena je detaljna karakterizacija dozirnog sustava temeljenog na biorazgradivim PLGA kopolimerima, razvijenog za produljeno oslobađanje indometacina. Morfološka analiza dozirnog sustava provedena je primjenom mikroskopskih tehnika (SEM, ESEM) i rendgenske difrakcije (XRPD), s ciljem razumijevanja površinske i unutarnje strukture dozirnog sustava.
Kromatografija na propusnom gelu (GPC) s višestrukom detekcijom korištena je za praćenje promjena u molekulskim masama PLGA kopolimera tijekom vremena. Paralelno je analizirana i kemijska stabilnost indometacina kako bi se utvrdile moguće degradacijske promjene tijekom dugotrajnog otpuštanja lijeka.
Dobiveni rezultati ukazuju na kompleksan mehanizam oslobađanja lijeka, koji uključuje difuziju, degradaciju polimera i interakcije između djelatne tvari i polimerne matrice. Identificirani su ključni procesi koji su uključeni u cjelokupni mehanizam oslobađanja lijeka te njihova dinamika, čime se omogućuje bolje razumijevanje i optimizacija formulacija za dugotrajnu terapijsku primjenu.

[1] Y. Su et al., Drug Deliv. 28 (2021) 1397-1418.
[2] J. Siepmann, F. Siepmann, Elsevier (2025) 10
[3] K. Hasegawa et al., RSC Adv. 14 (2024) 4129.



PRIPRAVA I KARAKTERIZACIJA BIOPOLIMERNIH PREVLAKA S HITOZANOM I PROPOLISOM NA TEKSTILU

PREPARATION AND CHARACTERISATION OF BIOPOLYMER COATINGS WITH CHITOSAN AND PROPOLIS ON TEXTILES

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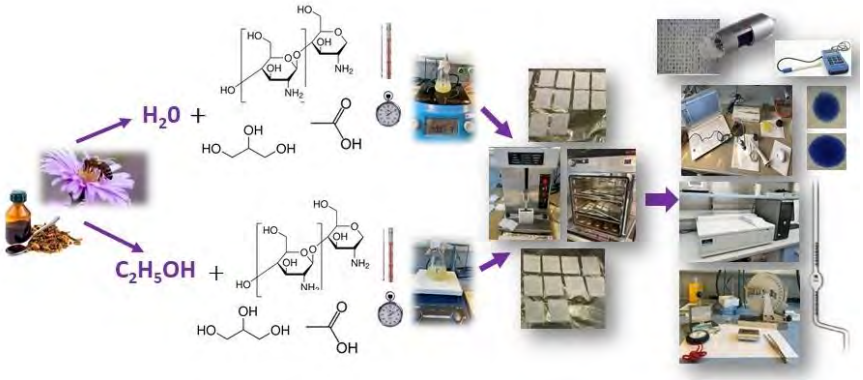
The development of environmentally friendly biopolymer coatings for medical and cosmetic textiles represents an important step prior to their practical application. Propolis and chitosan are recognized as natural materials with pronounced antibacterial and antiseptic properties, making them suitable for use in functional textile materials. In this study, aqueous and alcoholic extracts of propolis, as well as chitosan solutions with and without the addition of glycerol containing propolis, were analyzed. Prior to application onto planar textiles (surgical fabric), the surface tension of propolis solutions was determined using the stalagmometric method, while the presence of active compounds was examined by UV–VIS spectrophotometry. Textile modification was carried out using the dip-coating method to form biopolymer coatings. The samples were characterized in terms of physicochemical properties, treatment uniformity, recovery angle, and pH values. The unmodified sample was additionally analyzed with respect to its morphological, structural, and dimensional characteristics.

The results show that the fabric thickness increased by a maximum of 1.35% after modification, while the mass of the samples increased from 1.72% to 11.74%, which does not represent a significant burden for the materials prior their potential surgical, medical or cosmetic application. The drop test confirmed hydrophilicity and immediate absorption of methylene blue, which are highly favorable characteristics for materials intended for direct contact with the skin. Furthermore, the pH values of the modified samples were compatible with skin pH, and recovery angles ranging from 81.25° to 103.75° indicate preserved elastic behavior of the fabric. UV–VIS analysis demonstrated that ethanol was the most effective pure solvent for propolis, while the chitosan–glycerol mixture enabled a significantly higher amount of dissolved active compounds compared to all tested pure solvents. Moreover, the alcoholic extract of propolis exhibited the presence of additional active compounds, as confirmed by UV–VIS spectrophotometric analysis.

The obtained results confirm that fabrics modified with aqueous and alcoholic propolis extracts, as well as chitosan with added propolis, are suitable for usage as medical and cosmetic materials. The development and characterization of such coatings represent a significant advancement in the functional modification of textiles, with strong potential for application in surgical, cosmetic, and other medical products, while enabling further development of advanced, innovative, and functional textile materials.



TEXTURAL PROPERTIES OF Ca–Si ADSORBENTS SYNTHESIZED FROM NATURAL OPOKA

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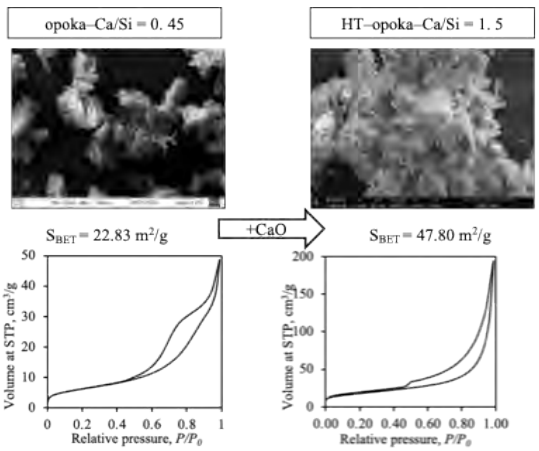
Currently, low-cost and effective wastewater purification has gained worldwide attention. Natural opoka has recently been recognized as a suitable reactive medium for onsite wastewater treatment systems due to its high phosphorus sorption capacity. However, the effectiveness of natural opoka as a phosphorus sorbent is strongly influenced by its mineralogical composition and a range of physicochemical properties, including silica crystallinity, calcium content, specific surface area, porosity, particle size distribution, surface charge, and pH-dependent reactivity, all of which collectively govern phosphorus adsorption capacity, binding mechanisms, and long-term stability. As a result, there is increasing interest in modifying naturally occurring materials, including the aforementioned natural opoka, to enhance their surface characteristics, stability, and adsorption capacity, thereby boosting their potential as affordable adsorbents for sustainable wastewater treatment.

To achieve this goal, the effects of calcination and hydrothermal treatment on the texture and mineralogical composition of Ca–Si based adsorbents derived from natural opoka were studied. Initially, opoka was calcined at 850 °C to produce the first adsorbent with a Ca/Si molar ratio of 0.45. To improve textural properties, hydrothermal treatment was also applied during the further synthesis of the second adsorbent. Low surface area is likely caused by low calcium content in opoka (25 wt.%); thus, to increase surface area up to 150 m^2/g (value reported in the literature), the Ca/Si molar ratio was increased to 1.5 by adding calcium oxide. Hydrothermal synthesis was conducted in unstirred suspensions under saturated steam at 200 °C for 16 hours. The synthesized adsorbents were characterized by X-ray diffraction (XRD), specific surface area (S_{BET}), and scanning electron microscopy (SEM) analysis.

XRD results showed that the first Ca–Si based adsorbent, consisted primarily of wollastonite, quartz, and tridymite. The sample exhibited both mesoporous and macroporous structures with a specific surface area of 22.83 m^2/g. This adsorbent demonstrated moderate phosphorus removal efficiency (18–25%). After hydrothermal treatment, the XRD results of the synthesized second Ca–Si based adsorbent showed the formation of crystalline calcium silicate hydrates, tobermorite, and α-C_2SH, alongside unreacted quartz and calcite. This sample also contained mesopores and macropores, similar to the previously described first adsorbent, but its specific surface area increased to approximately twice that value, reaching 47.80 m^2/g. SEM analysis revealed agglomerated particles ranging from 3 to 20 μm in both adsorbents; however, the second Ca–Si based adsorbent sample displayed distinct honeycomb-like particles with an open-framework structure characteristic of semicrystalline calcium silicate hydrates, thereby enhancing surface area and pore accessibility. Further experiments demonstrated that the second adsorbent exhibited significantly improved phosphorus adsorption performance, achieving up to 98% removal efficiency.

[1] M. Akhtar et al., Desalin. Water. Treat. 321 (2025) 100914.
[2] S. Gubernat et al., Materials. 13 (2020) 3377.
[3] H. Alkhaldi et al., RSC Advances 14 (2024) 33143–33190.



TOPLINSKA SVOJSTVA FORMULACIJA POLI(LAKTIDNIH-*KO*-GLIKOLIDNIH) KOPOLIMERA I LIJEKA KAO POTENCIJALNIH SUSTAVA ZA ISPORUKU S PRODULJENIM OSLOBAĐANJEM

THERMAL PROPERTIES OF POLY(LACTIDE-*CO*-GLYCOLIDE) COPOLYMER AND DRUG FORMULATIONS AS POTENTIAL DELIVERY SYSTEMS WITH EXTENDED RELEASE

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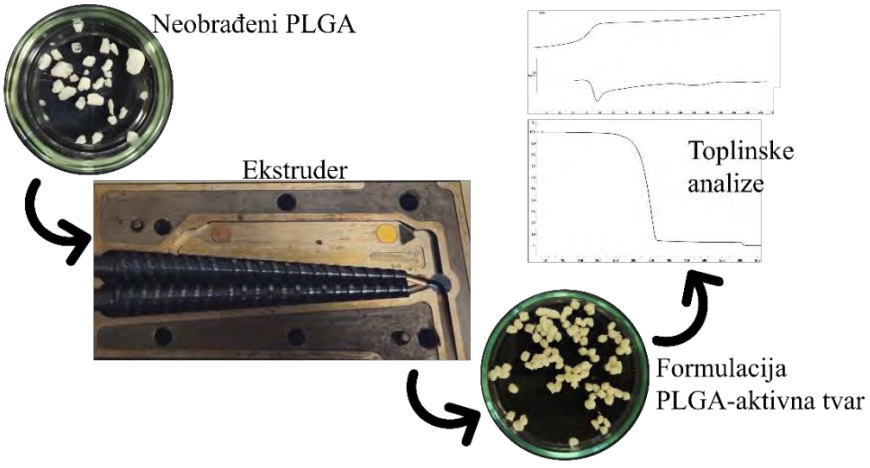
Bolesti mišićno-koštanog sustava kao osteoartritis zahvaćaju 528 milijuna ljudi globalno.[1] Nesteroidni protuupalni lijekovi (NSAID) koriste se za ublažavanje simptoma navedenih bolesti. Učestala oralna primjena NSAID lijekova može oštetiti probavni trakt, stoga je potrebno pripremiti formulaciju polimer-lijek s produljenim oslobađanjem lijeka, čime se smanjuje potreba za učestalom primjenom.[2] Upravo se zbog toga koristi sustav parenteralne primjene lijeka koja zaobilazi probavni trakt te ujedno poboljšava apsorpciju lijeka i lokalizira njegovu primjenu.[3] Poli(laktid-*ko*-glikolid) PLGA kopolimer, zbog svoje biokompatibilnosti i biorazgradivosti učestalo se koristi kao nosač u sustavima s produljenim oslobađanjem lijeka.[4] Kako bi se ispitali utjecaji vrste PLGA kopolimera (molarna masa, udio laktida/glikolida, efekte krajnjih skupina) na toplinska svojstva formulacija, pripremit će se smjese kopolimera (PLGA) i lijeka. Za pripremu formulacija polimera i lijeka korišten je ekstruder, a smjesa se zamiješavala pri sljedećim parametrima: temperatura od 80 °C, brzina mješanja kontrarotacijskih vijaka od 60 min^{-1} te vrijeme mješanja od 5 minuta. Smjesa je karakterizirana toplinskim metodama – razlikovnom pretražnom kalorimetrijom (DSC) i termogravimetrijskom analizom (TGA) u cilju određivanja utjecaja dodatka lijeka i obrade na toplinske prijelaze i stabilnost sustava.

[1] World Health Organization, WHO Fact Sheets (2023).
[2] M. Arabia et al., Part. Part. Syst. Charact. 42 (2025) 2400135.
[3] N. Gulati and H. Gupta, Recent Pat. Drug Deliv. Formul. 5 (2011) 133–145.
[4] J. Walker et al., Drug Deliv. Transl. Res. 13 (2023) 237–251.



PRIPRAVA MEZOSTRUKTURIRANIH $Ce_{1-x}Zr_xO_2$ ČVRSTIH OTOPINA METODOM MEKOG PREDLOŠKA

PREPARATION OF MESOSTRUCTURED $Ce_{1-x}Zr_xO_2$ SOLID SOLUTIONS USING THE SOFT TEMPLATE METHOD

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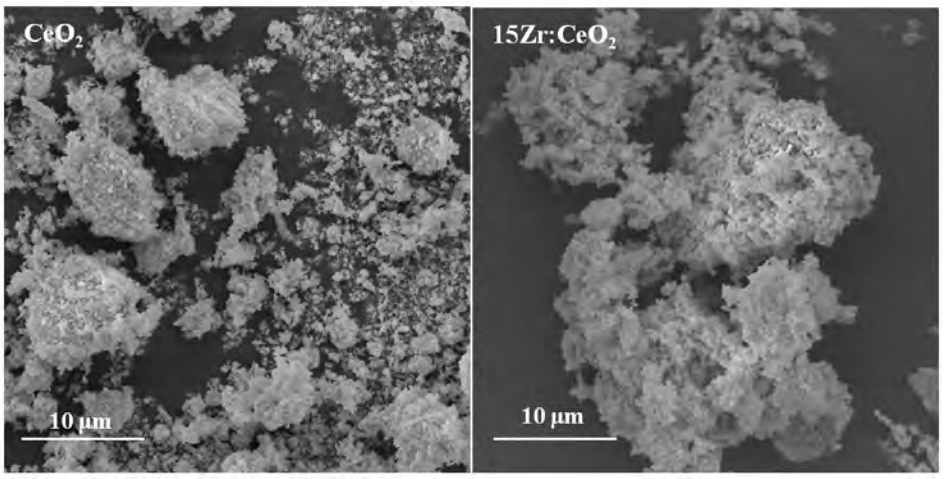
Cerijev(IV) oksid (CeO_2) jedan je od najčešće primjenjivanih oksida lantanoida, ponajprije zbog svoje ekonomske prihvatljivosti te sposobnosti reverzibilnog skladištenja i otpuštanja kisika, što mu osigurava važnu ulogu u katalitičkim procesima. U praktičnoj primjeni, primjerice u katalitičkim konverterima s trostrukim djelovanjem, CeO_2 se često kombinira s cirkonijem. Ugradnjom Zr^{4+} iona u kristalnu rešetku CeO_2 dolazi do stvaranja strukturnih defekata koji povećavaju pokretljivost kisika, reducibilnost Ce^{4+} iona i kapacitet skladištenja kisika. Čvrste otopine $Ce_{1-x}Zr_xO_2$ pokazuju poboljšana redoks svojstva, veću toplinsku stabilnost i otpornost na sinteriranje u odnosu na čisti CeO_2, pri čemu omjer Ce/Zr značajno utječe na katalitičku aktivnost. Mezoporozni materijali posebno su zanimljivi u katalizi zbog velike specifične površine te mogućnosti kontrole veličine, oblika i raspodjele pora. Prikladnim metodama sinteze moguće je pripraviti i mezoporozne materijale uređene mikrostrukture [1]. U ovom radu provedena je sinteza mezostrukturiranih čvrstih otopina $Ce_{1-x}Zr_xO_2$ (x=0; 0,05; 0,1 i 0,15) metodom mekog predloška. Pripravljeni uzorci karakterizirani su rendgenskom difrakcijom na prahu (XRD), infracrvenom spektroskopijom s Fourierovom transformacijom (FTIR), UV-Vis difuznom refleksijskom spektroskopijom (UV-Vis DRS), pretražnom elektronskom mikroskopijom (SEM) i energijski razlučujućom rendgenskom spektroskopijom (EDS). Katalitička aktivnost ispitana je u procesu katalitičke oksidacije modelnog hlapivog organskog spoja.

[1] M. G. Ruiz et al., J. Appl. Res. Technol. 16 (2018) 511-523.



UTJECAJ MODIFICIANJA TiO_2 NA POVRŠINSKA SVOJSTVA TiO_2/PLA KOMPOZITA

INFLUENCE OF TiO_2 MODIFICATION ON SURFACE PROPERTIES OF TiO_2/PLA COMPOSITES

Andrea Špoljarić, Elvira Vidović

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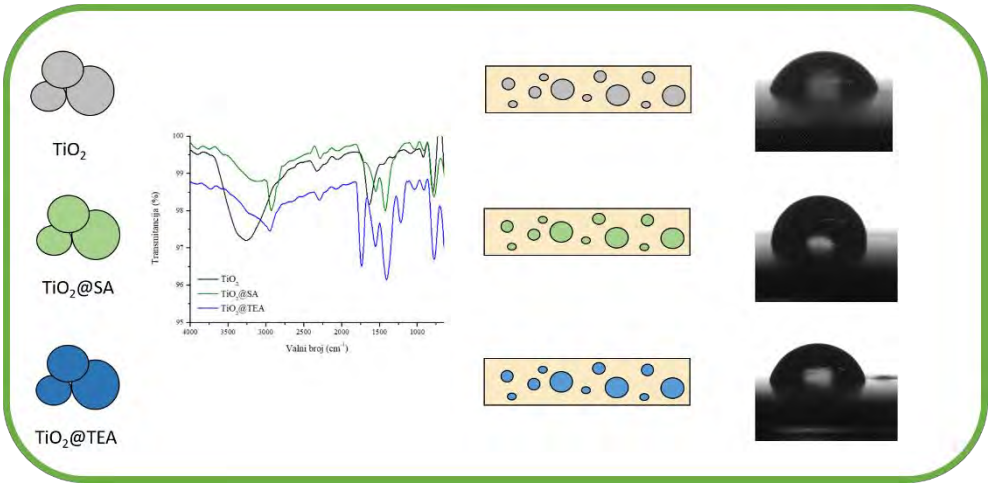
Poli(mliječna kiselina) ili polilaktid (PLA) prepoznat je kao prikladan biopolimer za primjenu u ambalažnoj industriji zbog svoje biorazgradivosti te lakoće prerade. Uvođenje anorganskih punila u PLA matricu dodatno proširuje funkcionalnost materijala, osobito u području aktivne i pametne ambalaže. Titanijev dioksid (TiO_2) ističe se kao punilo koje pridonosi fotokatalitičkom svojstvu materijala čime se može razviti ambalaža sa antimikrobnim učinkom i poboljšanom stabilnosti tijekom izlaganja UV zračenju. U kombinaciji sa PLA matricom, takvi kompoziti predstavljaju održivu i funkcionalnu alternativu konvencionalnim polimernim materijalima u industriji ambalaže [1]. Glavni izazov koji se susreće u pripravi nanokompozita i kompozitnih materijala postizanje je jednolike raspodjele punila kroz materijal. Homogeniju raspodjelu i bolju dispergiranost moguće je postići tretiranjem površine punila primjerice dodatkom modifikatora. Modifikatori su tvari koji se jednim dijelom svoje molekule površinski vežu sa česticama punila uz pomoć kemijskih interakcija, dok drugim dijelom molekule ostvaruju interakcije sa kompozitnom matricom.
Cilj ovog rada bio je pripremiti PLA kompozite s nemodificiranim TiO_2 te TiO_2 česticama modificiranima trietilaminom odnosno stearinskom kiselinom. Kompoziti su pripremljeni u Brabender gnjetilici te oblikovani u pločice prešanjem. Kako bi se utvrdila uspješnost površinske modifikacije i njen utjecaj na svojstva materijala, provedene su FTIR spektroskopija, mjerenje kontaktnog kuta i TGA analiza. Dobiveni rezultati pokazali su da je odabirom odgovarajućeg modificirajućeg sredstva moguće ciljno prilagoditi površinska svojstva kompozita, pri čemu njegova toplinska stabilnost ostaje očuvana.

[1] J. K. Nayak et al., J. Mol. Struct. (2024) 138892.



INFLUENCE OF SYNTHETIC CONDITIONS ON THE NUCLEARITY OF COPPER HYDRAZONE COMPLEXES

Juraj Toplak, Dino Kuzman, Višnja Vrdoljak

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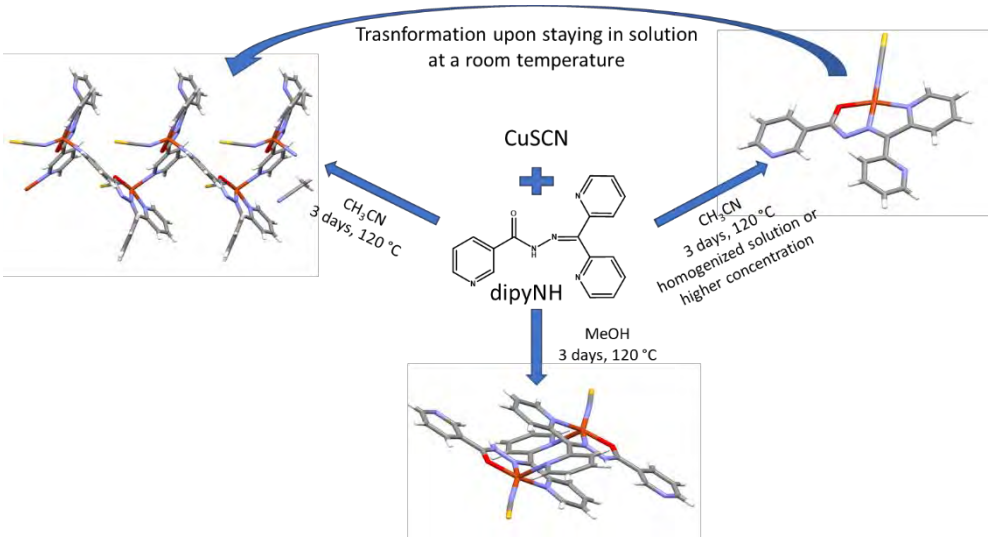
The nuclearity, and consequently the properties of a complex, is most strongly influenced by the nature of the metal center, ligand, and counterions. However, the synthetic conditions and methods often have a decisive effect on the reaction outcome. By varying reaction parameters, particularly the solvent, it is possible to obtain complexes with different geometries and nuclearities. As the number of publications increases, so does the number of syntheses that cannot be reproduced. A common reason for irreproducibility is the absence of a key procedural detail. Therefore, the main focus of this poster is the importance of synthetic conditions and their impact on reaction outcomes. To this end, new copper complexes with hydrazone ligands were synthesized. Interest in these compounds is growing due to their biological properties. Moreover, because of the rich coordination chemistry of copper and the versatile binding modes of polydentate hydrazone ligands, these complexes exhibit significant structural diversity. The new Cu(II) complexes were prepared via a solvothermal method by reacting copper(I) thiocyanate with a preformed tridentate hydrazone ligand. The synthesis was carried out under variations of solvent, stoichiometric ratios, concentration, and solution homogeneity. An unhomogenized reaction in acetonitrile resulted in the formation of a monomer, whereas homogenization produced a mixture of monomeric and polymeric species. Increasing the solution concentration led to the formation of only the monomer, regardless of homogenization. The stoichiometric ratio of CuSCN:ligand in these reactions was 1:2. When methanol was used as the solvent, a dinuclear complex was isolated from the filtrate, where the stoichiometric ratio in the unhomogenized solution was 1:1. The one-dimensional coordination polymer crystallizes as a solvate and, like the dimer, exhibits a square-pyramidal geometry at the copper center, in contrast to the planar geometry of the monomer. The reaction system is dynamic, as demonstrated by the transformation of the monomer into the polymer upon standing in solution for two weeks.

[1] R. G.Bergman, R. L. Danheiser, Angew. Chem. Int. Ed. 55 (2016) 12548-12549.
[2] Reproducing synthesis, Nat. Synth. 3 (2024) 419-420.
[3] V. P. Singh, Spectrochim. Acta, Part A 71 (2008) 17-22.
[4] V. Vrdoljak et al., New J. Chem. 40 (2016) 9263-9274.
[5] D. A. Tafere et al., RSC Adv. 15 (2025) 6191-6207.



ISTRAŽIVANJE MEHANIČKIH SVOJSTAVA SAVITLJIVIH KRISTALA STATIČKIM VLAČNIM POKUSOM

INVESTIGATION OF MECHANICAL PROPERTIES OF FLEXIBLE CRYSTALS BY STATIC TENSILE TESTING

Matteo Zausnig, Mateja Pisačić, Božena Lovrić, Marijana Đaković

University of Zagreb Faculty of Science, Department of Chemistry, Horvatovac 102a, 10 000 Zagreb, Croatia
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Advanced technologies continuously impose new and additional requirements on materials intended for use in smart devices, with flexibility among the most desired material properties. The inherent inelasticity of most crystalline materials, despite their numerous advantages, significantly limits their applicability in modern technological systems.[1-2] Over the past decade, a growing number of studies have focused on crystals capable of adapting to various external stimuli;[3-6] however, their effective implementation requires precise control of mechanical behaviour and a comprehensive understanding of the materials' mechanical characteristics.

In this contribution, the mechanical properties of crystals exhibiting mechanical flexibility are investigated, and their mechanical behaviour is analysed by static tensile testing. Particular emphasis is placed on the determination of Young's modulus of elasticity as a key parameter quantifying the resistance of a material to elastic deformation. Young's modulus is determined from the slope of the linear region of the stress–strain relationship, accounting for the geometric dimensions of the investigated crystals, thereby enabling the reliable determination of elastic properties within the elastic deformation regime.

Crystals of cadmium(II) coordination polymers with pyrazinamide and chloride or bromide ligands were examined, revealing noticeable differences in Young's modulus, which are in agreement with the theoretical model and our prior findings.[7] Measurements were carried out using a specially designed device for static tensile testing of small-scale samples. The setup allows gripping and fixation of individual crystals, the application of uniaxial force (0.1 mN to 500 mN), and simultaneous measurement of force and displacement. The system enables automated data acquisition, while data processing is performed using a Python script, yielding both graphical representations and numerical values of Young's modulus of elasticity.

[1] P. Naumov et al., Chem. Rev. 115 (2015) 12400–12490.
[2] S. Saha et al. Acc. Chem. Res. 51 (2018) 2957–2967.
[3] M. Đaković et al., Angew. Chem. Int. Ed. 57 (2018) 14801–14805.
[4] M. Pisačić et al., Chem. Mater. 33 (2021) 3660–3668.
[5] M. Pisačić et al., Chem. Mater. 34 (2022) 2439–2448.
[6] O. Mišura et al., Cryst. Growth & Des., 23 (2023) 1318 –1322.
[7] M. Đaković et al., J. Am. Chem. Soc. 147 (2027) 22219–22227.

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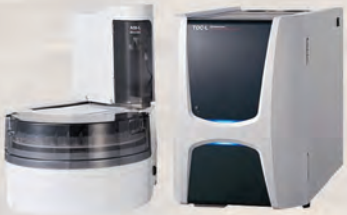
Sustavi za plinsku kromatografiju (GC) osiguravaju pouzdanu i osjetljivu analizu hlapljivih spojeva sadržanih u uzorku.

Masena spektrometrija s induktivno spregnutom plazmom (ICP-MS) je tehnika u kojoj se induktivno spregnuta plazma koristi kao ionizacijski izvor, a detekcija se vrši masenom spektrometrijom.

Spektrofotometri mjere intenzitet svjetlosti koju apsorbiraju ili emitiraju kemijske tvari.

Analizatori ukupnog organskog ugljika (TOC) mjere ukupnu količinu organskog ugljika u vodi, plinovima i čvrstim tvarima. Zadovoljavaju raznolik raspon potreba u područjima kao što su istraživanje okoliša, kontrola kvalitete i upravljanje procesima.



Sustavi za plinsku kromatografiju - masenu spektrometriju (GC/MS) omogućuju brzu identifikaciju nepoznatih komponenti i preciznu kvantitativnu analizu, čak i za komponente u tragovima.

Sustavi za visoko učinkovitu tekućinsku kromatografiju (HPLC) podržavaju širok raspon aplikacija, uključujući analizu hrane, lijekova te uzoraka iz okoliša.

Sustavi za tekućinsku kromatografiju (LC) uspješno razdvaja tvari na osnovi razmještanja između čvrste stacionarne faze i tekuće mobilne faze.

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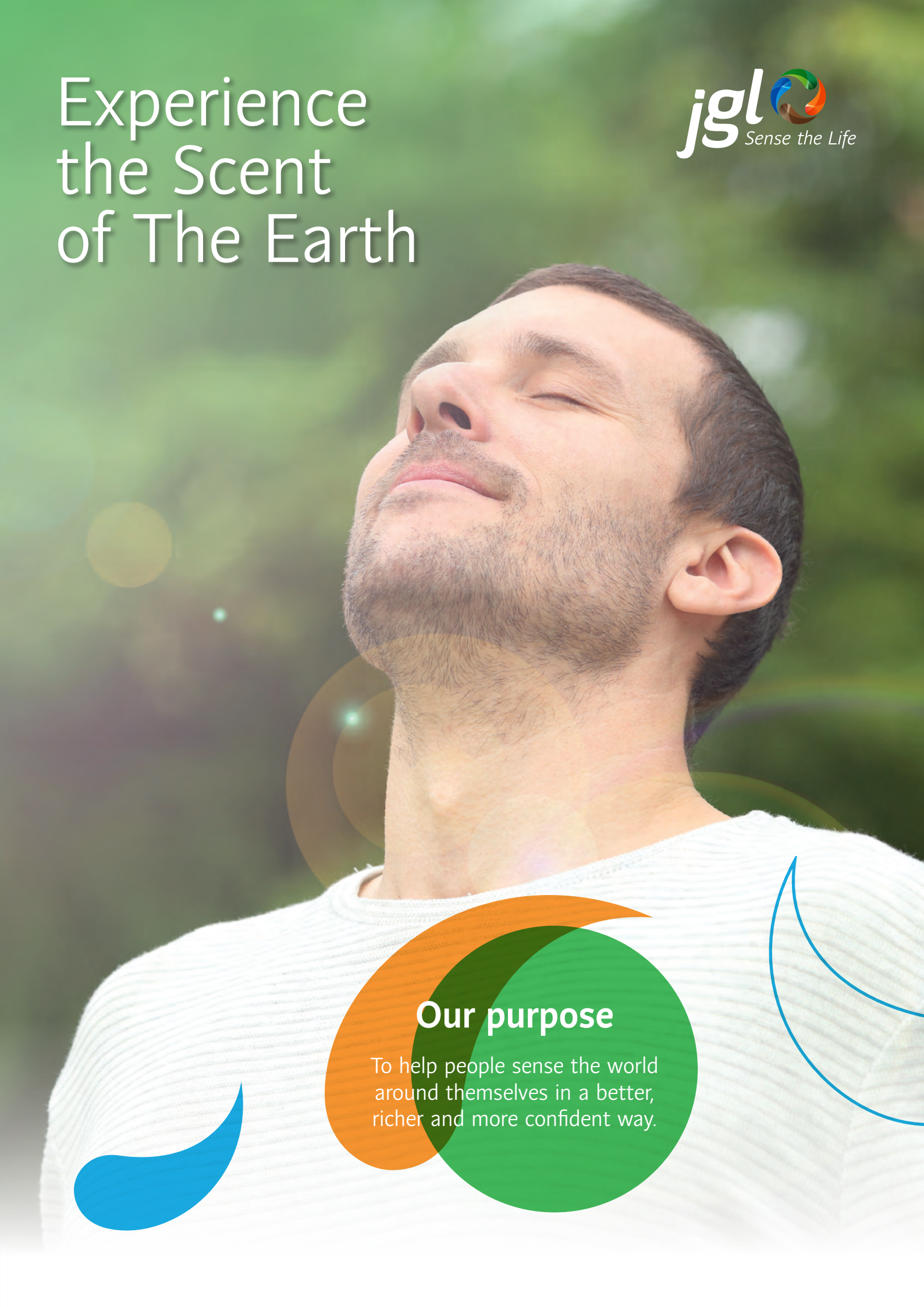

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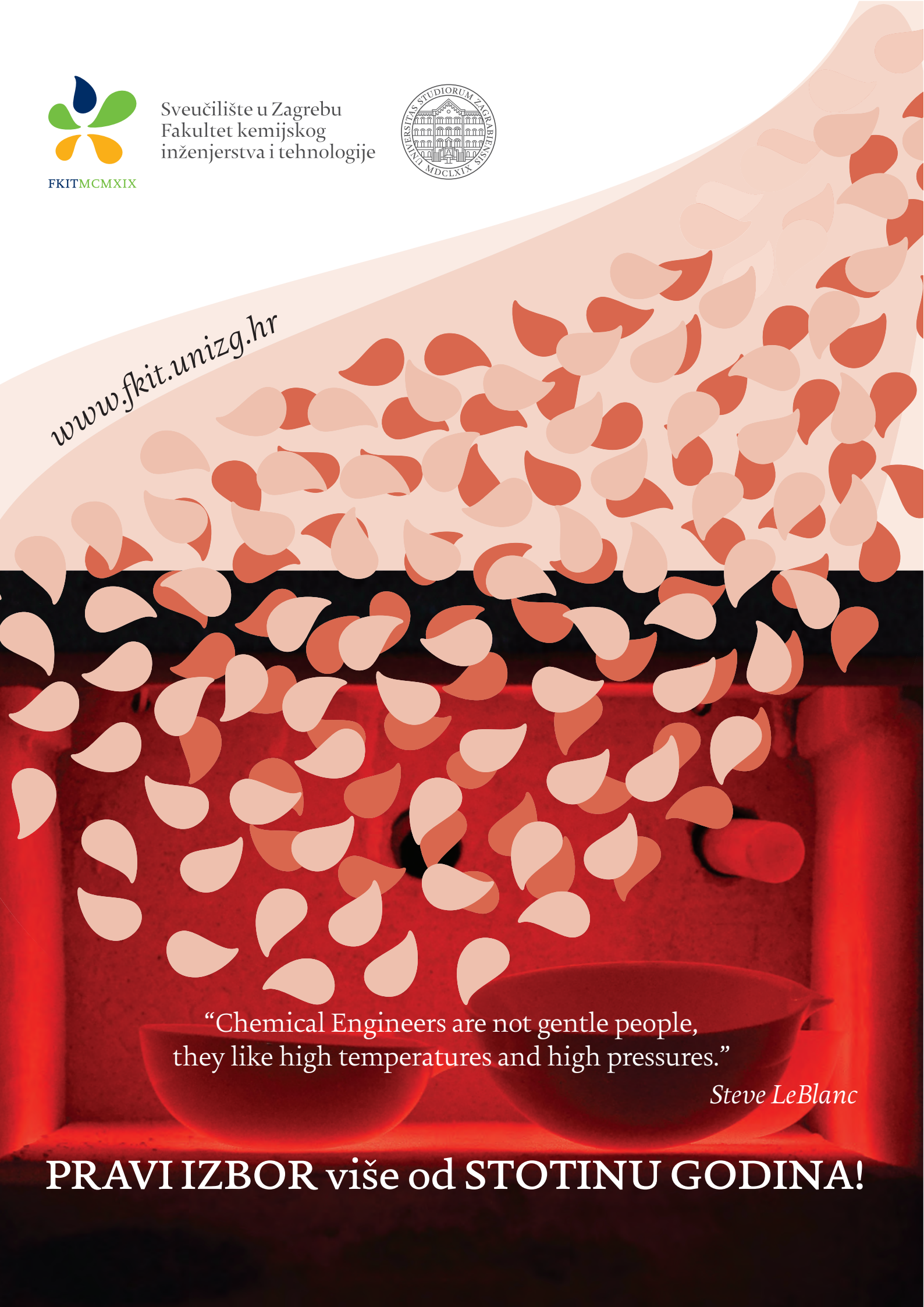

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