BOOK OF ABSTRACTS

10th Symposium of Chemistry Students

10th and 11th of October 2025

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Zagreb, Croatia

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PREFACE BY THE PRESIDENT OF THE ORGANIZING COMMITTEE

Dear participants,

on behalf of the Organizing Committee, it is my great pleasure to welcome you to the 10th Symposium of Chemistry Students taking place at the Department of Chemistry, Faculty of Science, University of Zagreb.

Since this is the jubilee Symposium, we as organizers had the daunting task of not letting down those who brought the idea of SiSK to life and helped develop the Symposium into the event it is today. Eleven years and nine symposia later, our mission is still the same: to host a scientific event organized by students for students to present their research, meet peers of similar interests, connect with professionals from industry and academia, and most importantly, ask questions. Dedicating time to research, on the path to becoming a chemist, provides students with a strong foundation for their future careers and is necessarily marked by passion, hard work, and curiosity [1]. Since seemingly few chemists have died of curiosity [2], I invite you all to ask questions, listen to various presentations and lectures, participate in discussions during the roundtables and the poster section, and enjoy the Symposium.

We are deeply grateful to the Croatian Chemical Society, led by Professor Vladislav Tomišić, for the ongoing support of this event. Also from the CCS, we would like to thank Danijel Namjesnik and Andrea Usenik for their guidance, support, and many well-placed critiques. Additionally, we would like to thank the Department of Chemistry, formerly headed by Professor Snežana Miljanić and currently by Professor Višnja Vrdoljak, for enabling us to host the Symposium at the Department of Chemistry. We would also like to thank all our sponsors, donors, and partners, because their generous support once again made it possible to organize the Symposium as a free scientific conference.

Most of all, I must thank the whole team of talented and passionate individuals who came together and made this event possible. I believe all our efforts will pay off as we try to inspire and interconnect the next generations of young chemists.

Finally, dear participants, I hope this Book of Abstracts Preface finds you well, and you find new ideas and bonds at the 10th Symposium of Chemistry Students!

Jakov Borovec

President of the Organizing Committee of the 10th SiSK

[1] D. Cinčić, *The Role of Skill Development in Scientific Research Work on Education and Professional Growth of Students*, 10th Symposium of Chemistry Students, Zagreb, 2025, Book of Abstracts, 23.

[2] Not supported by statistical data from a reliable source.

PREFACE BY THE HEAD OF STUDENT SECTION OF CCS

Dear students, professors, assistants, and all other participants of the Symposium,

It is my honor to write this preface for the fourth time. My long period as Head of the Student Section has now brought me to this 10th jubilee SiSK. Unfortunately, it is also my last one in this role… Over the years, I have exhausted most of the words I could use in such a preface, and as I mentioned last year, it might be expected that I have nothing new left to say. But I repeat – this is SiSK! There is always something new!

We are keeping the two-day event format after introducing it experimentally last year. Although it is more difficult and complicated to organize, it has proven to be a more diverse program, more interesting for students and Symposium visitors, and most importantly – more educational. The number of student oral presentations has been increased, since we must not forget that this is, above all, a student conference! Its purpose is to give students the chance to present their research results in front of a familiar audience, to learn from one another, and to gain experiences that will ease their paths in the future.

Over the four years of my leadership of the Section, and indirectly of the Symposium, I can say that the progress has been enormous. When we started with the 7th SiSK, completely inexperienced in organizing such an event and thrown into a whole new world, we still managed to create a one-day event that became a turning point and a high standard for us to follow. More than 300 participants – a day to remember. And then we continued, introducing the teaching section, expanding to a two-day program, adding roundtables and panels… the standard kept rising, and SiSK became more and more recognizable! And just when it seemed like the right moment to step down, the jubilee 10th SiSK did not allow us to do so. This one had to be special. That was the goal my deputy Karla and I set, and one which the next generation, who took over from us, is now making a reality.

In addition to a larger number of student presentations, panels, and invited lecturers, the 10th SiSK is also hosting two plenary speakers. One of them is, none other than, a Nobel Prize winner in Chemistry; the other is the very person who started it all – the one who inspired the first generation, the organizers of the very first SiSK, to launch and organize this Symposium. The generation succeeding us has done this job very well! Although this is the first time for all of them, with the guidance and instructions we left behind, they are more than ready for the future! I congratulate them and thank them deeply for taking this task seriously, and I am confident they will organize this Symposium successfully. I do not want to say "perfectly," because this is SiSK, and SiSK can always be better!

To you, dear colleagues and fellow students, I wish that, as before, you see this as something created for you. May you engage even more with the world of science, and may those of you who are active encourage those who are still passive to begin their journey into research. Exchange knowledge, but even more importantly – develop enthusiasm!

This preface, unlike the previous ones, is more personal… I would also like to take this opportunity, besides thanking Jakov, my successor Josip, and their team, to once again

express my gratitude to all those who have been on this path to the 10th SiSK. Especially to my Jelena, Dario, and Magda, who, by leading the previous three Symposia, kept raising the bar higher and higher, all while putting up with me ;) None of this would have been possible without our sponsors and donors, to whom I also extend my thanks. To the professors, assistants, and all other advisors of the Symposium – a huge thank you as well! And finally, my greatest gratitude goes to my Karla, my deputy, who could well be described as the "shadow Head." Without her, none of these Symposia would have been what they were.

Enjoy the 10th SiSK!

Antonio Magnabosco

Dear students, professors, assistant professors and other Symposium participants,

it is an honor to greet you for the first time in the name of the Student Section of the Croatian Chemical Society and wish you a warm welcome to the great tenth edition of the Symposium of Chemistry Students.

During the past four years, my predecessor Antonio and his amazing team have established a very successful set of projects which enrich chemistry students' university experience. I can only hope to properly uphold their work and strive to raise it to an even higher level. A great recognition also goes out to Jakov, President of this year's Organizing Committee, who has, with his sharp and thorough leadership, secured another successful Symposium edition.

For a full decade now, SiSK represents a conference tailored specifically for students. I believe we are all familiar with the challenges of navigating adulthood, and especially the challenging period of starting your professional career after graduation. Therefore, I would like to speak to all fellow students – you are not alone. The Symposium is created exclusively with you in mind, and we will continue to offer as many students as possible a chance to gather valuable skills and to present you and your experimental interests.

I wish you all a fantastic conference experience!

Josip Mikulić

Head of the Student Section of the Croatian Chemical Society

PROGRAMME

FRIDAY

10th of October 2025

11:30	**REGISTRATION OPENING** (hall of the Department of Chemistry, main entrance)	
13:30 – 14:00	**OPENING CEREMONY (A1)**	
	SECTION I (A1) chair: Luka Sumić	
14:00 – 14:45	**PLENARY LECTURE**	**Dominik Cinčić** (Faculty of Science, University of Zagreb): THE ROLE OF SKILL DEVELOPMENT IN SCIENTIFIC RESEARCH WORK ON EDUCATION AND PROFESSIONAL GROWTH OF STUDENTS
14:45 – 15:00	short break	
	SECTION II (A1) chair: Josip Mikulić	
15:00 – 15:30	**INVITED LECTURE**	**Tomislav Begušić** (Institute of Physical and Theoretical Chemistry, University of Würzburg): SIMULATING MOLECULAR QUANTUM DYNAMICS AND SPECTROSCOPY WITH "CLASSICAL" COMPUTERS
15:30 – 15:40	**SHORT PRESENTATION**	**Serbian Young Chemists' Club**
15:40 – 15:50	**SHORT PRESENTATION**	**Leon Poljanić** - UCLouvain
15:50 – 16:10	short break	
16:10 – 17:40	**ROUNDTABLE DISCUSSION (A1)** **From Student to Scientist**	**Katarina Mužina** (chair), **Lara Štorga, Stjepan Dolić, Borna Ferčec, Danijela Barić, Nikola Basarić**
17:40 – 18:30	not-so-short break	
18:30 – 20:00	**POSTER SECTION** (1st and 2nd floor of the Department of Chemistry)	
20:00 – 21:00	**And Now for Something Completely Different: Beer Tasting** (ground level of the Department of Chemistry, -1)	

SATURDAY

11th of October 2025

9:00	**REGISTRATION** (hall of the Department of Chemistry, main entrance)	
9:40 – 10:00	**ANNOUNCEMENTS (A1)**	
	SECTION III (A1) and plenary lecture livestream in A2 chair: Antonio Jularić	
10:00 – 10:45	**PLENARY LECTURE**	**Morten Peter Meldal** (Faculty of Science, University of Copenhagen): MOLECULAR CLICK ADVENTURES: THE INTRAMOLECULAR INAIC-CLICK REACTION
10:45 – 11:15	break	
	SECTION IV (A1) chair: Antonio Jularić	
11:15 – 11:45	**INVITED LECTURE (online lecture)**	**Ivan K. Ilić** (Istituto Italiano di Tecnologia): POWERING EDIBLE ELECTRONICS
11:45 – 12:15	**INVITED LECTURE**	**Tanja Poljak** (Selvita): THE SEARCH FOR MEDICINES: A CHEMIST'S STORY
12:15 – 12:30	short break	
	SECTION V (A1, eng) chair: Ema Begović	**SECTION VI (A2, eng)** chair: Jakov Borovec
12:30 – 12:45	**Adrian Jablan:** THE EFFECT OF FENOFIBRATE ON THE *N*-GLYCOSILATION OF TOTAL SERUM PROTEINS IN PATIENTS WITH TYPE 1 DIABETES MELLITUS	**Ana Francesca Stama:** CROSS-MODAL MOLECULAR REPRESENTATION FUSION FOR ENHANCED MOLECULAR PROPERTY PREDICTION
12:45 – 13:00	**Mislav Vorkapić:** EFFECT OF PHENOL OXIDASE STIMULATION ON *ASPERGILLUS NIGER*–MEDIATED BIOSYNTHESIS OF SILVER NANOPARTICLES	**Antun Zelić:** ENHANCING CHEMICAL PROPERTY PREDICTION THROUGH COMBINED ATOMIC AND MOLECULAR DESCRIPTORS

13:00 – 13:15	**Domagoj Bosiljevac:** POLYPHENOLIC PROFILE AND ANTIOXIDANT CAPACITY OF SELECTED FLOWERING PLANTS BEFORE AND AFTER *IN VITRO* DIGESTION	**Bruna Bakota:** CHOLINESTERASE INHIBITION BY 2-(ACYLAMINO)ACETAMIDES: INSIGHTS FROM QUANTUM CHEMICAL DOCKING
13:15 – 13:30	**Marina Varga, Marija Varga:** NMR ANALYSIS OF OLEUROPEIN AND OTHER BIOACTIVE PHENOLIC COMPOUNDS IN OLIVE LEAF EXTRACT	**Jana Panovska:** MULTI-CRITERIA OPTIMIZATION OF THERAPEUTIC RADIOISOTOPES VIA QUANTITATIVE MCDA
13:30 – 13:45	**GROUP PHOTO**	
13:45 – 15:15	**LUNCH BREAK**	
15:15 – 16:45	**ROUNDTABLE DISCUSSION (A1)** **This Roundtable was Brought to You by ChatGPT**	**Andrea Usenik** (chair), **Luka Sumić, Milica Bogdanović, Predrag Pale, Ernest Meštrović**
16:45 – 17:30	**Chemistry over Coffee** PARTNERS' AND SPONSORS' STANDS (main hall of the Department of Chemistry)	
	SECTION VII (A1, eng/cro) chair: Maria Magdalena Koprek	**SECTION VIII (A2, cro)** chair: Josip Mikulić
17:30 – 17:45	**Sven Marinac:** CALIXARENE-SOLVENT ADDUCTS FORMATION: A COMPREHENSIVE THERMODYNAMIC AND COMPUTATIONAL STUDY	**Mirna Sabol:** ALDEHYDES AS STRUCTURE-DIRECTING AGENTS IN THE MECHANOSYNTHESIS OF ZINC IMIDAZOLATE SOLID FORMS
17:45 – 18:00	**Vito Mijailović:** ADSORPTION OF POLY(4-VINYLPYRIDINE) DERIVATIVES ONTO QUARTZ NANOPLATES: SIDE CHAIN LENGTH IMPACT	**Mila Grgurić:** A ROUTE TO ISOSTRUCTURAL METAL-ORGANIC HALOGEN-BONDED (MOXB) COCRYSTALS WITH DIFFERENT MAGNETIC PROPERTIES
18:00 – 18:15	**Olga Jerković Perić:** CORROSION PROTECTION OF COPPER BY POLY(ALLYLAMINE HYDROCHLORIDE)/POLY(ACRYLIC ACID) MULTILAYER	**Marin Knežević:** FERROCENE PEPTIDES AS MODELS FOR SELECTIVE CATALYSTS
18:15 – 18:30	**Luka Klemen:** CALIXARENES – YES, THEY FLUORESCE!	**Patricija Klanac:** NIOBATE-PHOSPHATE-BASED GLASSES: INFLUENCE OF STRUCTURAL FEATURES ON MOBILITY OF LITHIUM CATIONS
18:30 – 18:45	short break	
	SECTION IX and CLOSING CEREMONY (A2) chair: Ema Begović	
18:45 – 19:15	**INVITED LECTURE**	**Sanja Belić** (Faculty of Sciences, University of Novi Sad): FROM EVIDENCE TO TRUTH: FORENSIC APPROACHES IN CRIME SCENE INVESTIGATION
19:15 - ∞	**Closing Ceremony and Explosive Conclusions by PO Entropija**	
	SYMPOSIUM AFTERPARTY (ground level of the Department of Chemistry, -1)	

PROGRAMME LEGEND

biochemistry

inorganic chemistry

computational chemistry

organic chemistry

engineering

physical chemistry

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SECTION LECTURES

POSTER PRESENTATIONS

PLENARY LECTURES

THE ROLE OF SKILL DEVELOPMENT IN SCIENTIFIC RESEARCH WORK ON EDUCATION AND PROFESSIONAL GROWTH OF STUDENTS

Dominik Cinčić

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As we celebrate the 10th Symposium of Chemistry Students (SCS – *SiSK*), I recognize a noticeable impact of student-led initiatives in promoting scientific research. The SCS (*SiSK*), organized by and for students, has become one of the important steps for chemistry students to share their work, connect with peers, and develop key skills that shape their academic and professional paths.

Based on my experience, engaging in scientific research allows chemistry students to go beyond theory and apply their knowledge in research laboratory. Through lab work and research projects, they develop the skills of critical thinking, experimental design, data analysis, independence in using instruments, problem-solving abilities, and scientific communication. Also, research experience of students builds up their confidence, professional identity, and is a strong foundation for future careers in academia, industry, or education. Organizing and participating in events like SCS (*SiSK*) strengthens leadership, teamwork, and organizational competencies. Students take ownership of their growth, not only as researchers, but also as active contributors to the scientific community. The SCS (*SiSK*) is a nice example of how student passion and dedication can shape them. By dedicating their time to research, students are not only learning chemistry—they are becoming chemists.

MOLECULAR CLICK ADVENTURES: THE INTRAMOLECULAR INAIC-CLICK REACTION

Morten Meldal

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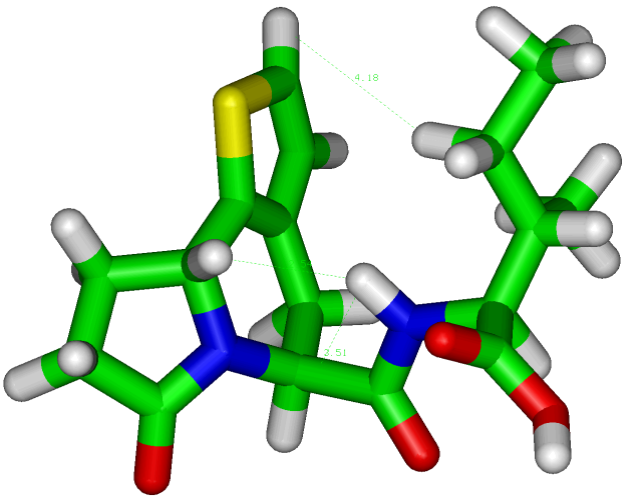
The presentation will take you through the journey of the 2022 chemistry Nobel Prize. During the development solid phase organic combinatorial chemistry, we investigated a large variety of reactions for merger with peptide diversity. It was during this development we discovered the extreme Cu(I) catalysis of triazole formation from azides and alkynes leading to the CuAAC click reaction. We also attempted to use peptide-linked aldehydes as electrophiles for a range of external nucleophiles. However instead, we observed the entropy driven formation of hydroxylactams with further transformation into highly reactive *N*-acyliminium ions through reaction of the aldehydes with upstream amide bonds. This allowed for one of the richest collections of peptide-based heterocycle templates to be accessed through an acid catalysed intramolecular *N*-acyliminium tandem cascade (INAIC) reaction of the aldehyde electrophile, first with one nucleophile, then with a second side chain or backbone nucleophile, both driven by entropy and with complete stereo-control [1]. In addition, carbamides could also be used as a first nucleophile leading to another range of novel molecular scaffolds through the INAIC reaction including heterocycles with interesting fluorescent properties [2]. The fluorescence properties of the novel scaffolds could be developed through mild oxidation conditions and were environment dependable. For both reactions, the heterocycle formation could be performed either during or after assembly of the peptide precursors. The reaction is possessing the properties of a click reaction in being quantitative under benign conditions, completely stereoselective and it can be performed inside a preassembled peptide, which makes it a valuable addition to our structural tools in chemical biology.



[1] T. E. Nielsen, M. Meldal, *J. Org. Chem.* **69(11)** (2004) 3765-3773.

[2] F. Diness, J. Beyer, M. Meldal, *Chemistry* **12(31)** (2006) 8056-8066.

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INVITED LECTURES

SIMULATING MOLECULAR QUANTUM DYNAMICS AND SPECTROSCOPY WITH "CLASSICAL" COMPUTERS

Tomislav Begušić

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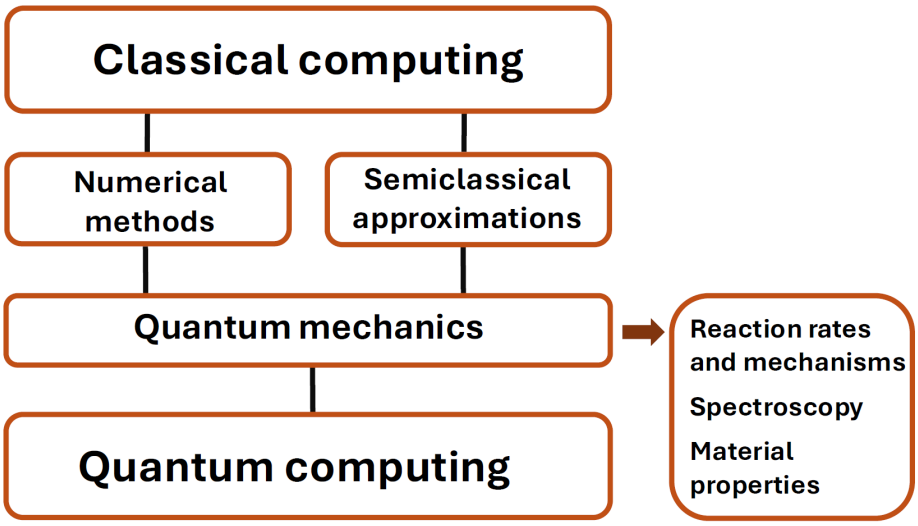
Quantum mechanics describes the microscopic world of atoms and molecules that make up complex, macroscopic materials. Molecular quantum dynamics underlies many observable quantities, such as reaction rates and molecular spectra. Despite the extremely unfavourable formal complexity of simulating quantum dynamics with ordinary (classical) computers, theoretical chemists can often provide accurate estimates of common observables. We achieve this either by identifying tractable numerical procedures for describing quantum-mechanical effects or by resorting to (semi)classical approximations that can be efficiently simulated on modern-day computers. Quantum computing offers an alternative approach, where one hopes to directly emulate the real-world quantum mechanics in a controlled quantum device. In my talk, I will show how our tools for classical computers can be improved and extended to describe quantum-mechanical phenomena and argue that the true utility [1] of quantum computers has yet to be demonstrated. First part of the talk will focus on semiclassical dynamics methods [2] and their application to time-resolved vibrational spectroscopy of liquids [3]. In the second part, I will present more recent work on the numerical simulation of quantum dynamics in discrete systems, such as qubits in a quantum computer [4].



[1] Y. Kim *et al.*, *Nature* **618** (2023) 500–505.
[2] T. Begušić, G. A. Blake, *Nat. Commun.* **14** (2023) 1950.
[3] M. Grechko *et al.*, *Nat. Commun.* **9** (2018) 885.
[4] T. Begušić, J. Gray, G. K.-L. Chan, *Sci. Adv.* **10** (2024) eadk4321.

FROM EVIDENCE TO TRUTH: FORENSIC APPROACHES IN CRIME SCENE INVESTIGATION

Sanja Belić

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Crime scene investigation represents one of the key segments of forensic practice, as it ensures the proper collection, preservation, and interpretation of material evidence that is crucial for judicial proceedings. The reliability of this process directly influences the outcome of investigations and criminal cases, which makes its methodological precision of exceptional importance.

This lecture examines the forensic approach to crime scenes through its main phases: gathering initial information, securing and marking the scene, numbering and photographing traces, as well as the proper sampling, packaging, transport, and storage of evidence. Special emphasis is placed on biological traces and DNA material, given their high evidentiary value and susceptibility to contamination. Furthermore, the importance of modern technologies, such as digital imaging and three-dimensional reconstruction of crime scenes, is highlighted as a means of improving the quality of investigations.

Through a case study of homicide, it is demonstrated how coordinated cooperation between the police, forensic experts, and criminal-technical services enables the successful resolution of complex criminal offenses and reduces the risk of judicial errors. This confirms the indispensable role of forensic methodology in transforming traces into legally valid evidence and in strengthening the integrity of the criminal justice system.

POWERING EDIBLE ELECTRONICS

Ivan K. Ilić[1], Valerio Galli[2], Mario Caironi[1]

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Edible electronics attracted great attention recently, due to their potential to revolutionize not only food industry, but also healthcare of gastro-intestinal tract [1]. Large amount of food is wasted every year as end-consumers, unsure if it is suitable for consumption, discard it as its past the best use before date. Edible sensors integrated as a part of food packaging could solve this problem, as they could detect potentially harmful chemicals and microorganisms. Furthermore, the healthcare of gastro-intestinal tract is often neglected, as diagnostic techniques, gastroscopy and colonoscopy, are complicated, risky, and painful. Edible electronic devices could replace these techniques by detecting variety of factors that indicate potential illnesses. While many edible electronic devices, such as transistors, antennas, and sensors, have been developed, a device delivering current at almost constant potential was missing. In our team we developed an edible battery that can deliver current at constant potential (around 0.65 V) [2]. The battery utilizes riboflavin and quercetin, common food additives, as anode and cathode materials, respectively. While this battery is made from food-grade materials only, its working principle is similar to any other rechargeable battery, such as Li-ion. Lastly, we demonstrate this battery can power variety of devices, such as LED, showcasing its applicability.

[1] A. Sharova *et al.*, *Adv. Mater. Technol.* **6** (2021) 2000757.

[2] I. K. Ilić *et al.*, *Adv. Mater.* **35** (2023) 2211400.

THE SEARCH FOR MEDICINES: A CHEMIST'S STORY

Tanja Poljak

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The landscape of modern drug discovery has been transformed over the past two and a half decades [1]. While small molecules continue to dominate in number, the field has seen a proliferation of new therapeutic modalities, including biologics, peptides, and oligonucleotides. New approaches like PROTACs have already validated their potential in the clinic [2], while macrocycles and peptidomimetics are enabling the targeting of previously inaccessible, broad and flat protein-protein interaction sites [3]. Parallel to this shift in modalities, our understanding of biological targets has evolved. Following successful campaigns against kinases and GPCRs, the scientific community is now pursuing what many consider the new holy grail of drug discovery: RNA [4].

Throughout these rapid changes, the chemist has remained at the centre of innovation. Their diverse expertise, from small and large-scale synthesis to computational modelling, analytical and solid-state chemistry, is essential for every stage of the drug development pipeline. To navigate this dynamic environment, chemists must cultivate a mindset of continuous learning, creativity, and curiosity. They must build and grow their technical knowledge, stay up to date of the scientific literature, and apply this knowledge to solve the complex challenges of drug discovery.

[1] N.A. McGrath, M. Brichacek, J.T. Njardarson, *J. Chem. Ed.* **87** (2010) 1348.

[2] G. Zhong, X. Chang, W. Xie, X. Zhou, *Sig Transduct Target Ther* **9** (2024) 308.

[3] M.L. Peterson, *American Pharmaceutical Review* (2017).

[4] S. Kovachka, M. Panosetti, B. Grimaldi, S. Azoulay, A. DiGiorgio, M. Duca, *Nature Reviews Chemistry* **8** (2024) 120.

SECTION LECTURES

CHOLINESTERASE INHIBITION BY 2-(ACYLAMINO)ACETAMIDES: INSIGHTS FROM QUANTUM CHEMICAL DOCKING

Bruna Bakota, Jakov Borovec, Toni Divjak, Alma Ramić,
Ines Primožič, Tomica Hrenar

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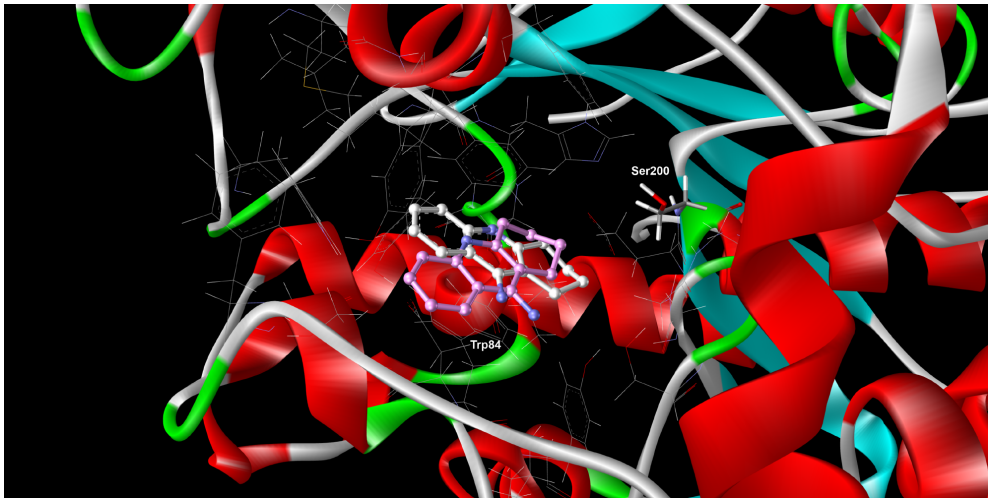
Alzheimer's disease is a serious and progressive brain disorder leading to substantial memory loss and cognitive impairment. A leading theory, the *cholinergic hypothesis*, suggests that a decline in the neurotransmitter acetylcholine plays a key role in the disease's development. Acetylcholine, crucial for learning, memory, and attention, is regulated by the enzymes acetylcholinesterase (AChE) and, to a lesser extent, butyrylcholinesterase (BChE). Given the association between reduced acetylcholine and Alzheimer's disease, cholinesterase inhibitors are used to increase acetylcholine levels in synapses and mitigate symptoms [1,2].

To explain the experimental data on the reversible inhibition of hAChE and hBChE by the prepared compounds, the binding modes of 2-(acylamino)acetamides to cholinesterases were investigated using semi-flexible quantum-chemical molecular docking. A recently developed parallelized *Monte Carlo* algorithm was used for generating diverse conformational ensembles, accounting for translational, rotational, and torsional degrees of freedom, while eliminating structures with steric clashes [3]. Binding enthalpies within the enzyme active site were estimated using PM7 single-point quantum chemical calculations, whereas the method was validated using the known crystal structures of AChE and commercial drugs. The resulting 1000 lowest-energy configurations were later optimized, clustered, and ranked by the binding energy. Finally, docked structures were analyzed using an automated hydrogen bond search module and visual inspection.



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

[1] A. V. Terry, J. J. Buccafusco, *Pharmacol. Exp. Ther.* **306** (2003) 821–827.

[2] D. Madhubala, A. Patra, M. R. Khan, A. K. Mukherjee, *Phytother. Res.* **38** (2024) 2993–3019.

[3] T. Hrenar, ***qcc***, *Quantum Chemistry Code*, rev. 0.68268, 2025.

POLYPHENOLIC PROFILE AND ANTIOXIDANT CAPACITY OF SELECTED FLOWERING PLANTS BEFORE AND AFTER *IN VITRO* DIGESTION

Domagoj Bosiljevac[1], Valerija Vujčić Bok[1], Ivana Šola[2], Ana Vukres[2], Gordana Rusak[2], Željan Maleš[1]

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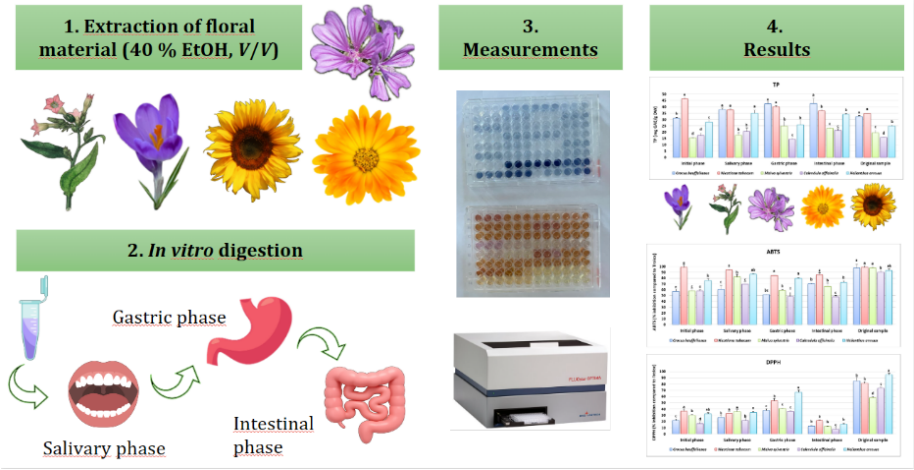
Despite its potential as a valuable source of nutraceuticals, floral biomass from industrial crops such as tobacco, sunflower, and saffron is often discarded as agricultural waste [1]. This study aimed to determine and compare, during *in vitro* digestion, changes in content of total polyphenols (TP), flavonoids (TF), hydroxycinnamic acids (THA) and proanthocyanidins (TPAN), as well as the antioxidant capacity of ethanolic extracts prepared from the petals of tobacco (*Nicotiana tabacum* L., Solanaceae) and black mallow (*Malva sylvestris* L., Malvaceae), tepals of Heuffel's saffron (*Crocus heuffelianus* Herb., Iridaceae), and ray flowers of sunflower (*Helianthus annuus* L., Asteraceae) and marigold (*Calendula officinalis* L., Asteraceae). Ethanolic (40 %, *V*/*V*) extracts were prepared by rotary extraction with the tube revolver rotator. Extracts from Heuffel's saffron exhibited high levels of TP (32.4 mg GAE/g DW), THA (41.7 mg CAE/g DW) and TPAN (4.17 mg CATE/g DW). Tobacco and sunflower extracts were rich in TP (34.8 and 24.9 mg GAE/g DW, respectively) and TF (23.5 and 22.3 mg CATE/g DW, respectively), whereas mallow extracts contained high amounts of TPAN (4.32 mg CATE/g DW). Most phytochemicals showed good stability under digestion conditions. In the intestinal phase, Heuffel's saffron retained the highest values of TP (42.7 mg GAE/g DW), THA (33.3 mg CAE/g DW) and TPAN (3.6 mg CATE/g DW), whereas sunflower was richest in TF (23.7 mg CATE/g DW). All original extracts had high antioxidant capacity (> 70 % inhibition) in the ABTS and DPPH assays, except for original mallow extract, which exhibited moderate DPPH activity. A reduction in antioxidant capacity was observed during digestion for both assays, although the reduction was much more pronounced for DPPH assay. Tobacco and sunflower extracts consistently retained the highest antioxidant activity across all assays. These results indicate that extracts may represent promising sources of bioactive compounds with potential applications in functional foods, dietary supplements, and cosmetics.



[1] O. Santana-Méridas, A. González-Coloma, R. Sánchez-Vioque. *Phytochem Rev* **11** (2012) 447-466.

A ROUTE TO ISOSTRUCTURAL METAL-ORGANIC HALOGEN-BONDED (MOXB) COCRYSTALS WITH DIFFERENT MAGNETIC PROPERTIES

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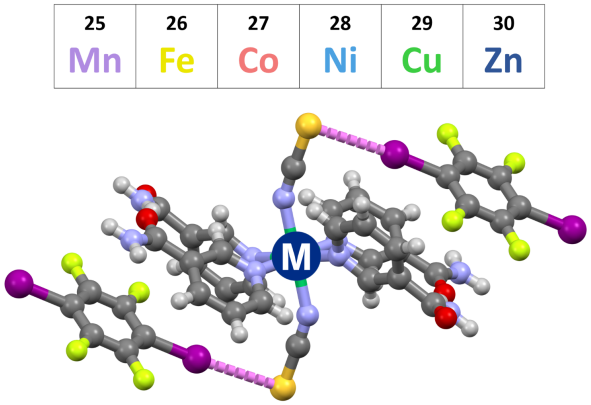
The construction of isostructural metal-organic halogen-bonded (MOXB) cocrystals and salts by replacing the metal ion is an attractive way of producing a series of materials with significant differences in some properties, while keeping the cocrystal architecture unchanged [1,2,3]. In this work, we have synthesized an isostructural series of six MOXB cocrystals containing an isothiocyanate coordination compound and 1,4-diiodotetrafluorobenzene (**14tfib**) as a halogen bond donor, differing only in the central metal atom of the coordination entity, [M(nicotinamide)$_4$(NCS)$_2$](**14tfib**) (M = Mn, Fe, Co, Ni, Cu and Zn). All MOXB cocrystals were characterized by powder and single crystal X-ray diffraction, thermogravimetric analysis and SQUID magnetometry, revealing interesting insights into their properties and differences. In addition, the mean cell similarity indexes, Hirshfeld surfaces and maps of electrostatic potential were calculated, which further characterized these systems. Structural analysis revealed that carbonyl oxygen atoms of nicotinamide ligands participate in the connection of metal-organic units in 2D networks by N-H···O hydrogen bonds, while each isothiocyanate ligand is connected to one **14tfib** by S···I halogen bonds, which additionally bridge the 2D networks of metal-organic units. All studied MOXB cocrystals with a magnetic transition metal ion (except Zn) show Curie-Weiss-like temperature dependence of susceptibility. However, analysis reveals that only Cu and Ni ions in the cocrystals have the expected magnetic moment for their respective spins in the octahedral environment. Co, Fe and Mn cocrystals show a possible mixture of high-spin and low-spin states, signifying that the octahedral arrangement is susceptible to small deformations which lead to different spin states.



[1] V. Nemec, L. Fotović, T. Friščić, D. Cinčić, *Cryst. Growth Des.* **17** (2017) 6169–6173.

[2] V. Stilinović, T. Grgurić, T. Piteša, V. Nemec, D. Cinčić, *Cryst. Growth Des.* **19** (2019) 1245–1256.

[3] J. E. Ormond-Prout, P. Smart, L. Brammer, *Cryst. Growth Des.* **12** (2012) 205.

THE EFFECT OF FENOFIBRATE ON THE N-GLYCOSILATION OF TOTAL SERUM PROTEINS IN PATIENTS WITH TYPE 1 DIABETES MELLITUS

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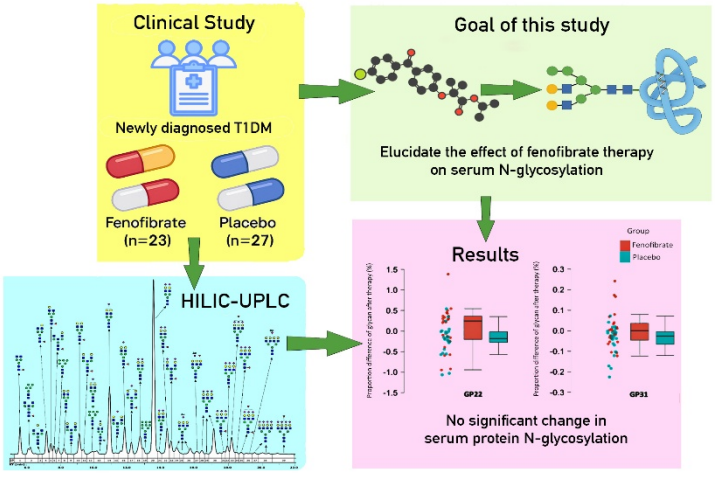
Type 1 diabetes mellitus (T1DM) is a chronic disease characterized by autoimmune mediated destruction of functional beta cell mass, leading to absolute insulin deficiency. Disease management revolves around substitution of the insulin deficiency with insulin analogues, and it is a lifelong therapy regiment. Several studies have shown that fenofibrate has the potential to preserve beta cell function and inhibit disease progression in patients with T1DM [1]. Glycosylation is a dynamic and sensitive post-translational modification. N-glycosylation patterns are susceptible to change under the influence of pathophysiological processes, medication and other environmental factors [2]. Alterations of plasma N-glycosylation patterns have already been identified in patients with newly diagnosed T1DM. However, the possible effect of fenofibrate on plasma *N*-glycosylation has not been extensively researched. With that in mind, a HILIC-UPLC analysis of the plasma N-glycome was performed, with the goal of elucidating the possible effect of fenofibrate therapy on inflammatory status and the progression of T1DM. Serum samples were received from a double-blind randomized clinical study, in which 56 patients with newly diagnosed T1DM were enrolled. The patients received either fenofibrate or placebo during a three-month therapy period. Of the original 56, the serum samples of 50 patients were analyzed (age range 18-39 years), with 23 belonging to the fenofibrate group, and 27 to the placebo group. Results between the therapy and control group were compared using an independent sample t-test, with an added Benjamini-Hochberg correction of calculated p-values to reduce the likelihood of false positive results. No statistically significant difference in the relative abundance of each serum N-glycan was confirmed. In addition, changes in relative abundance of glycans categorized by relevant structural similarities failed to reach significance. Based on these results, it was concluded that fenofibrate does not affect plasma protein N-glycosylation in patients with T1DM.



[1] Hostrup, P. E. *et al.*, *Diabetologia* **68** (2025) 29–40.

[2] Saldova, R. *et al.*, *J Proteome Res* **11** (2012) 1821–1831.

CORROSION PROTECTION OF COPPER BY POLY(ALLYLAMINE HYDROCHLORIDE)/POLY(ACRYLIC ACID) MULTILAYER

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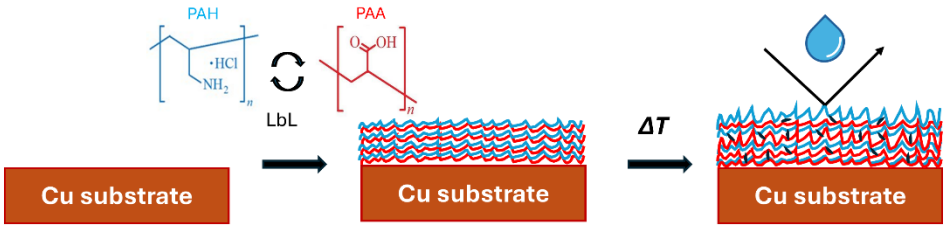
Corrosion of metals is one of today's main financial and technological problems. Consequently, the need for new, effective methods of protecting metals from corrosion is extremely important. Polyelectrolyte multilayers (PEMs) are versatile coatings formed by successive depositions of positively and negatively charged polyelectrolytes on solid substrates [1]. The properties of PEMs can be fine-tuned by changing the preparation conditions [2]. Moreover, further improvements of PEM properties can be achieved by post-fabrication methods such as thermal annealing [3]. In this study, surface topography of a polished copper sample and thickness of its native oxide layer were determined using atomic force microscope and ellipsometer. After that, PEM was prepared on copper substrate via layer-by-layer (LbL) assembled poly(allylamine hydrochloride) (PAH) and poly(acrylic acid) (PAA). PEM growth on copper substrate was monitored by ellipsometry. After preparation, the PAH/PAA multilayer was thermally cross-linked by heating in a vacuum drying oven at 175 °C for 120 minutes. Attenuated total reflectance IR spectroscopy confirmed the presence of amide bonds between PAH and PAA after heating treatment. The PEM thickness, as well as its surface roughness, increased slightly after thermal cross-linking. Finally, thermally cross-linked PEM was examined by electrochemical impedance spectroscopy, and enhanced corrosion protection effectiveness was observed.



Acknowledgments: HAZU financially supported the research under the project CORPEM.

[1] G. Decher, *Science* **277** (1997) 1232–1237.
[2] S. T. Dubas, J. B. Schlenoff, *Macromolecules* **32** (1999) 8153–8160.
[3] T. Klačić, K. Bohinc, D. Kovačević, *Macromolecules* **55** (2022) 9571–9582.

NIOBATE-PHOSPHATE-BASED GLASSES: INFLUENCE OF STRUCTURAL FEATURES ON MOBILITY OF LITHIUM CATIONS

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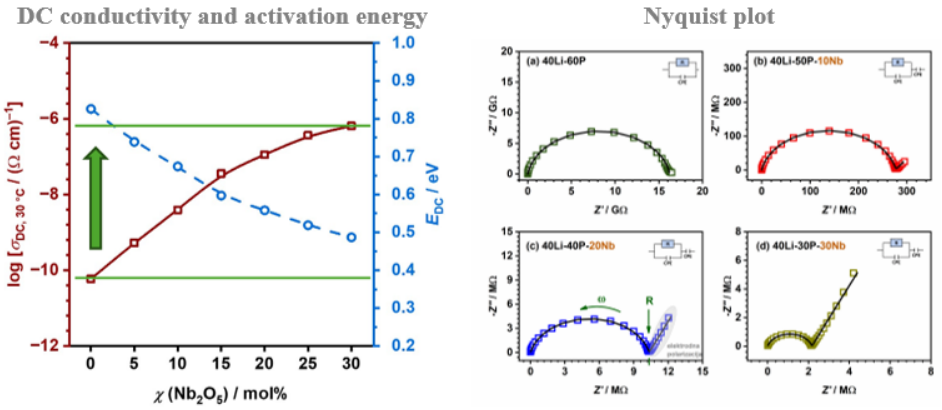
Lithium niobate-phosphate-based glasses are emerging as promising solid electrolytes or electrode material for solid-state batteries offering higher energy density and safety. However, binary alkali-phosphate glasses, in general, suffer from low conductivity and poor chemical durability. These issues can be addressed by incorporating intermediate oxides like Nb_2O_5, which create a mixed network through P–O–Nb bonds, enhancing durability and stability, along ion transport via the so-called mixed-glass former effect (MGFE) [1,2].
This study investigates the Li_2O–P_2O_5–Nb_2O_5 glass system prepared with classical melt-quenching technique in wide compositional range. Structural characteristic of such glasses along with thermal properties are studied with PXRD, IR-ATR and DTA. Nature of electrical transport and influence of structural features on it is evaluated through solid-state impedance spectroscopy (ss-IS) over a broad frequency and temperature range. Results show up to four orders of magnitude enhancement in ionic conductivity, highlighting the role of MGFE and elucidating structure-property relationships.



This work is supported by the internal RBI funding scheme KP-2023 program (KP1-2025) through National Recovery and Resilience Plan 2021-2026 (NPOO), funded by the European Union's NextGenerationEU program.

[1] S. Marijan *et al.*, *J. Physics and Chemistry of Solids* **181** (2023) 111461.
[2] S. Renka *et al.*, *Inorg. Chem.* **64** (2025) 11412–11425.

CALIXARENES – YES, THEY FLUORESCE!

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Calixarene derivatives have been widely recognized as promising fluorescent sensors when suitably functionalized with fluorophoric groups [1], as it has been believed that these compounds are not sufficiently intrinsically fluorescent [2]. In this work, we investigated the intrinsic fluorescence of several calix[*n*]arene derivatives (*n* = 4 or 6, Figure 1) lacking additional fluorescent moieties and explored the possibility of quantitative fluorimetric examination of their cation-binding processes taking place in different solvents (water, methanol, and acetonitrile) [3]. Despite the low intrinsic luminescence of the studied compounds, a significant fluorescence enhancement was observed upon their complexation with alkali and alkaline earth metal cations. In contrast, an opposite trend was noticed for monomeric compound **4**, which constitutes tertiary-amide calixarene derivative **2**. The results of excited-state lifetime measurements and quantum chemical calculations provided insight into the emission mechanisms and explained the differences between photophysical properties of the ligands and their cation complexes. Overall, the results of this comprehensive and integrated investigation indicate that, contrary to current opinion, spectrofluorimetry can be successfully employed as an effective and sensitive technique for the quantitative monitoring of complexation reactions involving calixarene derivatives and related compounds, regardless of whether additional fluorophores are present in their structures.

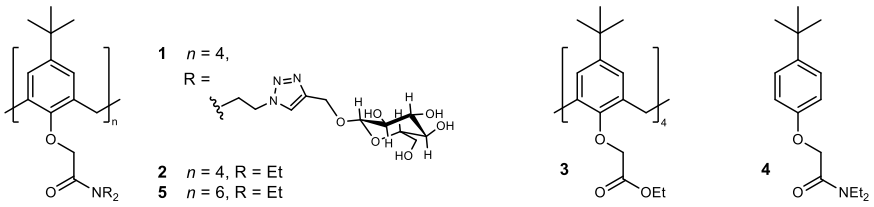

Figure 1. Structures of investigated calixarenes.

Acknowledgements. This research was funded by Croatian Science Foundation (project CalixCORE, Grant No. IP-2024-05-3012) and European Regional Development Fund (infrastructural project CIuK, Grant No. KK.01.1.1.02.0016).

[1] J. S. Kim, D. T. Quang, *Chem. Rev.* **107** (2007) 3780–3799; M. Tranfić Bakić *et al., RSC Adv.* **5** (2015) 23900–23914; R. Kumar *et al.*, *Chem. Rev.* **119** (2019) 9657–9721; K. Leko *et al.*, *ACS Omega* **8** (2023) 43074–43087; M. Modrušan *et al.*, *Croat. Chem. Acta* **97** (2024) 189–203; A. Usenik *et al.*, *Int. J. Mol. Sci.* **26** (2025) 1264.

[2] P. Neri, J. L. Sessler, M. X. Wang, Eds., *Calixarenes and Beyond*, Springer International Publishing, Cham, 2016.

[3] A. Usenik, I. Nikšić-Franjić, M. Belovari, M. Jurković, L. Klemen, N. Cindro, N. Došlić, I. Piantanida, V. Tomišić, *Anal. Chim. Acta* **1377** (2025) 344648.

FERROCENE PEPTIDES AS MODELS FOR SELECTIVE CATALYSTS

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The design of new selective catalysts is often based on the induction of chirality [1]. Ferrocene peptides are an important class of compounds in which chirality is induced through intramolecular hydrogen bonding [2]. The synthesis of different monosubstituted and 1,*n*'-disubstituted ferrocene peptides with and without a phenyl linker was carried out (Figure 1). The synthesis was performed in a one-pot reaction of ferrocene precursors and chiral amino acids using coupling reagents TBTU and HOBt in dichloromethane. The influence of different amino acids and *m*-phenyl or *p*-phenyl linker on the formation of intramolecular hydrogen bonds and induction of chirality, differences between the derivatives of alanine enantiomers as well as the difference between monosubstituted and 1,*n*'-disubstituted derivatives of the same amino acid were investigated. The methods used in the research include mass spectrometry, IR, ^{1}H NMR, ^{13}C NMR, UV/Vis and CD spectroscopy.

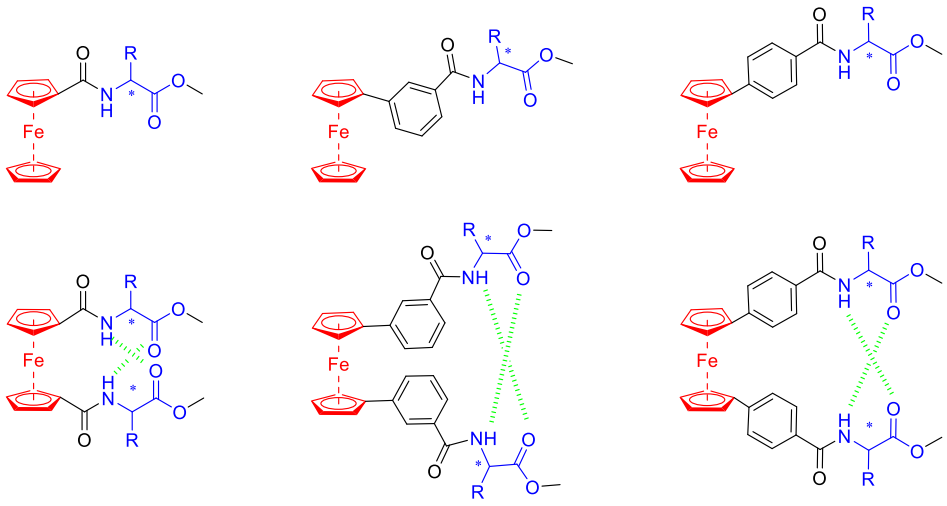

Figure 1. General formulas of the synthesized ferrocene peptides

[1] P. W. N. M. van Leeuwen, M. Raynal, *Supramolecular Catalysis: New Directions and Developments* (2022).

[2] S. I. Kirin, H.-B. Kraatz, N. Metzler-Nolte, *Chem. Soc. Rev.* **35** (2006) 348.

CALIXARENE-SOLVENT ADDUCTS FORMATION: A COMPREHENSIVE THERMODYNAMIC AND COMPUTATIONAL STUDY

Sven Marinac, Andrea Usenik, Matija Modrušan, Jakov Borovec, Katarina Pičuljan, Katarina Leko, Gordan Horvat, Josip Požar, Nikola Cindro, Tomica Hrenar, Vladislav Tomišić

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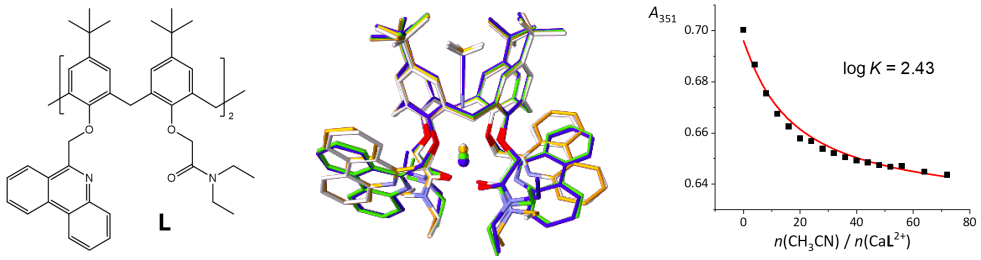
Calixarenes functionalized at the lower rim with electron-donating moieties, for instance those containing carbonyl groups, have been intensely investigated due to their ability to form stable complexes with various cations in different solvents [1]. Regarding solvation effect, the inclusion of solvent molecule into the calixarene hydrophobic *basket* plays a significant role in determining the extent of cation complexation reactions [2]. In our previous work [3], we studied the thermodynamics of first- and second-group metal cations complexation by calix[4]arene derivative **L** in acetonitrile, methanol, and ethanol. In the present study, the influence of solvent molecule inclusion in the *cone* of free and complexed ligand on the equilibria of binding reactions was particularly addressed from the thermodynamic and structural points of view. The structures of the ligand–solvent and complex–solvent adducts were examined using a combination of experimental and computational methods, including NMR spectroscopy, classical molecular dynamics simulations, and DFT calculations. The orientation of the solvent molecule inside the calixarene cavity was found to be the main difference between the adducts of the alkali and alkaline earth metal cation complexes. In the former, the solvent methyl group was oriented towards the cation, whereas in the latter the –CN or –OH group faced the metal ion and thereby coordinating it. The position/orientation of the included solvent molecule significantly affected the thermodynamic stability of the complexes. The solvent inclusion process was also quantitatively characterized by ITC and UV spectrophotometry, and the corresponding thermodynamic reaction parameters were determined and discussed.



Acknowledgements. This research was funded by Croatian Science Foundation (project CalixCORE, Grant No. IP-2024-05-3012) and European Regional Development Fund (infrastructural project CIuK, Grant No. KK.01.1.1.02.0016).

[1] A. F. Danil de Namor *et al.*, *Chem. Rev.* **98** (1998) 2495–2526; B. S. Creaven *et al.*, *Coord. Chem. Rev.* **253** (2009) 893–962.

[2] A. F. Danil de Namor *et al.*, *J. Chem. Soc., Chem. Commun.* (1991) 1546; A. F. Danil de Namor *et al.*, *J. Am. Chem. Soc.* **124** (2002) 12824–12836; G. Horvat *et al.*, *Inorg. Chem.* **52** (2013) 12702–12712; G. Horvat *et al.*, *Phys. Chem. Chem. Phys.* 19 (2017) 24316–24329; J. Požar *et al.*, *Molecules* **27** (2022) 470; M. Modrušan *et al.*, *Croat. Chem. Acta* **97** (2024) 189–203.

[3] K. Leko *et al.*, *ACS Omega* **8** (2023) 43074–43087; A. Usenik *et al.*, *Int. J. Mol. Sci.* **26** (2025) 1264.

ADSORPTION OF POLY(4-VINYLPYRIDINE) DERIVATIVES ONTO QUARTZ NANOPLATES: SIDE CHAIN LENGTH IMPACT

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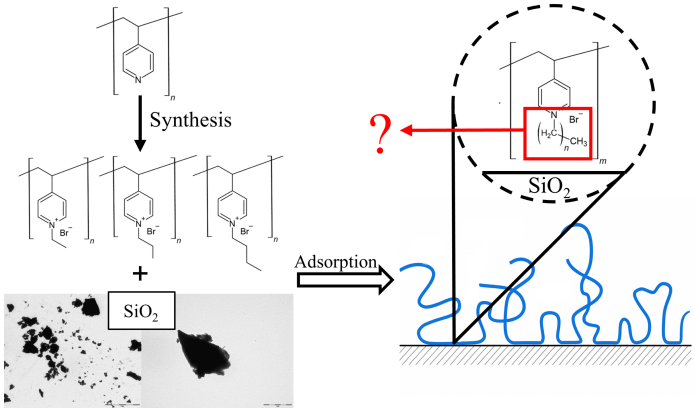
In this study, the adsorption of various derivatives of poly(4-vinylpyridine) on the surface of quartz nanoparticles was investigated with the aim of understanding the role of monomer structure in the adsorption process. Polyelectrolytes, as polymeric compounds with ionizable functional groups, exhibit the ability to adsorb onto nanoparticle surfaces through electrostatic and nonelectrostatic interactions. Three *N*-alkyl derivatives with different chain lengths were synthesized in order to compare their adsorption efficiency. The obtained compounds were characterized using NMR spectroscopy, IR spectroscopy, thermogravimetric analysis and potentiometric titration with a bromide ion-selective electrode [1]. After characterization of polyelectrolytes, nanoparticles were also characterized by transmission electron microscopy and electrophoretic light scattering. Their specific surface was also determined. Adsorption experiments were carried out on quartz nanoplates under controlled conditions. The results, analysed with UV-Vis spectroscopy were processed using Hesselink's model [2]. It was shown that derivatives with a smaller alkyl substituent on the monomer unit exhibited higher adsorption capacity compared to derivatives with larger substituent. This confirms the initial hypothesis that hydrophobicity and steric effects play a key role in the adsorption process.



Acknowledgements: Croatian Science Foundation financially supported the research under the project POLYMIN2 (IP-2020-02-9571).

[1] K. Mavronasou *et al.*, *Polymers* **14** (2022) 804.

[2] F. T. Hesselink, *J. Colloid Interface Sci.* **60** (1977) 448-466.

MULTI-CRITERIA OPTIMIZATION OF THERAPEUTIC RADIOISOTOPES VIA QUANTITATIVE MCDA

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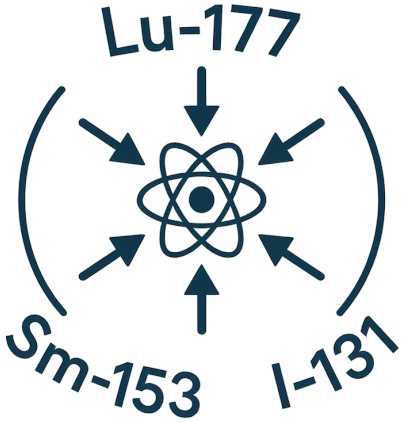
Selecting therapeutic radioisotopes for nuclear medicine was treated as a multi-factor optimization problem affecting clinical efficacy, imaging feasibility, and supply logistics, motivating a transparent quantitative method aligned with current theranostics practice. A multi-criteria decision analysis (MCDA) framework was developed and applied to eight candidates (Lu-177, Y-90, Re-188, I-131, Sm-153, Ho-166, Ac-225, Ra-223), using evaluated nuclear-data libraries to parameterize four a priori criteria and weights: half-life suitability 0.30 (2–10 d therapeutic window), therapeutic emission energy 0.40 (500–2500 keV (β) or 5000–8000 keV (α)), imaging γ yield/energy 0.20 (100–300 keV), and production accessibility 0.10 (reactor vs generator). Criterion values were normalized to 0–1 and aggregated by weighted summation $S=\sum w_i x_i$; robustness was tested via ±20% weight perturbations with rank-order tracking to evaluate model fragility. The analysis identified Sm-153, Ra-223, and I-131 as the highest-scoring isotopes with composite scores of 0.992, 0.959, and 0.940, respectively, and a cohort mean of 0.88 ± 0.09 across all eight nuclides, indicating meaningful separation among alternatives. Sensitivity analysis preserved the leading order and retained Sm-153 as the top candidate under all scenarios, demonstrating low susceptibility of conclusions to plausible weighting shifts. The MCDA provided a reproducible, adaptable tool for isotope prioritization that can be tuned to local clinical pathways and supply constraints, enabling rapid preclinical screening and informing procurement choices while maintaining imaging compatibility and practical production feasibility.



[1] B. J. Burkett, P. L. Choyke, *Radiol Imaging Cancer* **5(4)** (2023) e220157.
[2] I. Özşahin *et al.*, *Diagnostics* **13(8)** (2023) 1542.

ALDEHYDES AS STRUCTURE-DIRECTING AGENTS IN THE MECHANOSYNTHESIS OF ZINC IMIDAZOLATE SOLID FORMS

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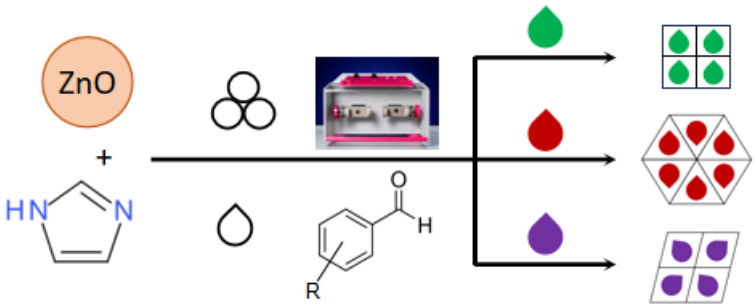
Zeolitic imidazolate frameworks (ZIFs) [1] are a subtype of metal-organic frameworks (MOFs) composed of tetrahedral metal atoms linked by imidazolate linkers, yielding polymeric structures which can form various topologies, similar to their zeolite namesakes. The simplest ZIF is the unsubstituted zinc imidazolate (Zn**Im**$_2$), for which at least 19 different topologies are currently known. The synthesis of these diverse topologies is predominantly achieved via solvothermal methods, frequently resulting in (pseudo)polymorphic mixtures. Alternatively, targeting desired polymorphs has been accomplished with mechanochemical methods, using the structure-directing effects of different liquids and salts [2,3].

In this study we used different aromatic aldehydes as structure-directing liquids for mechanochemical screening of new Zn**Im**$_2$ topologies. The obtained products were analyzed using infrared spectroscopy, powder X-ray diffraction and solid state nuclear magnetic resonance. It was found that the synthesis was directed by aldehyde choice, but also by specific reaction conditions, demonstrating a large diversity in form.



[1] Y.-Q. Tia *et al.*, *Chem. Eur. J.* **9** (2003) 5673.
[2] I. Brekalo *et al.*, *J. Am. Chem. Soc.* **147** (2025) 27413.
[3] P. J. Beldon *et al.*, *Angew. Chemie Int. Ed.* **49** (2010) 9640.

CROSS-MODAL MOLECULAR REPRESENTATION FUSION FOR ENHANCED MOLECULAR PROPERTY PREDICTION

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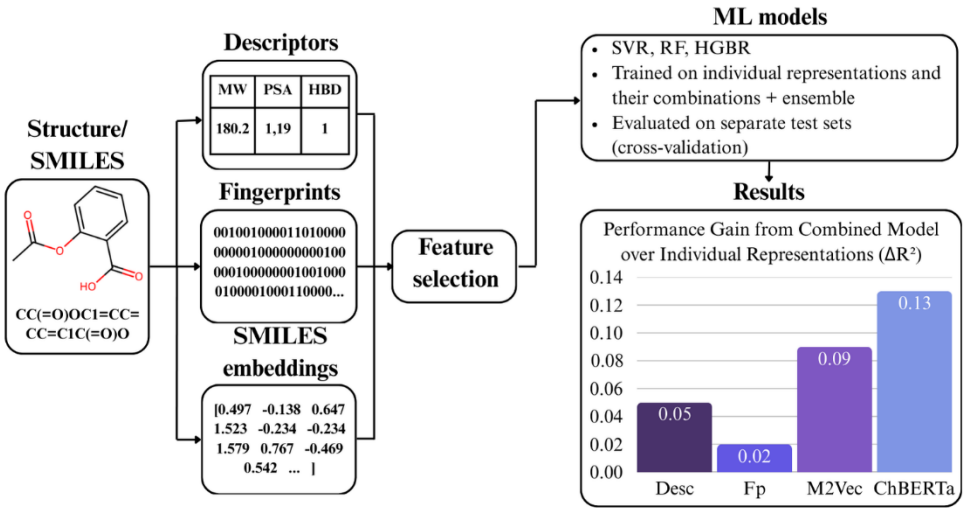
Molecular property prediction is a key task in cheminformatics for accelerating drug discovery, where predicting biological activity or physicochemical properties from molecular structure enables *in-silico* assessment prior to experimental testing, compound prioritization, and lead optimization. The quality of these predictions depends critically on chosen molecular representation. Common approaches include molecular descriptors (numerical values), structural fingerprints (bitstring), and latent embeddings derived from SMILES strings using NLP methods [1]. In this study, all three representations were generated from SMILES strings from two molecular datasets. Representations were simplified via feature selection to retain the most informative chemical features before being used to train Random Forest, Support Vector Regression, and Histogram-based Gradient Boosting ML models, separately and in combination, with an additional ensemble built from their outputs. Model performance was evaluated on independent test sets using R^2, MSE, and MAE measures. Combining multiple representations outperformed any single representation, and ensembles further improved prediction performance, enabling more reliable virtual screening, candidate selection, and fewer resources spent synthesising compounds unlikely to meet target profiles. While combining multiple representations increases complexity and computational cost, simpler single-representation models remain easier to implement with slightly reduced accuracy. The trade-off between complexity and predictive gain should be evaluated in the context of project goals and resources. This approach also shows potential in docking, generative design, and custom fingerprinting, where tailored representations may outperform conventional encodings.



[1] K. Zhang *et al.*, *Nat. Med.* **31** (2025) 45-59.

NMR ANALYSIS OF OLEUROPEIN AND OTHER BIOACTIVE PHENOLIC COMPOUNDS IN OLIVE LEAF EXTRACT

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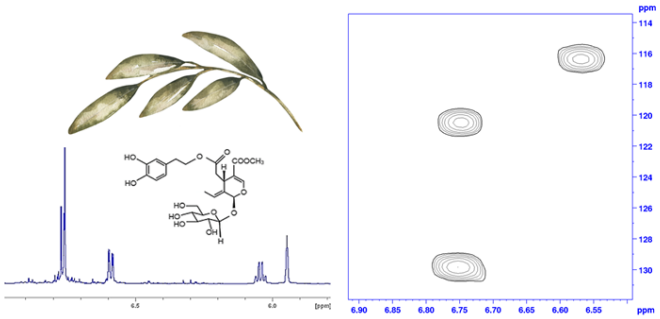
During pruning, olive groves produce a large amount of olive leaf waste, which is a valuable source of bioactive compounds. Olive leaves contain secoiridoid oleuropein and flavonoids, phenolic compounds which exhibit significant pharmacological activity, underscoring their potential applications in the prevention and treatment of cardiovascular and neurodegenerative diseases, diabetes, and cancer [1]. The increasingly employed NMR technique, due to its advantages such as lower solvent consumption and shorter analysis time, is still, unlike the standard HPLC technique, rarely used for the identification and quantification of phenols in olive leaves. In order to determine the oleuropein content in olive leaf extract by ^{1}H NMR spectroscopy, calibration curves were prepared in the concentration range (1) (0.20 - 6.58) and (2) (0.02 - 0.66) mmol/dm^3, where the oleuropein peak at 5.95 ppm was selected, and syringaldehyde was used as an internal standard [2]. By comparing the two NMR solvents, acetone-d6 was chosen due to its higher resolution of ^{1}H NMR spectra compared to methanol-d4. The method was validated: selectivity, linearity (r_1^2 = 0.9975 and r_2^2 = 0.9691) and sensitivity of the method (LOD = 0.13 mmol/dm^3, LOQ = 0.40 mmol/dm^3) underwent assessment. Using ^{13}C and 2D HMBC NMR spectroscopy, additional confirmation of the identification of oleuropein in olive leaf extract was performed. By comparing the ^{1}H NMR spectra with those of standard solutions of individual phenols, the absence of the notable olive oil secoiridoids oleocanthal and oleacein was confirmed. Simultaneously, the spectra indicated the presence of the flavonoids luteolin, luteolin 7-*O*-glucoside and apigenin, whereas kaempferol, naringenin and myricetin were not detected. The results of this research clearly indicate the possibility of characterizing the phenolic composition and determining the content of oleuropein in olive leaf by ^{1}H NMR spectroscopy.



[1] N. Talhaoui, A. Taamalli, A. M. Gómez-Caravaca, A. Fernández-Gutiérrez, A. Segura-Carretero, *Food Res. Int.* **77** (2015) 92–108.

[2] E. Mousouri, E. Melliou, P. Magiatis, *J. Agric. Food Chem*. **62 (3)** (2014) 660–667.

EFFECT OF PHENOL OXIDASE STIMULATION ON *ASPERGILLUS NIGER*–MEDIATED BIOSYNTHESIS OF SILVER NANOPARTICLES

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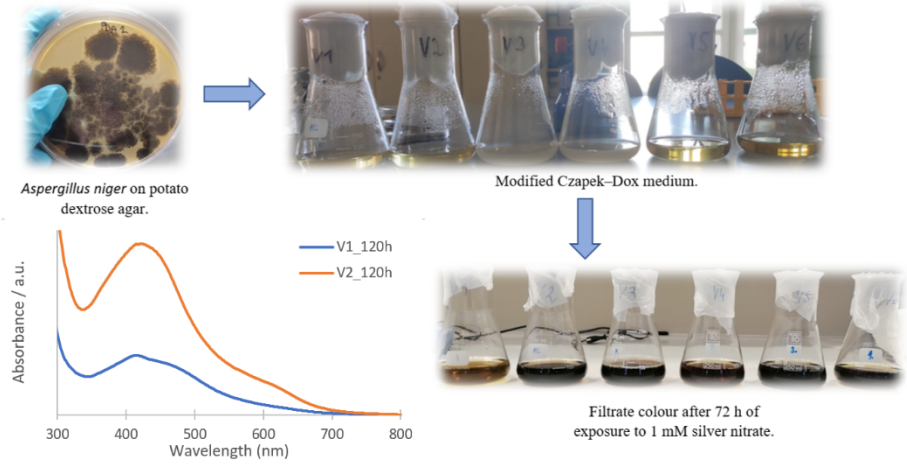
Green synthesis of silver nanoparticles (AgNPs) offers an environmentally friendly alternative to chemical routes, using biological reducing and capping agents produced by microbes. Filamentous fungi are particularly effective at reducing silver from silver nitrate because they secrete high levels of redox-active enzymes and metabolites. *Aspergillus niger*–mediated silver nanoparticle biosynthesis and the impact of Czapek–Dox modifications on nanoparticle biosynthesis were investigated. Six 50 mL Czapek–Dox variants were prepared with different carbon sources: sucrose (1, 2), starch (3, 4), and glucose (5, 6). Phenol oxidase activity was stimulated in variants 2, 4, and 6 by adding $CuSO_4 \cdot 5H_2O$ and H_2O_2; variants 1, 3, and 5 were unsupplemented controls. *A. niger* from potato dextrose agar was inoculated into each medium (pH 6.5) and incubated for 72 h. Biomass was collected (Whatman No. 1), washed, transferred to ultrapure water for 72 h to obtain extracellular extracts, and then removed by sequential filtration (Whatman No. 1 and then through a 0.45 µm membrane). Silver nitrate was added to each filtrate to 1 mM, and UV–Vis spectra (200-800 nm) were recorded at 72, 96, and 120 h. A brown colour appeared after ~72 h in all variants [1]. UV–Vis measurements showed a distinct AgNP surface plasmon resonance band at ~420 nm. Absorbance increased from 72 to 120 h and then plateaued [2]. At all time points, oxidase-stimulated variants (2, 4, 6) exhibited higher SPR absorbance than their corresponding controls (1, 3, 5), indicating enhanced silver nanoparticle formation under phenol-oxidase-promoting conditions. Medium engineering to stimulate phenol oxidases (Cu^{2+}/H_2O_2) increases the extent of AgNP biosynthesis and reveals a practical harvest window around 96–120 h. This study contrasts three common carbon sources with and without deliberate phenol-oxidase stimulation and shows that enzyme promotion consistently boosts AgNP formation across media. These results identify phenol oxidases as a tunable lever for yield in fungal AgNP production.



[1] L. R. Jaidev, G. Narasimha, *Colloids Surf. B Biointerfaces* **81** (2010) 430–433.
[2] K. Zomorodian *et al.*, *Biomed. Res. Int.* **2016** (2016) 5435397.

ENHANCING CHEMICAL PROPERTY PREDICTION THROUGH COMBINED ATOMIC AND MOLECULAR DESCRIPTORS

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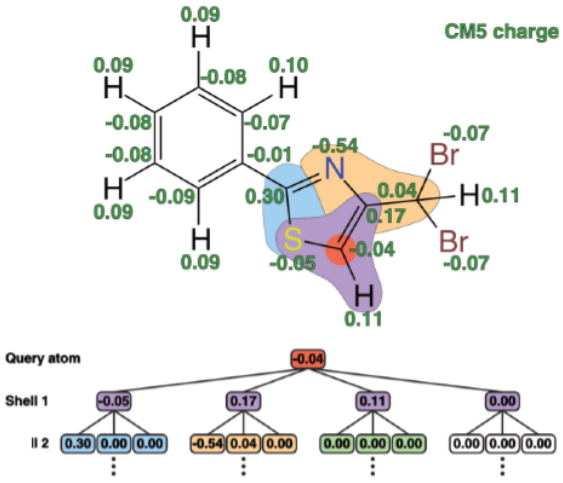
Computer-aided synthesis planning (CASP) has played a significant role in helping chemists since the second half of the last century. In recent years, there have been big advancements in the fields of machine learning, which resulted in better and broader methods used for CASP [1]. The only restriction is that the existing models cannot be successfully applied to different types of reactions or compounds which results in theoretical chemists trying to create new models utilizing different types of descriptors. Previous research identified shell descriptors utilizing charge model 5 (CM5) charges as good training data for models used for predicting different types of reactions [2]. The goal of this work is to combine these atomic shell descriptors of different properties to generate a new type of descriptor and test their prediction performance. We use these descriptors to train our model on a dataset containing 3910 C-H pK_a values and achieve mean absolute error (MAE) and root mean squared error (RMSE) values of 0.99 and 1.75 pK_a units, respectively. Furthermore, we created molecular descriptors from these atomic shell descriptors which we use to predict molecular log$P$ values from a dataset of 6000 diverse compounds achieving MAE and RMSE values of 0.62 and 0.81 log$P$ units, respectively.



[1] H. Gao *et al.*, *ACS Cent. Sci.* **4** (2018) 1465.
[2] A. R. Finkelmann, A. H. Göller, G. Schneider, *Chem. Commun.* **52** (2015) 681.

POSTER PRESENTATIONS

HPLC METHOD DEVELOPMENT AND VALIDATION FOR SIMULTANEOUS DETERMINATION OF FOUR ACTIVE PHARMACEUTICAL INGREDIENTS IN A COMBINED DOSAGE FORM

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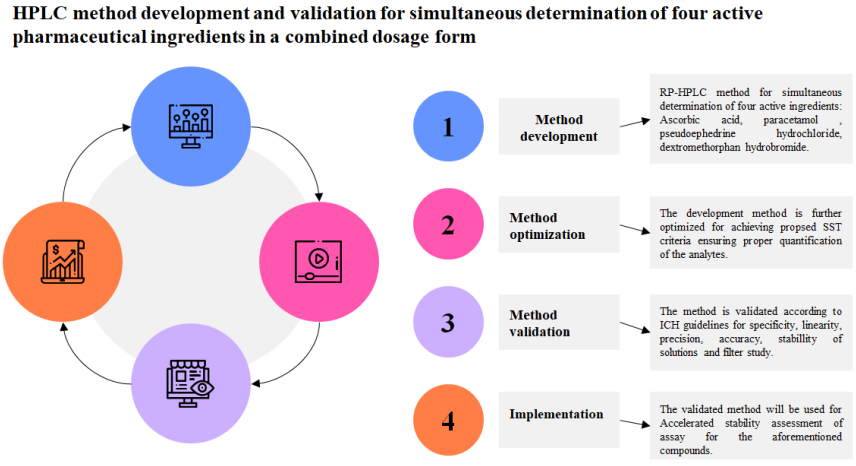
A high-performance liquid chromatography method for separation and simultaneous determination of ascorbic acid (AA), paracetamol (PAR), pseudoephedrine hydrochloride (PSE) and dextromethorphan hydrobromide (DEX) in a mixture was optimized. Due to the different properties of the target compounds, current methods require different chromatographic columns and conditions using a C18, SAX and SCX column for determination of each of the four compounds in a separate chromatographic run. The goal of this work was to develop and validate a suitable method for separation and quantification of these four compounds in a single run. Various RP-HPLC approaches were tested using a variety of columns with different stationary phases and dimensions, mobile phases with buffers in the pH range from 2-6, methanol and acetonitrile, in order to establish optimal chromatographic conditions and satisfactory resolution. It was found that using a C18 column (YMC-ODS AQ 250 mm × 4.6 mm, 5 µm) and mobile phase composed of A: 0.05 M KH_2PO_4 with pH = 4.5 and ion-pair reagent (0.075% heptane-1-sulfonic acid sodium salt), and B: CH_3OH gives satisfactory results with a proposed SST criteria for resolution better than 1.5 for all four active pharmaceutical ingredients within a run time of 20 minutes. The developed method was validated according to ICH guidelines for validation of analytical procedure [1,2] and its robustness confirmed in order to be used for accelerated stability studies of combined dosage forms containing the four aforementioned active compounds.



[1] Validation of Analytical Procedures – ICH Q2(R2). International council forharmonization of technical requirements for pharmaceuticals for human use, 2023.

[2] Analytical Procedure Development - ICH Q14. International council for harmonization of technical requirements for pharmaceuticals for human use, 2023.

SOL-GEL SYNTHESIS OF CERIA-BASED HIGH ENTROPY OXIDES AND THEIR POTENTIAL USE AS CATALYSTS FOR DYE DEGRADATION

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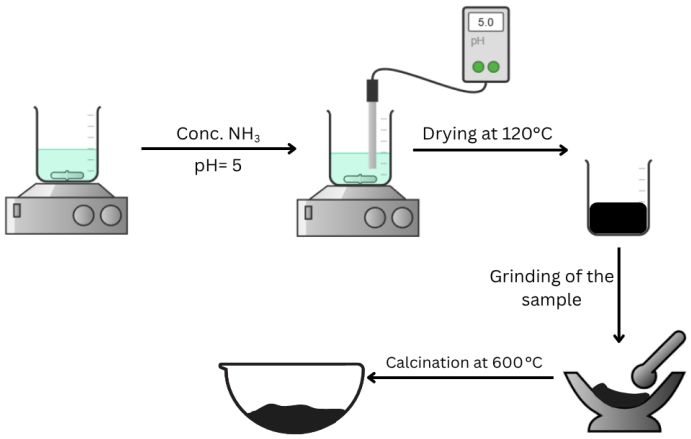
A family of materials known as high entropy oxides (HEOs) has a broad variety of possible uses because of its distinct composition and crystal structure. Due to the random distribution of cations within the crystal lattice, these single-phase solid solutions with five or more main metal cations in equiatomic proportions show remarkable stability [1]. In this work single- and dual-phase high entropy oxides were synthesized starting from CeO_2 and/or NiO as parent oxides: $Ce_{0.2}La_{0.2}Pr_{0.2}Sm_{0.2}Eu_{0.2}O_2$ (CLPSE), $Ce_{0.2}La_{0.2}Pr_{0.2}Sm_{0.2}Eu_{0.2}O_2$/NiO (CLPSE-N) and $Ce_{0.2}La_{0.2}Pr_{0.2}Sm_{0.2}Eu_{0.2}O_2$/$Ni_{0.25}Cu_{0.25}Mg_{0.2}Zn_{0.2}O$ (CLPSE-NCMZ). In the synthesis procedure metal nitrate salts were dissolved in citric acid solution (w = 10%) and the pH value was adjusted to 5 using concentrated ammonia solution (w = 25%). The solution was heated at 95 °C until a black resin was formed. The black resin was further dried overnight at 120 °C followed by a calcination at 600°C for 8 hours (heating rate 2 °C/min). The characterisation of yielded products was performed using a powder X-ray diffraction (PXRD), Raman spectroscopy and diffuse reflectance ultraviolet/visible light/near infrared spectroscopy (DRS UV/Vis/NIR). Their band gap values were calculated using Tauc method. Prior to monitoring dye degradation, solution containing methylene blue (MB) dye and catalyst dispersion was stirred in dark for 30 minutes. Tests for MB degradation were monitored by UV/Vis spectroscopy for 45 minutes *in situ* during the exposure to visible light in the spectrometer (halogen lamp, 20 W) in a kinetic mode at 664 nm (a maximum absorbance for MB dye solution, 10^{-5} mol/L). Results showed that synthesized compounds enhance the MB degradation compared to its self-degradation.



[1] A. Sarkar *et al.*, *Nat. Commun.* **9** (2018) 3400.

DETERMINATION OF ANTIVIRAL SUBSTANCES' ECOTOXICITY USING *PSEUDOMONAS PUTIDA* AND *LEMNA MINOR*

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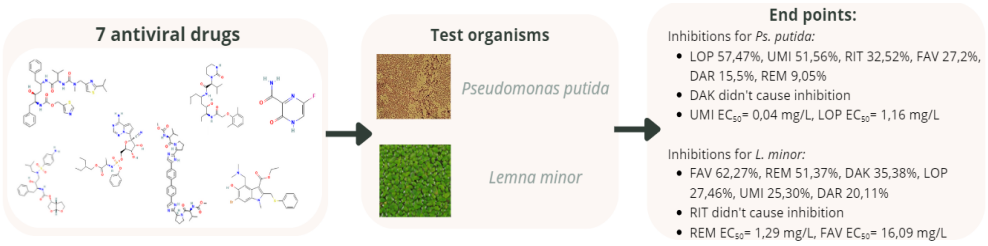
The COVID-19 pandemic, caused by the SARS-CoV-2 virus, began in 2019 and led to respiratory problems in millions of people worldwide, in many cases resulting in the death of patients. Antiviral substances are used to treat various viral diseases, and due to their widespread use, they end up in the environment, impacting aquatic ecosystems and soil. In this study, the ecotoxicity of antiviral substances was assessed using toxicity tests involving the bacterium *Pseudomonas putida* and the duckweed *Lemna minor*. Test organisms were exposed to the antiviral substance ritonavir (RIT), remdesivir (REM), and lopinavir (LOP) in concentration ranges from 0.00013 mmol/L to 0.002 mmol/L; favipiravir (FAV) and darunavir (DAR) in the range of 0.013 mmol/L to 0.2 mmol/L; daklatasvir (DAK) from 0.006 mmol/L to 0.1 mmol/L; and umifenovir (UMI) in concentrations from 0.000006 mmol/L to 0.0001 mmol/L. The test with the bacterium *Pseudomonas putida* was conducted over 16 hours and the *Lemna minor* test was conducted over 7 days. Among the tested antiviral substances, LOP showed the highest toxic effect on *Pseudomonas putida*, causing a 57.47% inhibition of bacterial growth at the highest tested concentration (0.002 mmol/L). UMI inhibited bacterial growth by 51.56% at a concentration of 0.0001 mmol/L, while DAK showed no ecotoxic effect on *Pseudomonas putida* within the tested concentration range. In the test with duckweed *Lemna minor* the highest growth inhibition (62.27%) was caused by FAV at a concentration of 0.002 mmol/L, while RIT did not inhibit growth and is considered as non-ecotoxic to *Lemna minor*. Toxicity tests have shown that the LOP is classified as moderately ecotoxic (1 mg/L<EC_{50}≤10 mg/L) and UMI as highly ecotoxic (EC_{50}≤1 mg/L), based on results obtained with the bacterium *Pseudomonas putida*. The REM is classified as moderately ecotoxic and FAV as slightly ecotoxic (10 mg/L<EC_{50}≤100 mg/L), according to the test with the duckweed *Lemna minor*.



The authors would like to acknowledge the financial support of the Croatian Science Foundation through project entitled Environmental Aspects of SARS-CoV-2 Antiviral Substances (EnA-SARS, IP-2022-10-2822).

[1] K. Kuroda, C. Li, K. Dhangar, M. Kumar, *Sci. Total Environ.* **776** (2021) 145740.

HALOGEN-BONDED COCRYSTALS OF 2D METAL-ORGANIC FRAMEWORKS BASED ON Mn(II), Fe(II), Co(II), Ni(II) AND Zn(II) CATIONS

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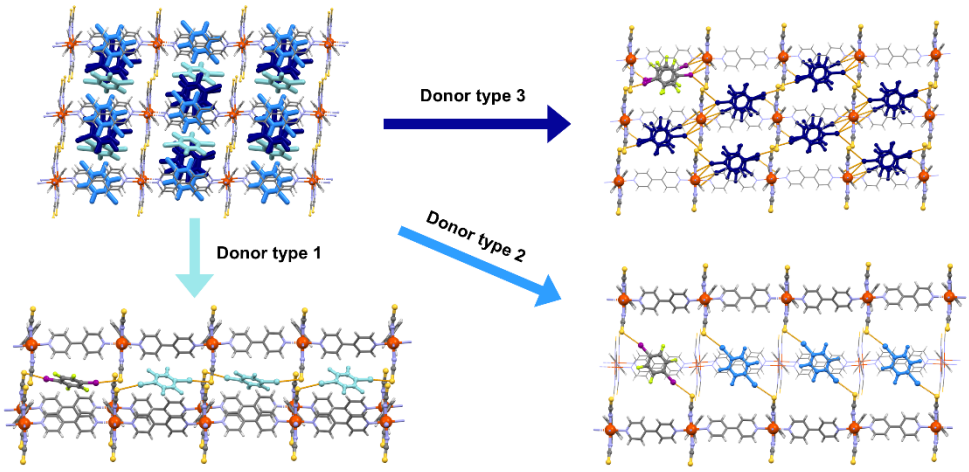
Although numerous advances in the preparation of halogen-bonded multi-component solids have been reported [1], the focus was almost exclusively on cocrystals comprising (relatively small) discrete constituents, whereas cocrystals of coordination polymers (CPs) remain unexplored. In this work we have prepared five isostructural two-dimensional (2D) metal-organic frameworks (MOF) of $[M(4,4'\text{-bipyridine})_2(NCS)_2]_n$ type (M = Mn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+}, Zn^{2+}) [2], whose pendant isothiocyanate groups are potential halogen bond acceptor sites [3]. We then cocrystallized them with 1,4-diiodotetrafluorobenzene (**14tfib**) as a halogen bond donor, both mechanochemically and via solution methods. The effectiveness of this strategy is indicated by the formation of five isostructural 2D MOF cocrystals, $[M(4,4'\text{-bipyridine})_2(NCS)_2]_n$(**14tfib**)$_{3n}$, including the first known crystal structure with zinc as a metal node in this CP family [4]. The systematic substitution of metal centers enabled us to study effects of metal centers on 2D framework geometry of the polymer itself and halogen bond parameters. The structural analysis revealed that the dominant non-covalent interactions in all cocrystals are I···S halogen bonds which connect adjacent layers of the polymer. However, of three **14tfib** molecules only two partake in strong halogen-bonding, while the third one is disorderd.



[1] V. Nemec *et al*., *CrystEngComm* **23** (2021) 3063.

[2] S.-Q. Wang, S. Darfish, D. Sensharma, M. J. Zaworotko, *Mater. Adv.* **3** (2022) 1240.

[3] L. Posavec, D. Cinčić, *Cryst. Growth and Des.* **24** (2024) 7514.

[4] C. R. Groom, I. J. Bruno, M. P. Lightfoot, S. C. Ward, *Acta Crystallogr. Sect. B Struct. Sci. Cryst. Eng. Mater.* **72** (2016) 171.

THE ROLE OF ENVIRONMENTAL BACTERIA IN THE REMOVAL OF PHARMACEUTICALS

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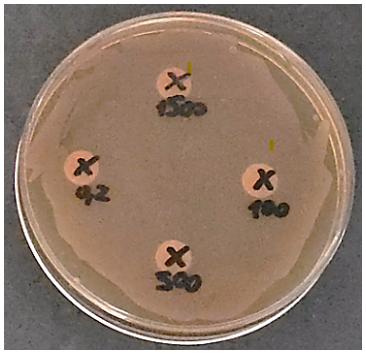
With the sharp rise in the population, the need for medicines is also increasing. Antibiotics are a group of pharmaceuticals used to treat bacterial infections. The excessive and irresponsible use of antibiotics poses a serious problem for the environment. Antibiotics can have harmful effects on aquatic organisms and increased concentrations of antibiotics in the environment could promote the development of antibiotic resistance in bacteria. Some environmental bacteria have been resistant to different types of antibiotics, especially those bacteria isolated from polluted areas [1]. Bacteria that are resistant to antibiotics can utilise them as substrates and use their metabolism and enzymes to convert harmful substances into compounds that are harmless to the environment [2]. This study investigated the ability of a Gramme negative, motile rod-shaped environmental bacteria to degrade an antibiotic belonging to the macrolide group. Studied bacteria showed no susceptibility. The removal efficiency of the tested antibiotic by biodegradation was 22.9 ± 12.0% within 3 days.



Acknowledgements: The financial support by NPOO.C3.2.R3-I1.05.0207 is greatly appreciated.

[1] D.G.J. Larsson, C.F. Flach, *Nat Rev Microbiol* **20** (2022) 257–269.
[2] S. Lakhani *et al.*, *CLCE* **4** (2022) 100073.

PHBV COMPOSITES WITH BIOACTIVE ADDITIVES: ANALYSIS OF MECHANICAL, THERMAL AND BARRIER PROPERTIES

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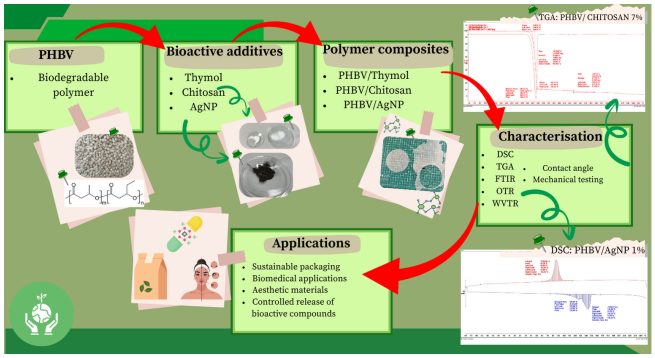
With the global shift towards environmentally responsible materials and increasing pressure to reduce pollution from conventional plastics, biodegradable polymers such as poly(3-hydroxybutyrate-*co*-3-hydroxyvalerate) (PHBV) have emerged as promising alternatives. Due to its biodegradability and biocompatibility, PHBV has emerged as a promising alternative in the development of eco-friendly materials, particularly in the packaging industry and beyond. However, the use of neat PHBV is limited by its poor mechanical and barrier properties. One of the strategies to enhance its performance involves the modification of the polymer matrix using bioactive additives capable of improving its structural and functional characteristics. In this research, PHBV-based composites with thymol, chitosan and silver nanoparticles were prepared and characterized. The composites were analyzed using differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), Fourier-transform infrared spectroscopy (FTIR), contact angle measurements, mechanical testing, and oxygen and water vapor transmission rate (OTR and WVTR) determination. The results indicated certain changes in crystallization behavior, thermal stability, and interfacial interactions. Variations in surface properties and permeability to gases and water vapor were observed, while some formulations demonstrated improvements in tensile strength and elasticity compared to neat PHBV. In conclusion, the use of bioactive additives showed potential in partially overcoming the limitations of unmodified PHBV, thereby broadening its range of possible applications. In addition to sustainable packaging the developed composites also demonstrated potential for use in biomedical and aesthetic materials, active surfaces, and systems for controlled release of bioactive compounds.



This research was conducted as part of the project „Production and development of compostable packaging from waste biomass for the packaging of industrially processed food products" (NPOO.C3.2.R3-I1 .04.0059) funded by National Recovery and Resilience Plan (funded by the European Union, NextGenerationEU).

EVALUATION OF BISQUATERNARY QUINUCLIDINIUM COMPOUNDS AS BUTYRYLCHOLINESTERASE INHIBITORS

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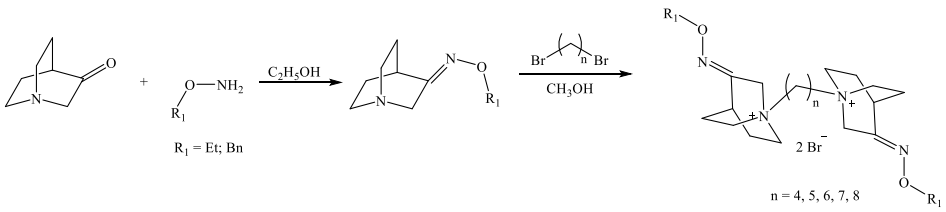
Quinuclidine, also known as 1-azabicyclo[2.2.2]octane, is a saturated, bicyclic amine with a nitrogen atom at a bridgehead position, resulting in its high symmetry and rigid structure that serves as a scaffold in organic and medicinal chemistry. Many natural alkaloids, including quinine, cinchonidine, and remijinine, contain the quinuclidine nucleus, which contributes to their diverse pharmacological profiles. Derivatives of quinuclidine display significant biological activities, including antimalarial, antibacterial, and antifungal [1]. They have also been investigated as potential therapeutics for neurological disorders because of their ability to interact with nicotinic acetylcholine receptors and cholinesterases [2]. In this work, we have prepared two oxime ethers of quinuclidine from commercially available quinuclidine-3-one and appropriate hydroxylamine hydrochloride by classic organic synthesis without the use of a base. A series of ten new bisquaternary quinuclidinium derivatives were prepared by the reaction of oxime ethers and alkyl dibromides with different chain lengths. The structure of the prepared compounds was determined by 1D and 2D ^{1}H and ^{13}C nuclear magnetic resonance spectroscopy. The inhibitory potential of prepared bisquaternary quinuclidinium derivatives toward the enzyme butyrylcholinesterase (BChE) was estimated using the Ellman method for colorimetric determination of cholinesterase activity [3]. The synthesized compounds were observed to exhibit notable inhibitory potential toward BChE.



[1] I. Maliszewska, A. Zdubek, B. Dziuk, P. Boratyński, *J. Nat. Prod.* **8** (2025) 1907–1918.

[2] S. Žunec *et al.*, *Int. J. Mol. Sci.* **25** (2024) 155.

[3] G. L. Ellman, K. D. Courtney, V. Jr. Andres, R. H. Featherstone, *Biochem. Pharmacol*. **7** (1961) 88–95.

UGI-BASED SYNTHESIS OF A STRUCTURALLY RELATED PEPTIDOMIMETIC LIBRARY

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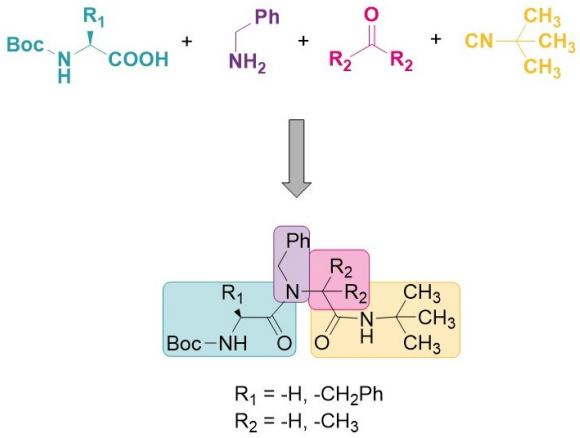
The Ugi multicomponent reaction enables the one-step synthesis of peptide-like molecules through the condensation of a carboxylic acid, an aldehyde, an amine, and an isocyanide [1,2]. It is an efficient tool in drug discovery research because it allows the synthesis of structurally diverse compounds in one step, which is important for identifying bioactive molecules with potential therapeutic effects [3]. These compounds often show broad activity against various biological targets. In this work, we have synthesized a small library of structurally related peptidomimetics through the Ugi reaction by using benzylamine, different *N-tert*-butyloxycarbonyl (Boc) protected amino acids, formaldehyde or acetone and *tert*-butyl isocyanide. In the preparation of compounds, we used two different approaches: classical organic synthesis and microwave assisted synthesis. Product yields were compared in relation to the synthesis method to determine the most appropriate method. The structure of all prepared compounds was determined with 1D and 2D ^{1}H and ^{13}C nuclear magnetic resonance spectroscopy (NMR) and high-resolution mass spectrometry.



[1] A. Dömling, I. Ugi, *Angew. Chem. Int. Ed.* **39** (2000) 3168–3210.

[2] C. Liu, L. G. Voskressensky, E. V. Van der Eycken, *Chem. Eur. J.* **30** (2024) e202303597.

[3] E. Fotopoulou, P. K. Anastasiou, C. Tomza, C. G. Neochoritis, *Tetrahedron Green Chem.* **3** (2024) 100044.

EFFECT OF PACKAGING TYPE ON ANTIMONY LEACHING INTO BOTTLED WATER

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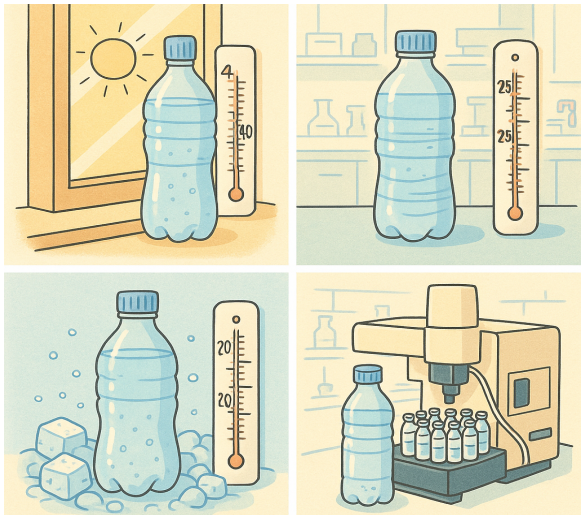
The type of packaging material is a critical factor influencing the safety of bottled water. Polyethylene terephthalate (PET) and glass are the most commonly used materials, with PET being widely applied due to its light weight and durability. However, antimony oxide, used as a catalyst in PET production, can leach into water, raising potential health concerns. In contrast, glass is generally chemically inert and does not contribute to antimony leaching [1,2]. The aim of this study was to compare antimony leaching from PET and glass packaging under different storage conditions. Six commercial bottled water brands were analyzed at three temperatures (−20 °C, 25 °C, and 40 °C) using inductively coupled plasma mass spectrometry (ICP-MS). In addition, the total Sb content of PET bottles was determined. The results confirmed Sb leaching exclusively from PET packaging, with the highest concentrations detected at 40 °C, exceeding the EU/EPA guideline value of 5 µg/L. In contrast, glass packaging showed stable Sb levels under all storage conditions, with the only exception being bottles sealed with PET-based caps, where measurable Sb leaching was observed. These results confirm that antimony leaching is associated with PET packaging and that glass packaging remains essentially inert under the studied conditions.



[1] C. Reimann, M. Birke, P. Filzmoser, *Appl. Geochem.* **27** (2012) 1492–1498.
[2] M. Ristić, I. Popović, V. Pocajt, D. Antanasijević, A. Perić-Grujić, *Food Addit. Contam. B* **4** (2011) 6–14.

SUSTAINABLE SYNTHESIS AND CHARACTERIZATION OF BIOCOMPATIBLE HYDROXYAPATITE FROM NATURAL CALCIUM CARBONATE SOURCES

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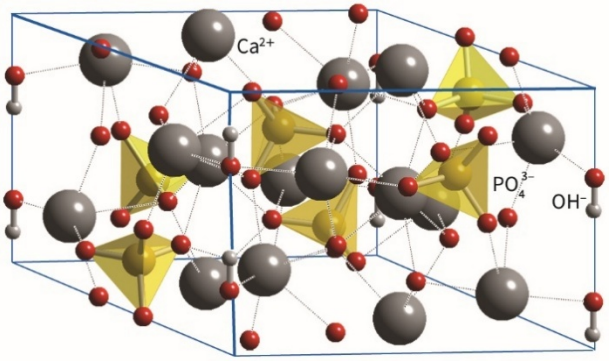
Hydroxyapatite (HAP), $Ca_{10}(PO_4)_6(OH)_2$, is a calcium phosphate biomaterial with remarkable biocompatibility and structural similarity to the mineral phase of human bones and teeth. Due to its excellent bioactivity and stability under physiological conditions, HAP is widely used in bone tissue engineering, dental implants and biomedical coatings. In this study, hydroxyapatite was synthesised by a precipitation method using calcium carbonate from natural waste materials, particularly chicken eggshells and mussel shells as an environmentally friendly and sustainable source of calcium [1,2]. The synthesis was carried out by stepwise addition of phosphoric acid to a calcium hydroxide suspension. Calcium hydroxide ($Ca(OH)_2$) was obtained by calcining calcium carbonate ($CaCO_3$) from natural starting materilas at 900 °C, producing calcium oxide (CaO), which was then hydrated by adding water. The pH being carefully adjusted using ammonia. The resulting HAP was isolated in powder form and then thermally treated. The synthesised material was characterised using Fourier transform infrared spectroscopy (FT-IR), powder X-ray diffraction (PXRD) and surface analysis using the Brunauer-Emmett-Teller (BET) method. FT-IR confirmed the presence of phosphate and hydroxyl groups, which are characteristic of HAP. PXRD analysis showed sharp diffraction peaks corresponding to a crystalline hexagonal HAP phase. BET analysis revealed a specific surface area suitable for biomedical applications. This approach not only demonstrates a cost-effective and environmentally friendly method for obtaining high-purity HAP, but also adds value to biowaste and thus contributes to the circular economy. The method offers the potential for scalable production of HAP for use in orthopedics, dentistry and as a scaffold material for bone regeneration. The work underlines the importance of green chemistry principles for the development of functional biomaterials.



[1] M. Vukomanovic *et al.*, *Cryst. Growth Des.* **8** (2008) 2217 – 2222.
[2] T. Suleyka, *et al.*, *J. Appl. Chem.* **17** (2024) 56 – 64.

COMPARISON OF THE ANTIOXIDANT ACTIVITY OF SELECTED HONEY TYPES FROM CROATIA

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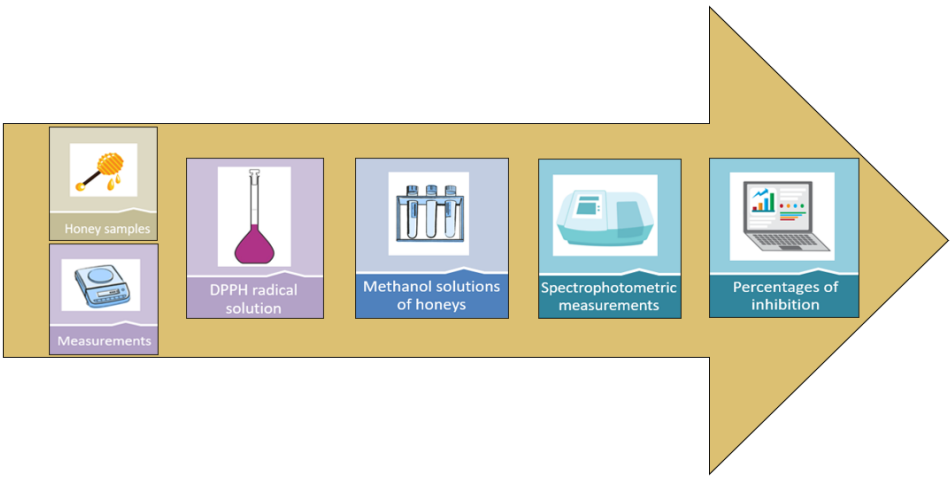
Honey is a complex natural product that is known for its health-promoting properties. The compounds contained in honey, such as phenolic compounds, ascorbic acid, some enzymes, carotenoid derivatives, products of the Maillard reaction, organic acids, amino acids and proteins, contribute to its antioxidant activity [1]. Since the composition of honey depends primarily on its botanical origin and geographical factors, the research and characterisation of monofloral honey varieties of known geographical origin is of particular interest [2,3]. In this work, a comparison of antioxidant activity was carried out between samples of light-coloured honey from the Croatian flora, comparing samples of three unifloral honey types (false indigo, black locust, and linden) and a multifloral honey sample. The botanical origin of the selected unifloral honey samples was confirmed by melissopalynological analyses. The antioxidant activity of the honey samples was evaluated by modified DPPH method reported by Gül and Pehlivan [3] using spectrophotometric measurements at 517 nm. The results are expressed as a percentage of DPPH inhibition. The highest percentage of DPPH inhibition was shown by multifloral honey, which is the darkest (95.18%), followed by linden (52.05%) and false indigo honey (29.84%), while the lightest black locust honey showed the lowest percentage of inhibition (9.14%). The results are consistent with previous findings [1] showing that antioxidant activity depends on the botanical source and colour of the honey, with darker honey having a stronger antioxidant power. Investigating the antioxidant capacity of different honey samples could indicate their therapeutic potential.



[1] M.I. Khalil, S.A. Sulaiman, L. Boukraa, *Molecules* **15** (2010) 9302–9324.

[2] I. Flanjak, D. Kenjerić, D. Bubalo, L. Primorac, *Eur. Food Res. Technol.* **242** (2016) 467–475.

[3] A. Gül, T. Pehlivan, *Saudi J. Biol. Sci.* **25** (2018) 1056-1065.

ELECTRON PARAMAGNETIC RESONANCE STUDY OF THE ANTIRADICAL ACTIVITY OF RED GOJI BERRY EXTRACTS

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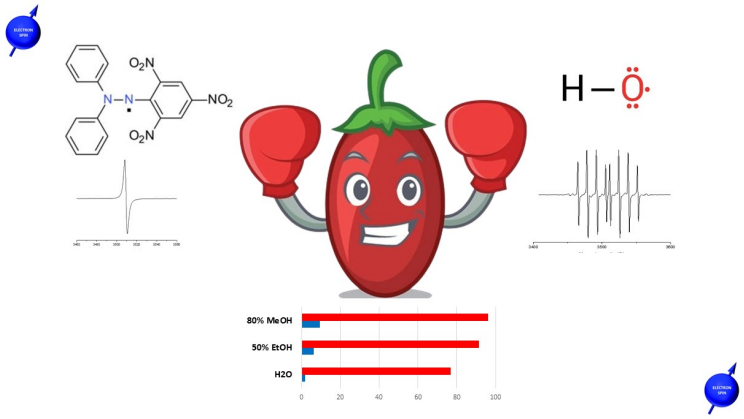
Goji berries (*Lycium barbarum* L.) are widely recognized for their bioactive phytochemicals, particularly polyphenols and carotenoids, which contribute to their antioxidant potential. In this study, electron paramagnetic resonance (EPR) spectroscopy was employed to investigate the antiradical activity of red goji berry extracts against two radical species: 2,2-diphenyl-1-picrylhydrazyl (DPPH) and hydroxyl radicals (˙OH). EPR spectroscopy was the method of choice because it enables direct, selective, and highly sensitive detection of free radicals and their scavenging, providing reliable insight into antioxidant activity. EPR spin trapping technique was used to detect ˙OH. Extracts were prepared using water, 50% ethanol, 75% ethanol, and 80% methanol at a 1:10 (w/v) ratio under ultrasound-assisted extraction. The results revealed a significantly higher scavenging capacity towards hydroxyl radicals compared to DPPH radicals. For DPPH, radical scavenging activity reached 1.96% (water), 6.41% (50% EtOH), and 9.44% (80% MeOH). In contrast, ˙OH scavenging was considerably stronger, with values of 76.92% (water), 91.47% (50% EtOH), and 96.28% (80% MeOH). The pronounced efficiency against hydroxyl radicals suggests that goji berry extracts may serve as effective natural protectants against highly reactive oxygen species. This study highlights the importance of solvent selection in maximizing the recovery of antioxidant compounds and demonstrates the utility of EPR spectroscopy in directly quantifying radical scavenging activity of natural products.



This research was funded by the Ministry of Science, Technological Development, and Innovation of the Republic of Serbia, contract numbers: 451-03-137/2025-03/200146 and 451-03-136/2025-03/200051

[1] D. Milosavljević *et al.*, *Plants* **11** (2022) 3566.
[2] Đ. Nakarada *et al.*, *HoPh* **8** (2021) 1004-1013.

IMGIIA PEPTIDES AS SELF-ASSEMBLING BUILDING BLOCKS: EXPERIMENTAL AND COMPUTATIONAL INSIGHTS

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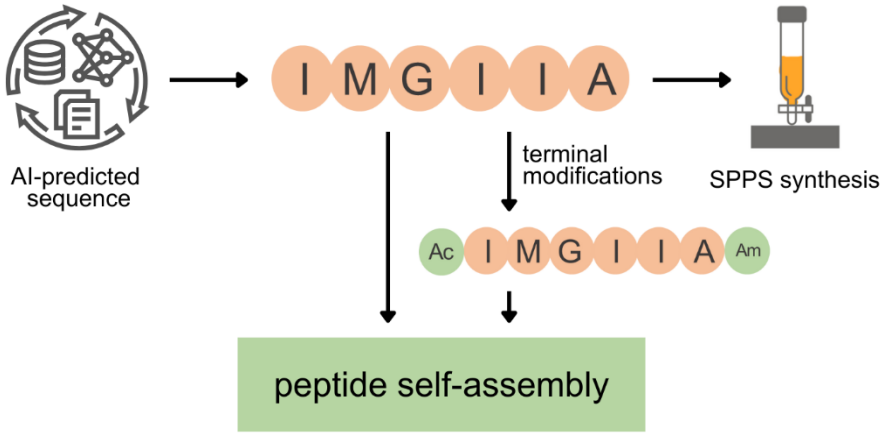
Peptides are versatile building blocks for nanomaterials, combining biocompatibility and tunable chemical properties. They can spontaneously organize into well-defined nanostructures through self-assembly, a process driven by noncovalent bonding such as π-π stacking, hydrogen bonding, electrostatic interactions and hydrophobic effects [1]. This self-assembly can be modulated by terminal modifications, including amidation and acetylation, which neutralize charges and adjust intermolecular interactions. Using AI, the IMGIIA sequence was generated with 99.4% probability of self-assembly [2]. The uncapped variant was synthesized using Fmoc-based solid-phase peptide synthesis, purified by reverse-phase high-performance liquid chromatography and characterized by liquid chromatography-mass spectrometry. Due to limitations in purifying capped IMGIIA, coarse-grained molecular dynamics simulations were employed to study both uncapped and capped peptides. The uncapped peptide showed aggregation in extended conformations, while capped IMGIIA consistently formed compact spherical assemblies, highlighting the effect of terminal charge removal on assembly behaviour. This combined approach demonstrated that experimental methods and *in silico* simulations provide complementary insights, with simulations offering predictive value for variants that are experimentally challenging to obtain. The results suggest IMGIIA peptides as promising candidates for the design of supramolecular nanostructures and peptide-based hydrogels, supporting future applications in biomedicine and nanotechnology.



[1] E. Dražić, D. Jelušić, P. Janković Bevandić, G. Mauša, D. Kalafatovic, *ACS Nano* **19** (2025) 20295-20320.

[2] M. Njirjak *et al.*, *Nat Mach Intell* **6** (2024) 1487–1500.

COPPER(II) COMPLEXES WITH BENZOPYRANONE LIGAND AND INCORPORATED PYRIDINE: SYNTHESIS, STRUCTURE, AND POTENTIAL BIOACTIVITY

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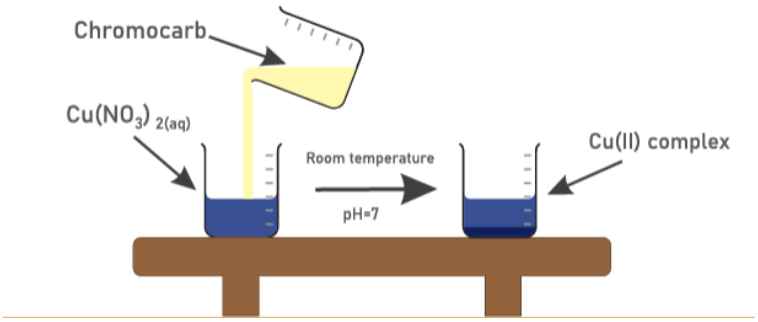
Coordination compounds of transition metals, particularly copper(II), are a subject of intensive research due to their wide range of chemical and biological properties. Copper, as an essential element, participates in numerous enzymatic processes, and its complexes show significant potential in the field of medicine, including antitumor and antimicrobial activity. Benzopyranones, such as chromone derivatives [1,2], are known for their diverse biological effects, including anti-inflammatory, antiallergic, and antitumor activity. As ligands in metal complexes, they can stabilize various coordination geometries and contribute to the properties of the compound. Pyridine is often used as a solvent in the synthesis of complex compounds, but its presence in the reaction system can also lead to supramolecular incorporation into the crystal structure of the product. Such incorporation can significantly influence the final geometry of the complex, its packing in the crystal lattice, and its physicochemical and biological properties. In this study, copper(II) complexes with benzopyranone ligand (chromocarb) were synthesized. After filtration and drying of the precipitate, the compound was recrystallized with pyridine to monitor its possible incorporation into the structure. The obtained compounds were characterized using spectroscopic and analytical methods, as well as single-crystal X-ray diffraction, in order to determine their structure and supramolecular organization. The potential antimicrobial activity will also be investigated to assess the influence of the ligand and the presence of pyridine on the biological efficacy of the compounds.



[1] C. Yu *et al.*, *Front. Chem*. **10** (2022) 50726.
[2] Z. Xiao, A.G. Wedd, *Nat. Prod. Rep*. **27** (2010) 768.

STRUCTURAL INSIGHTS AND CYTOTOXIC ACTIVITY OF A RHENIUM(V)–APIGENIN COMPLEX

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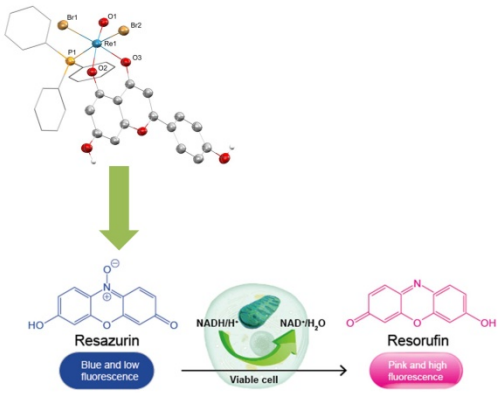
Apigenin is a flavonoid belonging to the flavone subclass, widely distributed in medicinal plants. It has been recognized as a bioactive compound exhibiting anti-inflammatory, antioxidant, and anticancer properties [1]. Oxorhenium(V) complexes have attracted considerable attention due to their structural versatility and stability, as well as their potential applications in medicinal chemistry [2].

A new complex of apigenin with $ReOBr_3(PPh_3)_2$ was synthesized, characterized, and used for biological studies. The complex was obtained by the reaction of apigenin with the rhenium(V) precursor ($ReOBr_3(PPh_3)_2$) in acetone (1:1) under reflux. Its chemical structure was confirmed using standard analytical techniques, including NMR and IR spectroscopy, and by single-crystal X-ray diffraction. The rhenium center in the complex exhibited a distorted octahedral geometry, with apigenin chelating through two oxygen atoms in an almost planar chelate. The oxo ligand was positioned *cis* to the two bromido ligands and trans to the oxygen donor atoms of apigenin.

Cytotoxicity assessment was conducted using the resazurin reduction assay across multiple cancer cell lines. This Re-apigenin complex showed significant cytotoxic potential toward Jukart cell line and moderate activity against other cell lines. Furthermore, IC_{50} values of all complexes were less than 5 μM for Jurkat and demonstrated enhanced cytotoxic activity.

In conclusion, the coordination of apigenin to the rhenium(V) center was shown to refine its cytotoxic potential, highlighting the role of oxorhenium(V) complexes as promising candidates for the development of novel anticancer agents.



[1] B. Salehi *et al.*, *Int. J. Mol. Sci.* **20** (2019) 1305.
[2] R. Alberto, R. Schibli, *Dalton Transactions* **39** (2010) 5851–5861.

THERMODYNAMICS OF STEROID DERIVATIVES' COMPLEXATION WITH CYCLODEXTRINS

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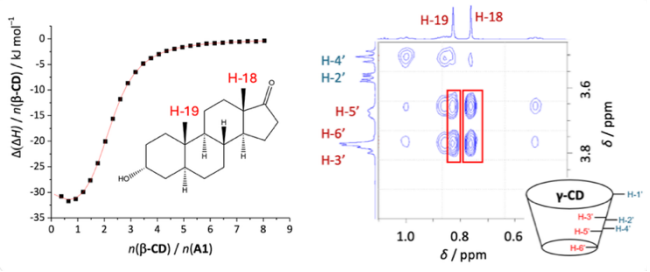
Cyclodextrins are widely recognized as host molecules for hydrophobic guests, whereby steroids represent particularly relevant targets due to their structural diversity, poor aqueous solubility, and important biological roles. Formation of steroid–cyclodextrin inclusion complexes enhances bioavailability and has found practical applications, such as cholesterol removal from food products [1]. Nevertheless, comprehensive thermodynamic and structural studies of these complexes remain relatively scarce, limiting a deeper understanding of the underlying binding thermodynamics.

In this study, the inclusion of several steroids and bile salts into β- and γ-cyclodextrins in aqueous solution was investigated at 25 °C using isothermal titration calorimetry (ITC) and 1D/2D NMR spectroscopy. Stable complexes with different stoichiometries were formed, influenced by the host's dimensions and functionalization, as well as the molecular structure of the guests. The reactions were enthalpically favorable, while in certain cases they were mainly governed by entropy. Temperature-dependent investigations revealed negative $\Delta_r C_p°$ values, as well as enthalpy–entropy compensation, resulting in nearly temperature-independent $\Delta_r G°$ for selected steroid–γ-cyclodextrin complexes [2-4].



[1] P. Fenyvesi, I. Puskás, L. Szente, in: E. Bilensoy (Ed.), *Cyclodextrins in Pharmaceutics, Cosmetics, and Biomedicine: Current and Future Industrial Applications*, Springer, 2018, *Cham*; pp. 25–60.

[2] K. Leko *et al.*, *Chem. Eur. J.* **26** (2020) 5208–5219.

[3] A. Usenik *et al.*, *J. Mol. Liq.* **388** (2023) 122774.

[4] A. Usenik *et al.*, *New J. Chem*. **47** (2023) 18745–18755.

ASSESSMENT OF THE ECOTOXICITY OF ADDITIVES IN BIODEGRADABLE PACKAGING USING DUCKWEED *LEMNA MINOR*

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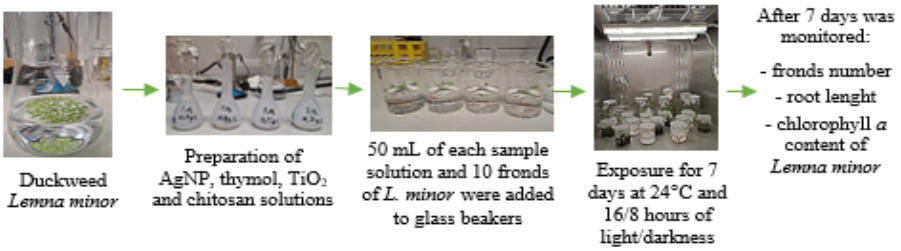
The extensive use of biodegradable polymers as alternatives to conventional plastic has led to the inclusion of various functional additives aimed at improving antimicrobial, barrier, and mechanical properties [1]. Among the most frequently used are silver nanoparticles (AgNPs), thymol, titanium dioxide (TiO_2), and chitosan. Although these substances enhance packaging performance, their potential release into the environment raises concerns regarding ecotoxicity [2]. In this study, the ecotoxicological effects of these additives were investigated using *Lemna minor*, a freshwater macrophyte commonly used as a sensitive bioindicator in aquatic ecotoxicity assessments. *Lemna minor* was exposed for 7 days to aqueous solutions of each additive under 24 ºC and 16/8 hours of light/darkness, and their effects were evaluated through changes in frond number, root length, and chlorophyll *a* content. The tested concentrations ranged from 1–10 g/L for AgNPs, from 10–100 g/L for thymol and from 0.1–1.0 g/L for TiO_2 and chitosan. AgNPs and thymol exhibited strong ecotoxic effects, with 100% growth inhibition observed at concentrations ≥3 g/L. No growth or root elongation was recorded for any thymol concentration. In contrast, TiO_2 showed no observable ecotoxicity, while chitosan caused moderate growth inhibition (10–17%) and a noticeable reduction in root length. The inhibition of chlorophyll *a* production corresponded with the growth inhibition results, with thymol and AgNPs causing the greatest reduction (91.16% was INH *Ca* for the highest concentration of thymol and 60.28% was INH *Ca* for the highest concentration of AgNP). The results suggest that despite the functionality added by such additive, their use in biodegradable packaging should be carefully evaluated to prevent unintended environmental harm. Ecotoxicological testing was therefore confirmed as an essential tool for evaluating the environmental safety of biodegradable packaging additives.



This research was conducted as part of the project "Production and development of compostable packaging from waste biomass for packaging of industrially processed food products" (NPOO.C3.2.R3- I1.04.0059) funded by the National Recovery and Resilience Plan (funded by the European Union, NextGenerationEU).

[1] K. Y. Perera, A. K. Jaiswal, S. Jaiswal, *Foods* **12** (2023) 2422.
[2] K. Kraśniewska, S. Galus, M. Gniewosz, *Int. J. Mol. Sci.* **21** (2020) 698.

2D MOLYBDENUM DISULFIDE: FROM ATOMIC LAYER TO DEVICE INTEGRATION

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Two-dimensional (2D) transition metal dichalcogenides (TMDs), such as monolayer molybdenum disulfide (MoS_2), have attracted considerable attention due to their exceptional mechanical, electronic and optical properties [1]. In the first part of this project, MoS_2 was synthesized by chemical vapor deposition (CVD) and subsequently transferred onto Si/SiO_2 substrates. Standard microfabrication steps, including photolithography and metal evaporation, were employed to prepare structures suitable for further studies. The MoS_2 layers were characterized by atomic force microscopy (AFM), Raman and photoluminescence (PL) spectroscopy, and scanning electron microscopy (SEM), confirming the quality and morphology of the layers. Given the strong interest in MoS_2 for nanoelectronic applications, in the second part of the project its potential was explored by integrating MoS_2 mono- and multilayers into 2D devices and by performing electrical characterization. Taken together, these results provide a foundation for future studies of MoS_2 and other 2D TMDs, whether through chemical functionalization strategies [2] or by advancing their use in sensing and electronic technologies.

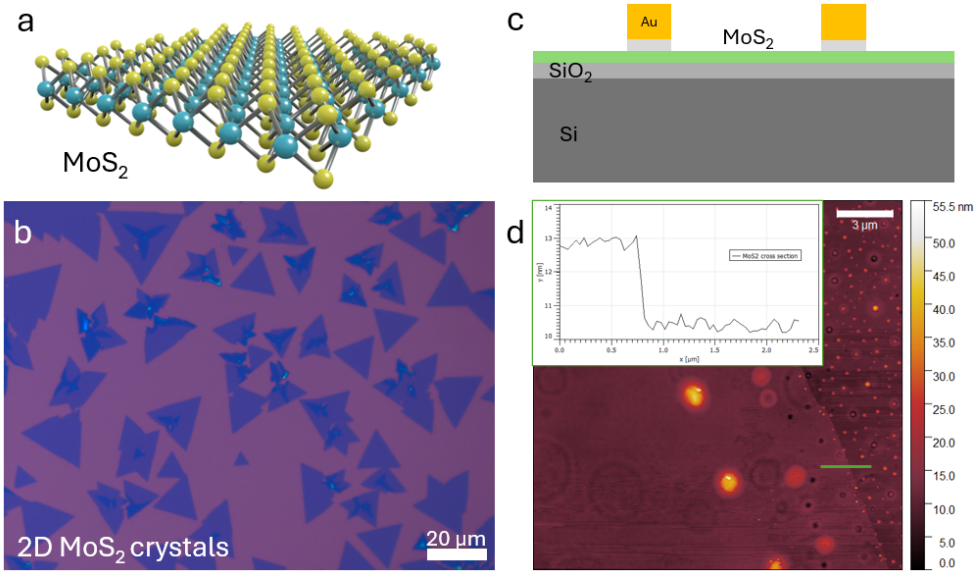

Figure 1. Atomic structure of MoS_2 monolayer (a). Optical micrograph of synthesized MoS_2 crystals (b). Cross-sectional schematic of a MoS_2-based device (c). AFM image of MoS_2 monolayer with cross-section line (green) and corresponding height profile (d).

[1] Q. H. Wang *et al.*, *Nat. Nanotechnol.* **7** (2012) 699–712.

[2] M. Lihter *et al.*, *ACS Appl. Nano Mater.* **4** (2021) 1076–1084.

CHARACTERIZATION OF GLUCOSE DEHYDROGENASE PRODUCED BY DIFFERENT MICROORGANISMS

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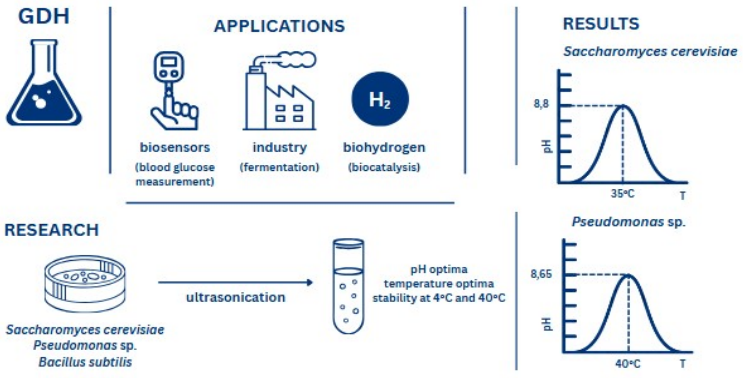
Glucose dehydrogenase (GDH) is an industrially and scientifically important enzyme that is widely used in various biotechnological processes. Its applications include the production of biohydrogen by enzymatic oxidation of glucose, integration into biosensor systems for monitoring blood glucose levels, and use as a biocatalyst in fermentation processes for the synthesis of various high value-added biochemicals.

In this study, GDH were characterised from three different microbial sources: *Saccharomyces cerevisiae*, *Bacillus subtilis* and *Pseudomonas* sp. The microorganisms were cultivated under controlled laboratory conditions and biomass concentration was monitored during the cultivation period. After reaching the stationary phase, the cells were separated from the medium and disrupted by ultrasonication to release intracellular enzymes. GDH activity was subsequently analysed in the crude extracts, and the activity was detected in the biomass of *S. cerevisiae* and *Pseudomonas* sp., while no significant activity was observed in *B. subtilis*.

Further characterization of GDH from different sources included the determination of their pH and temperature optima as well as their storage stability at different temperatures. GDH from *S. cerevisiae* showed optimal activity at $T = 35$ °C and pH = 8.80 while the GDH from *Pseudomonas* sp. showed its highest activity at $T = 40$ °C and pH = 8.65. Storage stability tests showed better enzyme stability at 4 °C compared to 40 °C for both enzyme sources, indicating temperature-sensitive deactivation at higher storage temperatures.



[1] S. Shah, A. V. Sunder, P. Singh, P. P. Wangikar, *Indian J. Microbiol.* **60** (2020) 87-95.

[2] A. Basner, G. Antranikian, *PLoS One* **9** (2014) 85844.

HALOGEN-BONDED COCRYSTALS OF $M(NCS)_2(3\text{-}Xpy)_4$ COORDINATION COMPOUNDS (M = Co, Ni, Fe; X = Cl, Br, I)

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Although less studied than halogenide ligands in halogen-bonded metal–organic compounds [1], isothiocyanate has proven to be a versatile halogen bond acceptor [2]. In this study we further evaluate its potential and additionally demonstrate how halogen atoms at the periphery of coordination compounds influence halogen-bonded cocrystal structures. To this end, we prepared nine octahedral coordination compounds (M-X) of $M(NCS)_2(3\text{-Xpyridine})_4$ type (M = Co, Ni, Fe; X = Cl, Br, I) and cocrystallized them with the halogen bond donor 1,4-diiodotetrafluorobenzene (**14tfib**). Characterization of (M-X)(**14tfib**)$_2$ cocrystals obtained by liquid-assisted grinding and recrystallization from solution was performed using powder and single crystal X-ray diffraction. Structural analysis of all cocrystals revealed double chains formed by I···S halogen bonds between **14tfib** and isothiocyanate ligands. In (M-I)(**14tfib**)$_2$, iodine atoms from 3-iodopyridine ligands emerged as halogen bond donors, forming weaker I···S halogen bonds between chains. In contrast, halogen-bonded chains in (M-Cl)(**14tfib**)$_2$ and (M-Br)(**14tfib**)$_2$ are connected via other non-covalent interactions. Beyond confirming the strong halogen-bonding propensity of isothiocyanate sulphur, this study demonstrates the halogen-bond donating ability of peripheral iodine atoms and shows that the metal center in (M-X)(**14tfib**)$_2$ cocrystals has no significant influence on the key features of the supramolecular architecture.

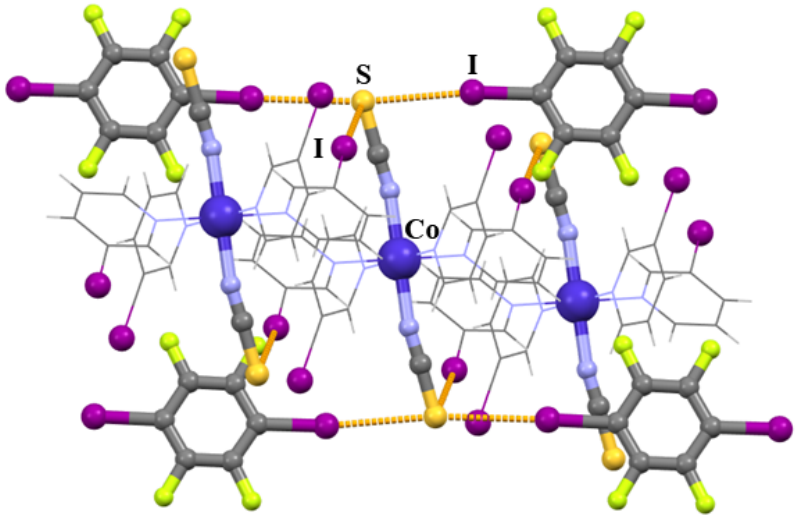

Figure 1 Halogen bonding in the (Co-I)(**14tfib**)$_2$ cocrystal.

[1] V. Nemec *et al*., *CrystEngComm* **23** (2021) 3063.

[2] L. Posavec, D.Cinčić, *Cryst. Growth Des.* **24** (2024) 7514.

SYNTHESIS AND CHARACTERIZATION OF COPPER(II) COMPLEXES WITH CHROMONE-2-CARBOXYLIC ACID: A GREEN CHEMISTRY APPROACH

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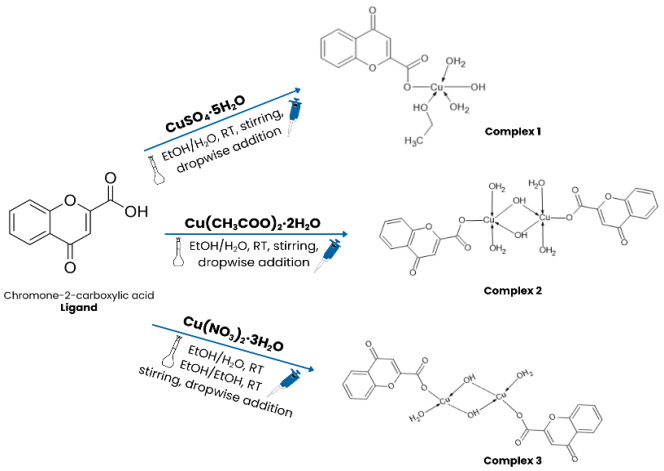
In this study, three novel copper(II) complexes were synthesized using chromone-2-carboxylic acid, a ligand from the benzopyrone group, in combination with copper salts, namely copper(II) sulphate pentahydrate, copper(II) nitrate trihydrate, and copper(II) acetate dihydrate. The synthesis followed green chemistry principles, using water and ethanol as solvents to minimize the environmental impact of the process [1,2]. The synthesis was carried out under mild conditions, ensuring an efficient process with minimal waste. The use of environmentally friendly reagents and solvents emphasizes the importance of sustainable methods in modern chemical synthesis. The synthesized complexes were characterized by FT-IR spectroscopy, thermal analysis, and X-ray powder diffraction (XRD). FT-IR spectra indicated the successful coordination of the ligand with copper(II) ions, showing the deprotonation of the carboxyl group in the chromone ligand. Specific absorption bands in the IR spectra were attributed to the vibrations of the functional groups, providing insight into the coordination environment and structural features of the complexes. Thermal analysis, supported by XRD, further complemented the characterization, revealing the stability of the copper component and the decomposition patterns of the complexes. The mass loss observed in thermogravimetric analysis was consistent with the proposed structures, indicating the ordered loss of water molecules and organic components with increasing temperature. XRD analysis on the polycrystalline sample confirmed the crystalline nature of the complexes, providing valuable structural data and supporting the FT-IR and thermal findings. This study demonstrates that the principles of green chemistry can be successfully applied in the preparation of organometallic complexes, promoting both sustainability and efficiency in the development of novel materials for various applications, including catalysis and material science.



[1] L. Toso *et al.*, *J. Inorg. Biochem*. **127** (2013) 220–231.
[2] J. Arshad, M. Hanif, *RSC Med. Chem*. **10** (2022) 1–10.

MONITORING THE FORMATION OF THE CINNARIZINE:HYDROXYPROPYL-B-CYCLODEXTRIN INCLUSION COMPLEX IN SOLUTION BY SPECTROSCOPY NMR

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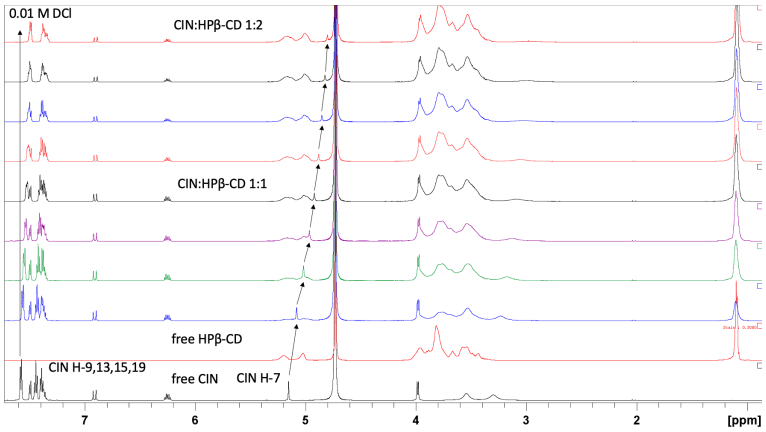
Cinnarizine, one of piperazine derivatives with multiple pharmacological activities, was limited in its clinical application due to poor solubility in aqueous media. One of the approaches to improve its solubility was the formation of inclusion complexes with cyclodextrins. Specifically, the possibility of cinnarizine complexation with hydroxypropyl-β-cyclodextrin (HP-β-CD) was examined using nuclear magnetic resonance (NMR) spectroscopy. The interaction between the two molecules was assessed by monitoring chemical shift changes during titration of cinnarizine with HP-β-CD solutions, and the results indicated inclusion of the cinnarizine molecule into the cavity of HP-β-CD, with the orientation being assumed only on the basis of molecular size. Titration of cinnarizine with HP-β-CD solutions was carried out at two different DCl concentrations (c = 1.0 mol dm^{-3} and c = 0.01 mol dm^{-3}) to examine the influence of medium acidity on complexation. At the higher acid concentration, no significant chemical shift changes were observed, suggesting that the predominantly diprotonated form of cinnarizine was not stable inside the cyclodextrin cavity. In contrast, at lower acidity, where both mono- and diprotonated forms were present, clear changes in the ^{1}H NMR spectra indicated inclusion complex formation, particularly evident for H-7, whose chemical shift systematically changed upon HP-β-CD addition, and for protons H-9,13,15,19, which shifted upfield. Although the observed patterns resembled those with β-cyclodextrin, detailed analysis of cyclodextrin protons was hindered by overlap and broadening of HP-β-CD signals in the 3–4 ppm region. Changes in the appearance of these signals further supported the conclusion of complex formation. The shift of the CIN H-7 signal did not level off at a cinnarizine:HP-β-CD ratio of 1:1 but continued up to 1:2, suggesting the possible involvement of one cinnarizine molecule in two HP-β-CD cavities. However, due to the limitations of the ^{1}H NMR technique, an unambiguous conclusion regarding the inclusion mode could not be drawn without additional complementary methods.



[1] Q. Li, J. Xiang, *J. Magn. Reson.* **23** (2025) 100199.

ELECTROSPUN PLGA NANOFIBERS AS CARRIERS FOR SUSTAINED INDOMETHACIN RELEASE

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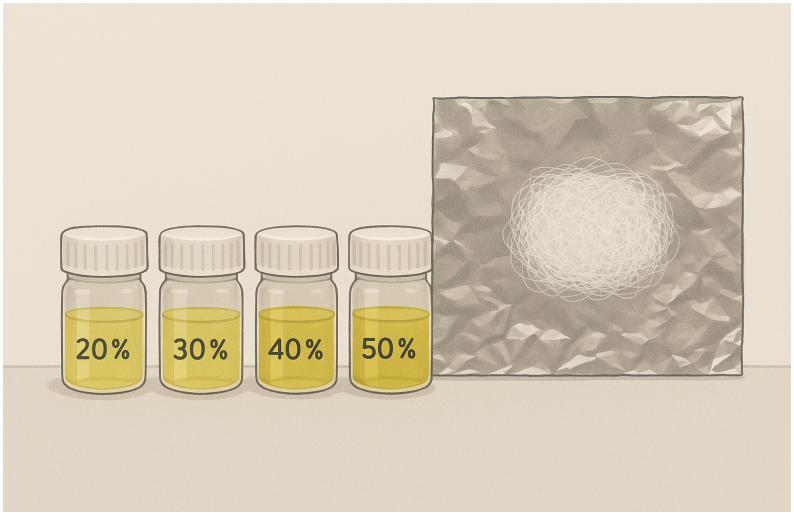
Indomethacin has been recognized as a valuable therapeutic option among nonsteroidal anti-inflammatory drugs, although its use has often been restricted by poor solubility and gastrointestinal side effects [1]. To address these limitations, poly(lactic-*co*-glycolic acid) (PLGA) nanofibers prepared by electrospinning were investigated as carriers for prolonged release. Fibers containing different amounts of indomethacin were fabricated and subsequently characterized by optical microscopy, FTIR, TGA, and DSC. These analyses confirmed that the drug had been successfully incorporated without compromising the structural and thermal stability of the polymer matrix. Release studies performed in alkaline medium demonstrated that indomethacin was gradually released from the fibers, indicating that electrospinning enabled sustained release kinetics. This release behavior suggested the possibility of maintaining therapeutic concentrations for longer periods while reducing dosing frequency and minimizing adverse gastrointestinal effects. Given the biodegradability and biocompatibility of PLGA [2], electrospun nanofibers were shown to represent a promising approach for the development of improved indomethacin formulations intended for long-term therapy.



Acknowledgements. 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.

[1] S. Lucas, *Headache Currents* **56(2)** (2016) 436-446.

[2] H. K. Makadia, S. J. Siegel, *Polymers* **3(3)** (2011) 1377-1397.

ECO-DESIGN OF PBS/PHBV POLYMER BLENDS: A STEP TOWARD BIODEGRADABLE MATERIALS

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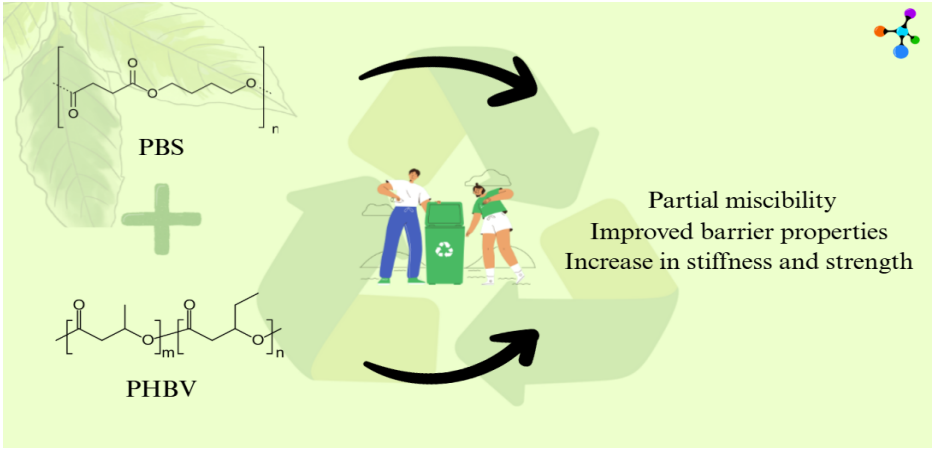
Over the past several decades, the search for environmentally responsible packaging materials has intensified, with biodegradable polymers emerging as a promising alternative. While traditional polymeric materials offer excellent functionality, their persistence in the environment raises serious ecological and waste-management challenges. Consequently, research has shifted toward biodegradable and compostable polymers that can be safely integrated into circular economy models. A clear understanding of the differences between biodegradable, compostable, and bio-based materials is essential to ensure their correct application within recycling and composting systems.

This study explores polymer blends of poly(butylene succinate) (PBS) and poly(3-hydroxybutyrate-*co*-3-hydroxyvalerate) (PHBV) prepared in varying ratios (100/0, 95/5, 90/10, 85/15, 80/20, 75/25, 70/30). The blends were analyzed using differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) for thermal properties, scanning electron microscopy (SEM) for morphology, as well as mechanical and barrier performance tests. Results indicate partial miscibility and noticeable phase separation, reflecting limited interfacial compatibility between the two polymers. Nevertheless, the incorporation of PHBV enhanced barrier resistance to gases and vapors, while mechanical analysis revealed improvements in stiffness and strength. These findings suggest that optimized PBS/PHBV compositions could provide promising pathways toward the development of advanced, eco-friendly packaging materials.



This research was conducted as part of the project „Production and development of compostable packaging from waste biomass for the packaging of industrially processed food products" (NPOO.C3.2.R3-I1 .04.0059) funded by National Recovery and Resilience Plan (funded by the European Union, NextGenerationEU).

PRODUCTION, CHARACTERIZATION AND APPLICATION OF RECOMBINANT [NIFE]-HYDROGENASE IN BIOHYDROGEN SYNTHESIS

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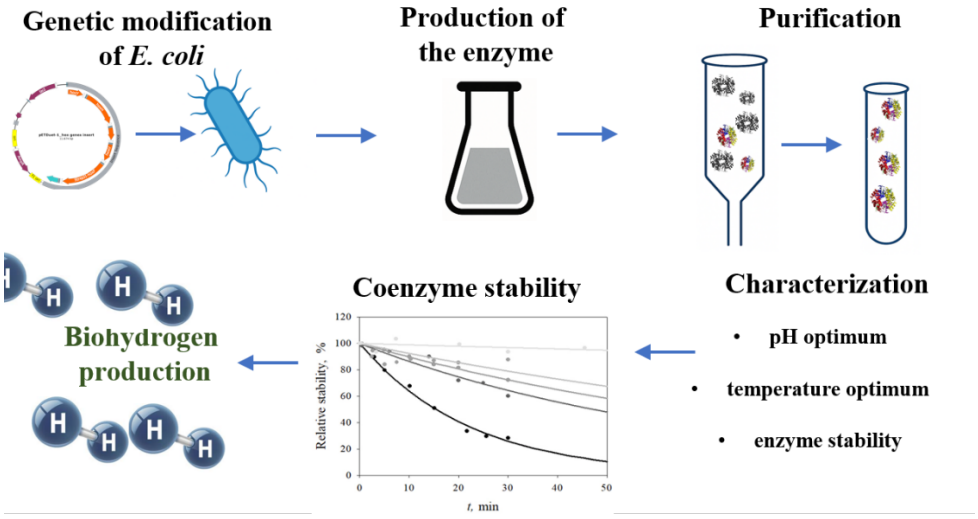
In recent decades, the problem of fossil fuel overuse has become one of the most important global issues due to its devastating impact on the environment. The use of biofuels has been cited as one of the solutions to this growing problem, and biohydrogen is a promising solution [1]. Hydrogenase enzymes play an important role in the production of biohydrogen as they catalyze the reactions of hydrogen oxidation and reduction. They are divided into three groups: [FeFe]-hydrogenases, [NiFe]-hydrogenases and [Fe]-hydrogenases, with [NiFe]-hydrogenases being the most interesting due to their resistance to the presence of oxygen [2].

The objective of this study was to produce, purify using StrepTrap XT column and characterize recombinant [NiFe]-hydrogenase and to evaluate its application in hydrogen production. Analysis of the crude extract showed that the recombinant [NiFe]-hydrogenase has two optimal pH values: pH = 4.25 (hydrogen oxidation), and pH = 7 (hydrogen production), and an optimal temperature T = 35 °C. Furthermore, the stability of the coenzymes NADH and NADPH which serve as essential substrates for biohydrogen production, was investigated, with NADH showing a higher stability. Finally, biohydrogen synthesis was carried out with crude extracts and the purified enzyme as well as with NADPH and NADH as substrates.



[1] F. Kanwal, A. A. J. Torriero, *Energies* **15** (2022) 1-3.

[2] R. Vičević, A. Šalić, A. Jurinjak Tušek, B. Zelić, *Sustainability* **16** (2024) 10650.

INFLUENCE OF PRECURSORS ON THE MECHANOCHEMICAL SYNTHESIS OF Ag_2MoO_4

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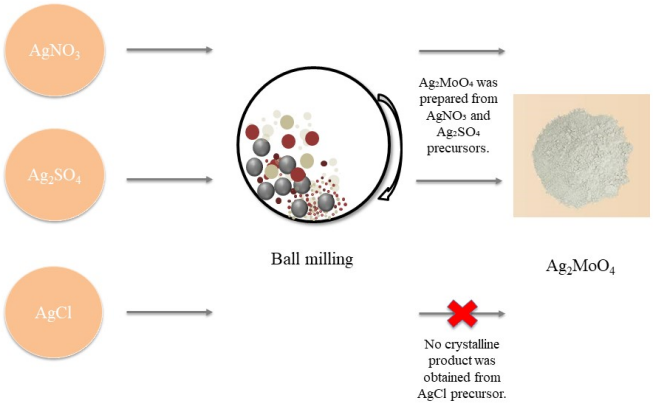
Silver molybdate (Ag_2MoO_4) has been widely investigated due to its photocatalytic and antibacterial properties [1]. Mechanochemical synthesis had emerged as a sustainable and solvent-free route for preparing metal oxides, where precursor choice strongly influenced structural and morphological outcomes [2]. In this work, Ag_2MoO_4 was synthesized mechanochemically using different selected precursors via ball milling. The precursors employed were AgCl, $AgNO_3$, and Ag_2SO_4. The resulting materials were characterized using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), scanning electron microscopy with energy-dispersive spectroscopy (SEM-EDS), and diffuse reflectance spectroscopy (DRS). It was found that precursor selection influenced the crystallinity, phase purity, thermal stability, and optical band gap. Furthermore, the product obtained by AgCl synthesis was identified as an unreacted and insoluble precursor, whereas nitrate and sulphate synthesis resulted in crystalline Ag_2MoO_4. These findings suggested that careful precursor control in mechanochemical synthesis enabled tuning of structural and functional properties of silver molybdate.



[1] N. T. Padmanabhan *et al.*, *ACS Physical Chemistry Au* **4** (2024) 247-258.
[2] A. A. Geciauskaitė, F. García, *Beilstein J. of Org. Chem.* **13** (2017) 2068–2088.

SYNTHESIS AND CRYSTAL STRUCTURE OF MULTICOMPONENT COPPER(II) MOF WITH SARCOSINE AND BISPYRIDYL LINKER

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Metal-organic frameworks (MOFs) are porous polymers comprised of metal ions and organic linkers [1]. MOFs are rising in prominence due to their wide applications in adsorption, catalysis, chiral separation and water harvesting [2,3]. They were even listed in the IUPAC Top Ten Emerging Technologies in Chemistry 2024 [4]. Multicomponent MOFs are assembled from two or more distinct organic linkers, allowing for enhanced structural complexity and wider range of functional properties. The key objective of our research is preparing MOFs with potential use as atmospheric water harvesters, addressing the urgent global challenge of limited access to safe drinking water, which currently affects one in four people worldwide [5]. A multicomponent MOF of copper(II) with sarcosine (HSar) and (*E*)-1,2-bis(pyridin-4-yl)ethene (bpe) was prepared by solution–based synthesis: $\{[Cu_2(NO_3)(Sar)(bpe)_3](NO_3)_2 \cdot \text{solvents}\}_n$ (**MOF1**). Compound **MOF1** was analysed by single-crystal and powder X-ray diffraction, FTIR and thermogravimetric analysis. The crystal structure (Figure 1) reveals that the compound is a 3D coordination polymer interwoven with 3D channels occupied by solvent molecules and nitrate ions. The **MOF1** demonstrated stability in ambient temperature and humidity, but underwent decomposition in arid environments – a behaviour that highlights its potential suitability for atmospheric water harvesting applications.

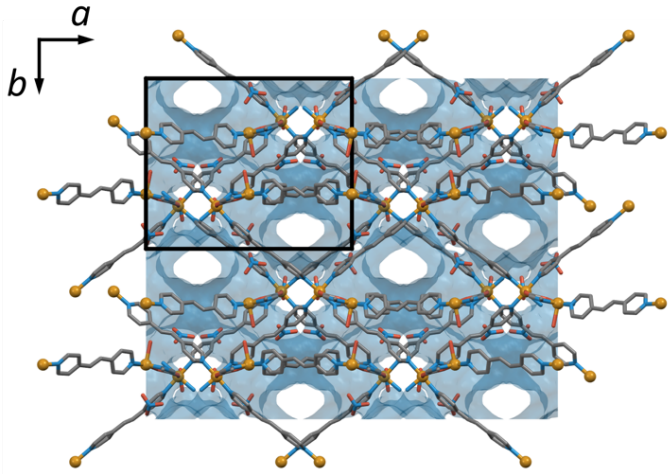

Figure 1. Crystal structure of $\{[Cu_2(NO_3)(Sar)(bpe)_3](NO_3)_2 \cdot \text{solvents}\}_n$. Contact surface of solvent molecules within the channels is shown in blue colour.

[1] M. J. Kalmutzki, C. S. Diercks, O. M. Yaghi, *Adv. Mater.* **30** (2018), e1704304.

[2] S. J. Lee, S. G. Telfer, *Angew. Chem. Int. Ed.* **62** (2023), e202306341.

[3] W. Xu, O. M. Yaghi, *Metal–Organic Frameworks for Water Harvesting from Air, Anywhere, Anytime*, *ACS Central Science* **6** (2020) 1348–1354.

[4] F. Gomollón-Bel, *IUPAC's 2024 Top Ten Emerging Technologies in Chemistry*, *Chemistry International* **46** (2024) 8–16.

[5] https://www.who.int/news/item/26-08-2025-1-in-4-people-globally-still-lack-access-to-safe-drinking-water---who--unicef (accessed 4 September 2025).

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 48h. 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. DMP motifs such as Boc-L-Ala-D-Glu(OBn)-OH **1** and Boc-L-Ala-D-*iso*glutamine(OBn)-NH_2 **2** (Fig. 1a) have been selected as target molecules. Standard solution-phase peptide coupling methods such as EDC/HOBt/TEA, HATU/DIPEA and *N*-hydroxysuccinimide/TEA 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. So far we have found that the Boc-L-Ala-OSu/TEA method in THF at 50 °C, 150 W, 250 psi and coupling time of 1 h 15 min (Fig. 1b) resulted in very good yield and purity of **1**. Therefore, the coupling time and efficiency for Boc-L-Ala-D-Glu(OBn)-OH synthesis has been improved significantly over the classical solution-phase peptide coupling method [2].

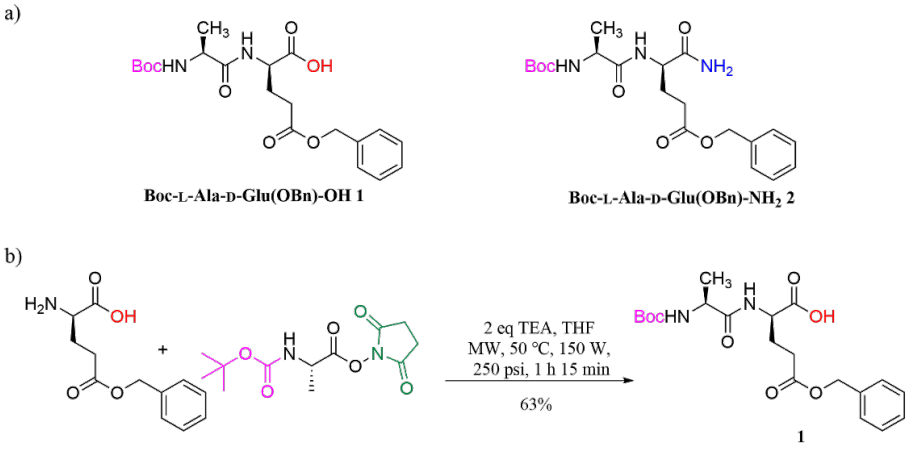

Fig. 1. a) Target DMP compounds we aim to prepare by MW solution-phase peptide method; b) MW-assisted coupling of D-Glu(OBn)-OH and Boc-L-Ala-OSu in preparation of **1**.

[1] V. P. Peroković *et al.*, *Int. J. Mol. Sci.* **25** (2022) 8628.

[2] V. P. Peroković, *et al.*, *Molecules* **26** (2021) 6352.

[3] A. Mahindra, K. K. Sharma, R. Jain, *Tetrahedron Letters* **53** (2012) 6931–6935.

MECHANOCHEMICAL SYNTHESIS OF 2-ANILINOPYRIMIDINES FROM 2-CHLORO-4,6-DIMETHYLPYRIMIDINE

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It is commonly recognized and extensively documented that anilinopyrimidines are a class of compounds known for their use as pesticides, especially as fungicides. Additionally, several derivatives of anilinopyrimidine have been evaluated as kinase inhibitors that prevent cancer cell lines from reproducing [1], which makes them very interesting as synthetic targets. There are several methods for preparing anilinopyrimidines, including aromatic nucleophilic substitution of halogenated pyrimidines with anilines, and cyclization of guanidines with β-diketones, ethyl acetoacetate or ethyl cyanoacetate. The main disadvantages of such procedures are requirement for harsh conditions and long reaction times [2]. Mechanochemistry was recently reintroduced as a method of chemical synthesis based on mechanical force that initiates and carries chemical transformations, with mechanical input typically being solvent-free milling or grinding. This technique requires far milder conditions than solution synthesis and, due to the exclusion of solvents, represents a much more environmentally acceptable approach [3]. In this work nucleophilic aromatic substitution reactions between 2-chloro-4,6-dimethylpyrimidine and aniline derivatives were examined, along with the effect of acidic catalysts and other reaction parameters.

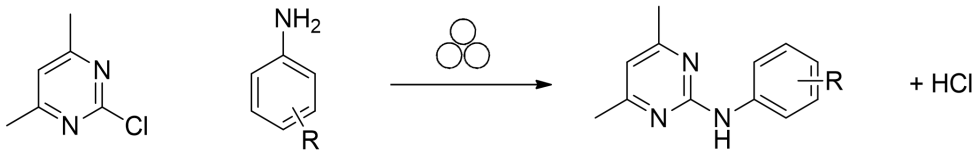

Figure 1. Mechanochemical synthesis of anilinopyrimidines.

[1] J. Joe *et al.*, *Bioorg. Med. Chem. Lett.* **29** (2018) 62–65.

[2] C. Campestre, G. Keglevich, J. Kóti, L. Scotti, C. Gasbarri, G. Angelini, *RSC Adv.* **10** (2020) 12249–12254.

[3] J. L. Do, T. Friščić, *ACS central science* **3** (2017) 13–19.

PHOTOCATALYST-FREE, VISIBLE LIGHT-INDUCED HYDROALKYLATION OF VINYL SULFONES WITH ALCOHOLS

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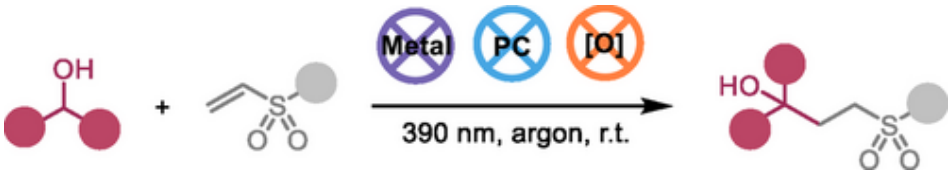
Sulfones are versatile and valuable building blocks in organic synthesis, and the sulfone group is characterized by its flexible reactivity. Moreover, sulfones comprise a class of compounds with diverse biological activity, highly relevant to the fields of pharmaceuticals and bioactive natural products. Herein, we report a direct intermolecular hydroalkylation of vinyl sulfones with alcohols under visible light irradiation. Remarkably, this transformation proceeds without photocatalysts, metals, or external redox agents, offering an atom-efficient and sustainable approach for the synthesis of γ-hydroxy sulfones. The reaction is compatible with a broad range of solvents and can be conducted with various alcohols and vinyl sulfones. Mechanistic investigations and kinetic analysis revealed an induction period and enabled the identification of a key intermediate within the reaction pathway, offering deeper insight into the transformation and supporting the proposed mechanism. The operational simplicity, mild conditions and synthetic utility position this protocol as a valuable addition to visible-light-mediated transformations.



This research was supported by the Science fund of the Republic of Serbia, Grant Number: 7750119, project acronym – New SMART Synthesis.

[1] B. Krnjaja *et al.*, *Eur. J. Org. Chem.* (2025) 000:e202500596.

[2] Y. Song *et al.*, *Green Chem*. **26** (2024) 6578.

PREPARATION AND CHARACTERIZATION OF BIODEGRADABLE PHBV/PBAT POLYMER BLENDS

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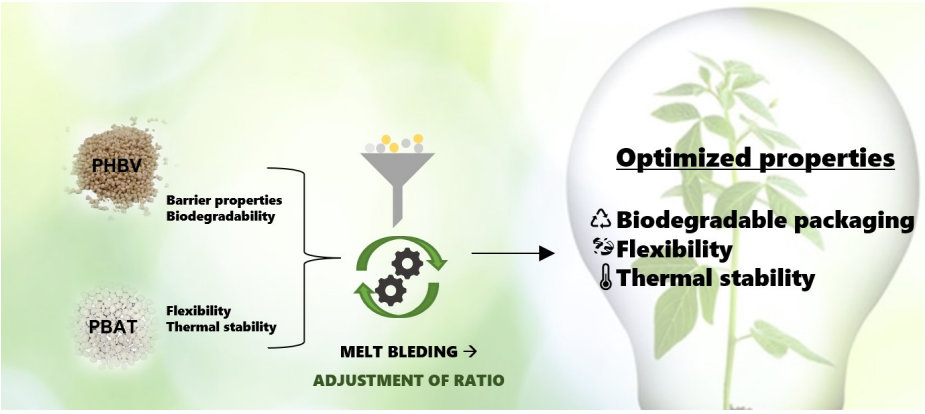
A growing demand for sustainable alternatives to conventional plastics has led to the development of biodegradable blends for food packaging applications. In this study, blends of poly(3-hydroxybutyrate-*co*-3-hydroxyvalerate) (PHBV) and poly(butylene adipate-*co*-terephthalate) (PBAT) were prepared in different mass ratios to investigate the influence of composition on material properties. The immiscibility of the two polymers posed a challenge to blend performance and was addressed by examining thermal, morphological, mechanical, and barrier properties. Differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) were used to assess thermal behaviour and stability, while scanning electron microscopy (SEM) was applied to evaluate phase distribution and morphology. Mechanical testing provided insight into tensile strength and flexibility, and barrier performance was assessed through gas permeability measurements. The results indicated that increased PBAT content led to improved flexibility but decreased thermal resistance, whereas higher PHBV content enhanced barrier properties and heat resistance, which are crucial for food contact applications. Morphological analysis showed how composition affects phase distribution and performance. By adjusting the blend ratio, flexibility, barrier properties, and thermal properties can be customized without having to resort to petroleum-based plastics. The results support the development of environmentally friendly packaging solutions that meet current market requirements and comply with current EU regulations.



This research was conducted as part of the project „Production and development of compostable packaging from waste biomass for the packaging of industrially processed food products" (NPOO.C3.2.R3-I1 .04.0059) funded by National Recovery and Resilience Plan (funded by the European Union, NextGenerationEU).

[1] P. Zytner *et al.*, *ACS Omega* **8** (2023) 1946-1956.
[2] M. Larsson, O. Markbo, P. Jannasch, *RSC Adv.* **6** (2016) 44354–44363.

IMPROVEMENT OF THE POLYPHENOLIC PROFILE OF ONION OUTER SCALES

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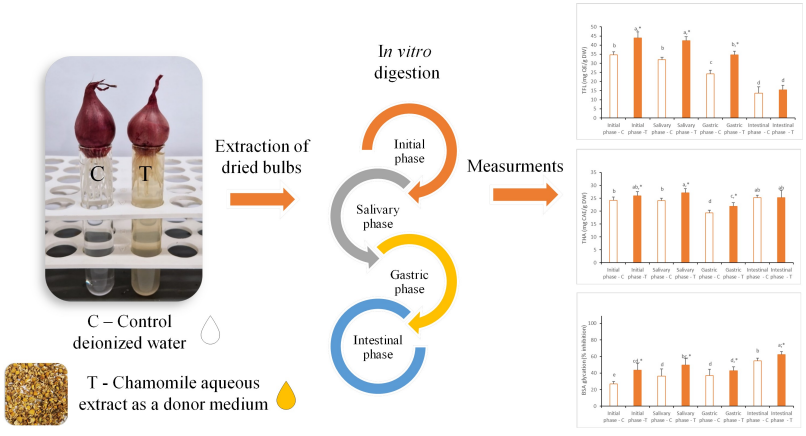
Using chamomile (*Matricaria chamomilla* L.) aqueous extract as a donor medium of apigenin, the aim was to improve the phytochemical properties of common onion (*Allium cepa* L.) through metabolite transfer between species. The purpose of this study was to evaluate, during *in vitro* digestion, the changes in flavonols, and hydroxycinnamic acids in extracts of onion outer scales treated with chamomile aqueous extract, as well as their antidiabetic potential. Prior to extraction, onion bulbs were treated with chamomile aqueous extract (12 g/L) for 24 hours. After treatment, plant material was dried in an oven at 90 °C. Ethanolic extracts of onion outer scales were prepared by rotary extraction using a tube revolver rotator for 60 min at room temperature. Total flavonols in the initial phase reached 44.0 mg QE/g DW in treated samples, compared to 34.6 mg QE/g DW in controls. Their content decreased during digestion with the lowest values of 15.4 mg QE/g DW (treated) and 13.6 mg QE/g DW (control) recorded in the intestinal phase. The concentrations of hydroxycinnamic acids were also higher in treated samples compared to controls in the early phases. In the initial phase, values were 25.9 mg CAE/g DW (treated) and 24.2 mg CAE/g DW (control). The highest content was found in the oral phase of treated samples (27.1 mg CAE/g DW), while a decline was observed in the gastric phase, especially in controls (19.3 mg CAE/g DW). In the intestinal phase, the values stabilized in both groups. The antidiabetic potential, measured by inhibition of bovine serum albumin glycation, showed significantly higher activity in treated samples at all digestion phases. The obtained results indicate that chamomile treatment of onion outer scales enhances the stability, and content of certain polyphenolic compounds – particularly flavonoids and hydroxycinnamic acids – and significantly improves their antidiabetic potential throughout the digestive process.



University of Zagreb and FarmInova (KK.01.1.1.02.0021) funded by the European Regional Development Fund.

DEVELOPING PRECURSORS FOR CHLORIDE-TEMPLATED CYCLIZATION: LINEAR TETRATYROSINE SYNTHESIS

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Peptides are essential biomolecules whose diverse biological roles are often limited by their susceptibility to enzymatic degradation and poor structural stability. Cyclization offers a strategy to overcome these limitations, as cyclic peptides typically have improved metabolic stability, enhanced bioavailability and greater target selectivity compared to their linear analogues. However, the cyclization of short peptides is often synthetically challenging due to conformational constraints, sequence-dependent inefficiencies and low yields [1,2]. Previous studies demonstrated that chloride anions can serve as templating agents by forming non-covalent interactions with nitrogen from backbone amides, thereby facilitating the alignment of peptide termini for efficient ring closure [2]. To demonstrate the method's applicability to amino acids with bulky side chains, a linear tetratyrosine precursor was synthesized from protected tyrosine derivatives. The peptide, containing *tert*-butyl (tBu) side-chain protecting groups, was obtained via solution-phase peptide synthesis through optimization of iterative coupling and deprotection reactions. Its structure was confirmed by ^{1}H and ^{13}C NMR spectroscopy. This peptide will serve as a precursor for the synthesis of linear penta- and hexatyrosines, as well as the foundation for testing the Cl^{-}-assisted macrocyclization strategy on tyrosine derivatives. Future work will focus on physicochemical characterization of cyclic tetra-, penta-, and hexatyrosines, as well as studies of their anion-binding properties using microcalorimetry and ^{1}H NMR titrations.

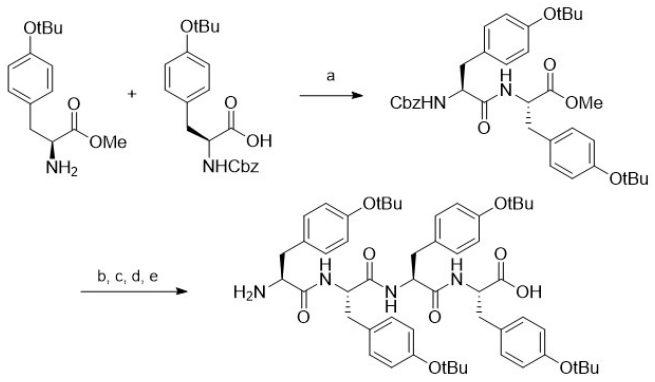

Figure 1: Synthesis of linear tetratyrosine. (a) HOBt, HBTU, TEA, DMF; (b) LiOH, MeOH/H_2O; (c) Tyr(OtBu)-OMe, HOBt, HBTU, TEA, DMF; (d) NH_4HCO_2, Pd/C, MeOH; (e) Cbz-Tyr(OtBu)-OH, HOBt, HBTU, TEA, DMF. Once the fully protected tetratyrosine was obtained, steps b and d were repeated to remove methyl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

[1] C. J. White, A. K. Yudin, *Nature Chemistry* **3** (2011) 509–524.

[2] N. Vidović *et al.*, *Organic Letters* **22** (2020) 2129–2134.

INNOVATIVE METHODS FOR THE TREATMENT OF XENOBIOTICS MIXTURES – EFFECTS ON ECOTOXICITY AND ENVIRONMENTAL SAFETY

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The preservation of water quality is one of the key challenges of modern society, given the growing burden of various pollutants on natural water resources. Xenobiotics – compounds that are not naturally present in the environment and known for their persistence and potential for bioaccumulation, may have long-term adverse effects on the environment and human health. Current wastewater treatment plants are often not efficient enough at removing xenobiotics, leading to further contamination of aquatic ecosystems. Therefore, it is important to monitor the removal efficiency of both individual xenobiotics and their mixtures to support the development of advanced wastewater treatment technologies.

The aim of this work was to investigate the efficiency of removing a mixture of six xenobiotics (clothianidin, acetamiprid, thiacloprid, mebendazole, albendazole, febantel) by applying UV irradiation and UV combined with hydrogen peroxide. The photooxidation process was carried out at three different concentrations of hydrogen peroxide (20, 50 and 100 mM). In addition, ecotoxicity tests with bioluminescent bacteria *Vibrio fischeri* were carried out at pH 4, 7 and 10 after 5 hours photolysis treatment and at pH 4 after 1, 3 and 5 hours photooxidation treatment.

After the implementation of the suntest treatment the results were read on the HPLC device. Photolysis did not result in significant removal of xenobiotics, but photooxidation is an indicator of better results. The best removal was achieved at a hydrogen peroxide concentration of 100 mM for all xenobiotics. Albendazole showed the highest removal rate at all concentrations. The results of the toxicity tests showed that the mixture of xenobiotics treated with hydrogen peroxide at a concentration of 50 mM, was the most toxic to *Vibrio fischeri*. The mixture of xenobiotics treated with hydrogen peroxide at a concentration of 20 mM was shown to be the least toxic. Also, the samples collected in the fifth hour did not show a significant reduction in toxicity. Such results are possible due to the formation of by-products, but also due to the fact that it is a mixture of xenobiotics that interact with each other.

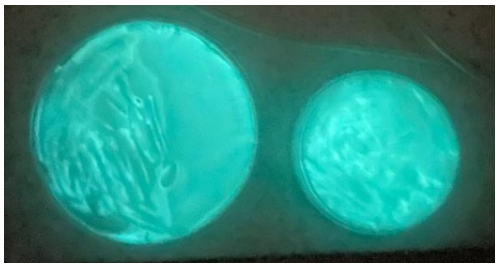

Figure 1. Bioluminiscence of pure bacterial culture *Vibrio fischeri*.

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

SYNTHESIS OF MANNOSE PRECURSORS FOR CLICK REACTIONS

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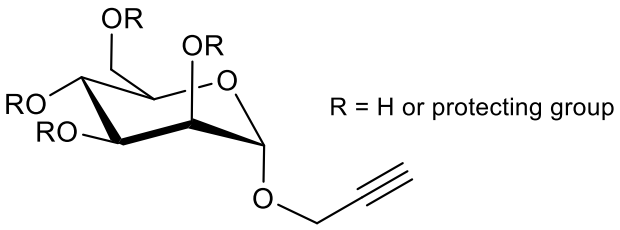
Copper(I) catalysed azide-alkyne 1,3-dipolar cycloaddition reaction (CuAAC) is a frequently used click reaction that results in the regioselective formation of 1,4-disubstituted 1,2,3-triazole derivatives [1]. The triazole subunit is one of the most common heterocyclic motifs in the structures of modern drugs with different biological effects because of its stability and resistance to metabolic degradation. In the field of carbohydrate chemistry, click chemistry, and especially the CuAAC reaction, is used to prepare a large number of compounds from simple glycosides to complex glycoconjugates [2].

Mannose is a monosaccharide that is recognized by special mannose receptors located on the surface of some cells [3]. The binding of mannose, among other things, enables targeted delivery of the drug and facilitates the entry of the drug into the cell by endocytosis. The introduction of mannose into the structure of a potential drug can also be achieved by CuAAC reactions, in which mannose derivatives can be used as an alkyne or an azide component. In this work, we report the synthesis of mannose derivatives, propargylated at the anomeric position, which was used as an alkyne component for CuAAC reaction with various azides with potential biological effect.



[1] a) M. Meldal, C. W. Tornøe, *Chem. Rev.* **108** (2008) 2952–3015.; b) E. Haldón, M. C. Nicasio, P. J. Pérez, *Org. Biomol. Chem.* **13** (2015) 9528−9550.

[2] M. Poláková, M. Belánová, K. Mikušová, E. Lattová, H. Perreault, *Bioconjugate Chem.* **22** (2011) 289–29.

[3] M. Paurević, M. Šrajer Gajdošik, R. Ribić, *Int. J. Mol. Sci.* **25** (2024) 1370–1392.

CHLORIDE-GUIDED PEPTIDE CYCLIZATION: EXPANDING THE SCOPE WITH ORNITHINE PRECURSORS

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

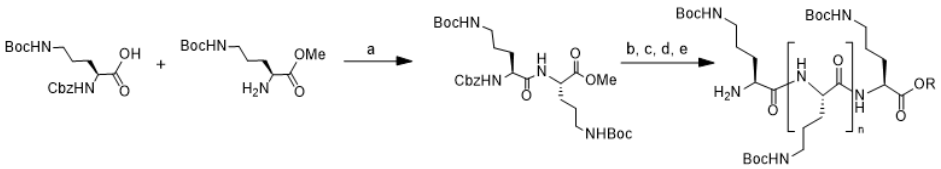

Figure 2: Synthesis of linear L-ornithine tetrapeptide: (a) HOBt, HBTU, DMF, TEA; (b) LiOH, MeOH, H_2O; (c) Orn(Boc)-OMe, HOBt, HBTU, DMF, TEA; (d) NH_4HCO_2, Pd/C, MeOH; (e) Cbz-Orn(Boc)-OH, HOBt, HBTU, DMF, TEA. Steps b and d were repeated in order to synthesize tetraornithine without OMe and Cbz.

[1] V. Apostolopoulos *et al.*, *Molecules* **26** (2021) 430.
[2] N. Vidović *et al.*, *Organic Letters* **22** (2020) 2129–2134.

SURVIVAL OF FREEZE-DRIED ENVIRONMENTAL BACTERIAL CULTURE

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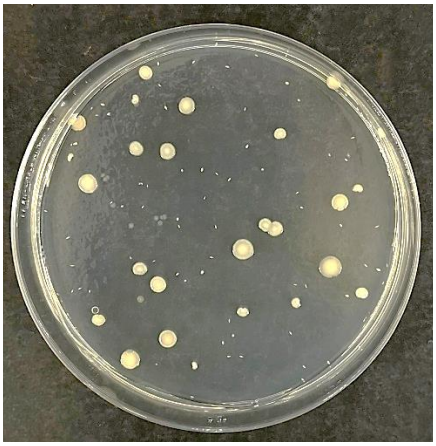
Freeze-drying is a widely used method for the long-term preservation of microorganisms in which a sample is frozen and then dried by sublimation under vacuum, followed by a second drying process. It has been used in various fields for the preservation of certain bacteria [1]. To ensure optimal survival of the bacteria, lyoprotectants are usually used to maintain the viability of the cells [2]. In this study, different proteins and sugars as lyoprotectants were investigated for the preservation of environmental bacteria and the viability of the cells was evaluated by the number of colony forming units (CFU) before and after freeze-drying. The survivability of lyoprotected samples compared to untreated controls averaged 11.0 ± 7.6 %.



Acknowledgements: The financial support by NPOO.C3.2.R3-I1.05.0207 is greatly appreciated.

[1] L. Luft, M.A. Mazutti, *Processes* **13** (2025) 2188.
[2] D.G. Farfan Pajuelo, M. Carpio Mamani, G.J. Maraza Choque, D.M. Chachaque Callo, C.J. Cáceda Quiroz, *Microorganisms* **11** (2023) 2705.

IN SILICO ANALYSIS OF OLFACTION-RELATED PROTEINS IN THE INVASIVE SPECIES *HALYOMORPHA HALYS*

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The invasive species *Halyomorpha halys* (brown marmorated stink bug) has posed a serious threat to global agriculture due to its broad host range, high resistance, and ability to rapidly spread. A key factor in its adaptability is the developed chemosensory system, which enables the detection of odorant and chemical signals from the environment. In this study, an *in silico* analysis of odorant-binding proteins (OBPs) relevant for the sense of smell in *H. halys* was carried out to elucidate their evolutionary relationships, structural properties, and potential functional roles [1,2]. Using bioinformatic databases and computational tools, multiple sequence alignments, phylogenetic analyses, and structural analysis were performed. To provide a comprehensive overview, both primary sequence features (pI, GRAVY index, amino acid composition) and three-dimensional structural predictions from AlphaFold were examined.

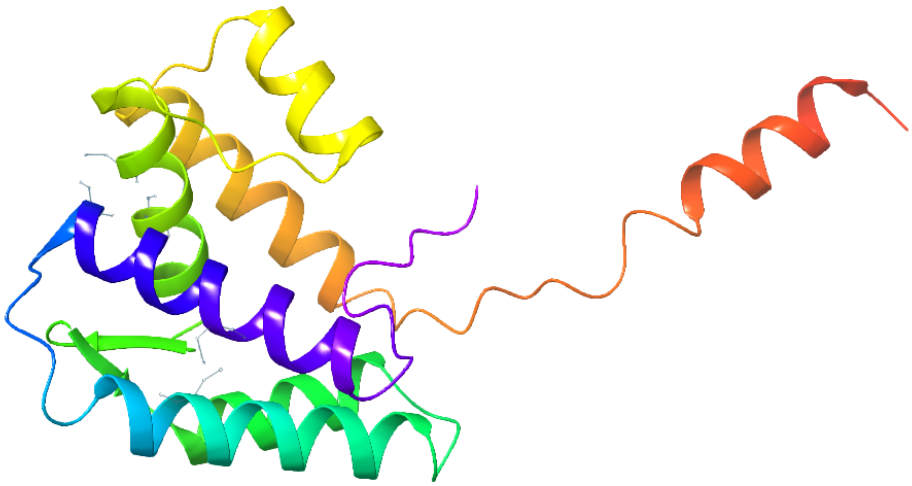

Figure 1. Predicted 3D structure of odorant-binding protein 15 (OBP15) from H. halys generated by AlphaFold and visualized in Maestro (Schrödinger).

[1] D. P. Paula *et al.*, *Insect Molecular Biology* **25** (2016) 580–594.
[2] M. E. Sparks *et al.*, *BMC Genomics* **21** (2020) 227.

DEVELOPMENT OF A POTENTIOMETRIC SENSOR BASED ON MOLECULARLY IMPRINTED POLYMER FOR DETERMINATION OF THIABENDAZOLE

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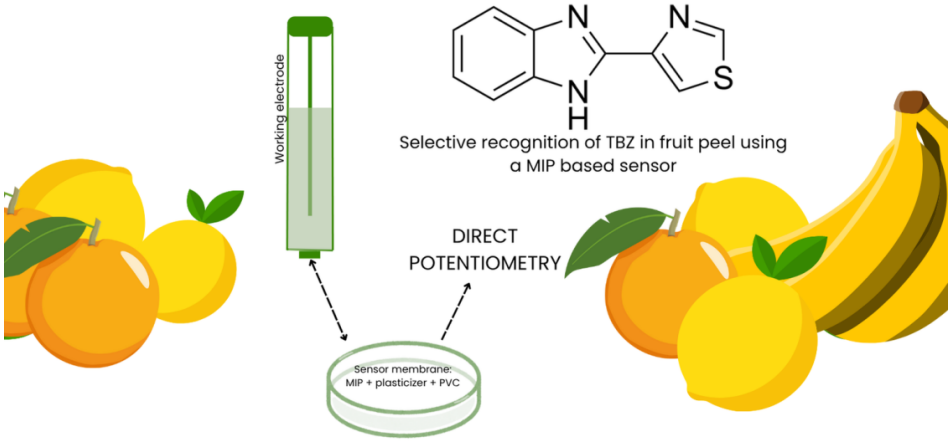
Thiabendazole (TBZ), an organic compound derived from benzimidazole and thiazole, was recognized for its broad-spectrum anthelmintic and antifungal activity [1]. It was widely used in medicine to treat infections caused by nematodes [2]. In agriculture, TBZ was employed as a postharvest fungicide and seed treatment, while in industry, it was utilized as a preservative. Despite its benefits, TBZ posed significant health risks. In high doses, it was shown to induce liver damage and neurological symptoms [3]. Chronic exposure to TBZ was associated with long-term health issues such as cancer, endocrine disorders, and neurotoxicity, particularly in agricultural workers and vulnerable populations [4]. In the environment, TBZ was transported via runoff and atmospheric dispersion, leading to its accumulation in soil and aquatic organisms, and contributing to biomagnification in food chains. Therefore, stricter regulatory measures, residue monitoring in food, and the development of safer alternatives were strongly emphasized [4,5]. A novel potentiometric sensor based on a molecularly imprinted polymer (MIP) for the selective detection of TBZ was developed. Its analytical performance was evaluated under controlled conditions. Calibration experiments were conducted to characterize the potentiometric response of the sensor and assess its sensitivity. The developed sensor was tested on fruit peel samples to evaluate its practical applicability in real matrices. It demonstrated excellent performance, showing high selectivity and reliable response for TBZ detection in the tested samples.



[1] M. Budetić, D. Kopf, A. Dandić, M. Samardžić, *Molecules* **28** (2023) 3926.

[2] K. Gourgiotou, E. Nicolaidou, A. Panagiotopoulos, E. Hatziolou, A. D. Katsambas, *J. Eur. Acad. Dermatol* **15** (2001) 578-580.

[3] A. M. Tabanez *et al.*, *Molecules* **25** (2020) 3083.

[4] Q. Sun *et al.*, *RSC adv.* **8** (2018) 20295-20303.

[5] C. Shekhar *et al.*, *Toxicol. Rep.* **13** (2024) 101840.

GENERATIVE DESIGN OF MOLECULES WITH DESIRABLE PROPERTIES USING REINFORCEMENT LEARNING

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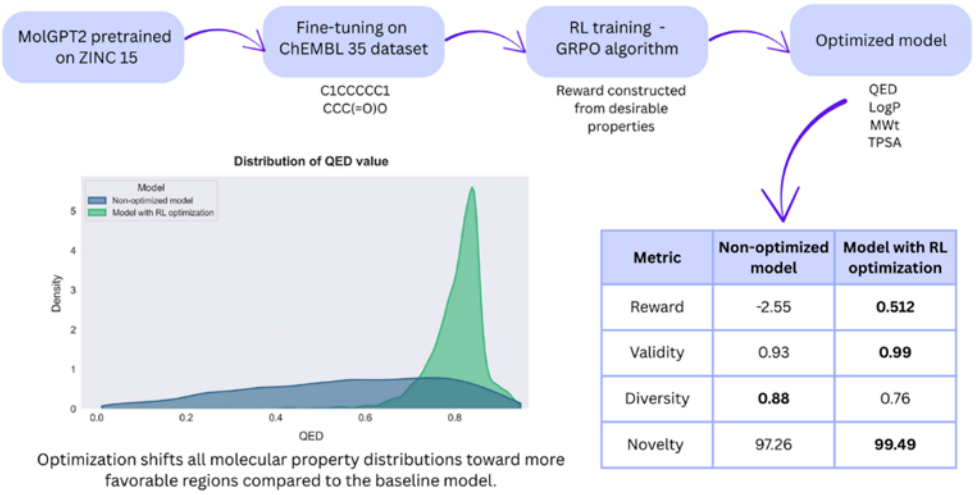
The discovery of new chemical compounds with desired properties represents one of the main challenges in modern chemical and pharmaceutical industries. In this work, a generative molecular design approach was implemented using reinforcement learning optimization. The problem was formulated as a causal language modelling task for predicting the next character in SMILES representations, where a large language model based on the GPT-2 Transformer architecture, specifically the MolGPT model pre-trained on the ZINC-15 database [1], was employed and subsequently fine-tuned on a custom dataset derived from the ChEMBL-35 database. The model was then optimized using the Group Relative Policy Optimization (GRPO) reinforcement learning algorithm, guided by a multi-objective reward function encompassing four molecular descriptors – quantitative estimate of drug-likeness, octanol-water partition coefficient, molecular weight, and topological polar surface area – selected according to the literature [2]. The reinforcement learning-optimized model demonstrated significant improvements, with the validity of generated molecules increasing from 93 % to 99 % and novelty remaining high at 99.49 % relative to the training datasets. The distributions of targeted molecular properties were significantly shifted toward desired values, although diversity was decreased due to focusing on a specific region of chemical space. The results established a foundation for further research and practical application in drug development scenarios, demonstrating the model's ability to explore new chemical entities with potentially relevant pharmaceutical properties.



Metric	Non-optimized model	Model with RL optimization
Reward	-2.55	**0.512**
Validity	0.93	**0.99**
Diversity	**0.88**	0.76
Novelty	97.26	**99.49**

Optimization shifts all molecular property distributions toward more favorable regions compared to the baseline model.

[1] V. Bagal, R. Aggarwal, P. K. Vinod, U. D. Priyakumar, *J. Chem. Inf. Model.* **62(9)** (2021) 2064–2076.

[2] H. Kim, H. Choi, D. Kang, W. B. Lee, J. Na, *Chem. Sci.* **15(21)** (2024) 7908–7925.

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