

# BOOK OF ABSTRACTS

9<sup>th</sup> Symposium of Chemistry Students

11<sup>th</sup> and 12<sup>th</sup> of October 2024

Department of Chemistry, Faculty of Science

Zagreb, Croatia



# **IMPRESSUM**

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## PREFACE

### BY THE PRESIDENT OF THE ORGANISING COMMITTEE

Dear participants,

on behalf of the Organising Committee, it is my great honour to welcome you to the 9th Symposium of Chemistry Students at the Department of Chemistry of the Faculty of Science of the University of Zagreb.

SiSK has always been a platform for students to gain invaluable experience in presenting their research, offering both poster and oral presentations that prepare them for future scientific conferences and professional opportunities. This year, we have made a concerted effort to ensure that even more students can participate, as we firmly believe that these experiences are key to both academic and social development. The increasing number of participants has prompted us to extend the Symposium to two days, allowing for more opportunities to learn, network, and foster collaborations among students and scientists. This year, we have also introduced new features, including roundtable discussions on studying abroad and the relationship between industry and science, as well as a bilingual format to expand the Symposium's reach to an international audience. We are excited to see how these additions will enrich the experience for all attendees.

I am incredibly grateful to the dedicated and talented team behind this event. Their hard work and passion have been vital in bringing our ideas to life, and I am excited to be part of a Symposium that continues to inspire and connect the next generation of chemists. I would like to extend my deepest gratitude to the Organizing Committee, especially to Karla, Ivan, and Antonio, whose leadership and tireless efforts were instrumental throughout the entire process. Their commitment has been exceptional, and together with the invaluable contributions of Ema, Ana, Paula, Sara, Emanuel, Nela, and Valentina, their unwavering dedication has truly been the backbone of this Symposium. A heartfelt thank you also goes to our advisor, Danijel Namjesnik, for his invaluable guidance, and to our reviewers, whose expertise has elevated this Symposium to new heights. We are deeply grateful to the Croatian Chemical Society, led by Professor Vladislav Tomišić, and to the Department of Chemistry, headed by Professor Snežana Miljanić, for their ongoing support and for hosting this event for the ninth time in the Department's halls.

On behalf of the Organizing Committee, I would like to express our sincerest thanks to our sponsors, donors, and partners, whose generous support has enabled us to host this free scientific conference, ensuring that students from all backgrounds have the opportunity to participate. Their contributions have created an inclusive space where knowledge can be shared freely and openly. Finally, a special thank you to our families and friends for their patience and understanding throughout this journey, as we have tirelessly spoken about the Symposium for the past year.

It is my sincere hope that the abstracts in this book will inspire new ideas and provide valuable insights. May this Symposium be a rewarding experience for all, sparking new connections and innovations that will shape the future of chemistry.

*Hvala i uživajte!*

Magda Topić

President of the Organising Committee of the 9th SiSK



## **PREFACE**

### **BY THE HEAD OF STUDENT SECTION OF CCS**

Dear students, professors, assistants, and all other participants,

for the third time, I am writing this introduction, and one would expect that I no longer have anything new to say, but with the Symposium of Chemistry Students, that is never the case! Like in previous years, this Symposium offers students a unique opportunity to try their hand at poster or oral presentations, thus preparing themselves for future appearances at "larger" scientific conferences. Oral presentations are a great practice for many students in public speaking, particularly for their upcoming thesis defences, and ultimately serve as a fantastic introduction to the professional world, where such public appearances will become a daily occurrence for some. The SiSK Symposium is gradually, and almost traditionally, introducing new features each year. Last year's introduction of the Teaching Section has sparked significant interest among students pursuing teaching paths to participate in the Symposium. Every year, the number of applications, both active and passive, increases, which means our goals are being achieved. However, this also requires us to extend the Symposium from a one-day event to a two-day one, ensuring that no interested student misses the opportunity to present their contribution to the world of chemistry. This year, for the first time, we are introducing roundtable discussions (panels) to the Symposium - one focusing on studying abroad and another dedicated to the relationship between industry and science. However, the biggest novelty of this Symposium is its bilingual nature, allowing students to give their oral presentations in English. This somewhat contradicts the initial concept of this Symposium, but we hope it will make the Symposium recognizable not only in the region but also beyond, attracting chemistry students from all over Europe to attend our Symposium. This year, we will have the pleasure of listening to six plenary lectures and four invited speakers. Additionally, students will, of course, have the unique opportunity to learn from their colleagues and exchange experiences, which traditionally happens not only during the presentations but also during breaks. I take this opportunity to thank and commend all the students who have applied to participate in the Symposium. I hope that the interaction and networking between students and scientists at the Symposium will inspire both active and passive participants to continue (or begin) their research work and potentially start new collaborations.

None of this would be possible without our faithful and dedicated people from the Organization who have been devoting their free time for months to make this ninth edition of the Symposium a reality. Starting with a slow pace at the beginning of the year, each month it became clearer that the Symposium was approaching; the pace kept increasing, the work kept piling up, but all these "primarily students," my dear colleagues, didn't give up, and I believe they are now proud of the result of their work. I am proud of the results, and therefore I am proud of them as well. A big thank you to the president of the Organization, Magda, and an equally big thank you to my and her "right

hands," Karla and Ivan, as well as all the other wonderful people from the SiSK team. They have all done a great job, raising this Symposium another notch. I would also like to thank all our advisors, especially Danijel, who was ready to help at any time of the day or night. Thanks to the Croatian Chemical Society and its president, Professor Tomišić, for all the support, to the Department of Chemistry at PMF and its head, Professor Miljanić, for providing the Department's space, and finally, thank you to all our loyal sponsors and donors, without whom it would be almost impossible to hold the Symposium.

I hope that this Symposium, like the previous ones, will encourage other students to get involved in the work of our Section.

Antonio Magnabosco  
Head of the Student Section of the Croatian Chemical Society





# PROGRAMME



**FRIDAY**  
**11th of October 2024**

9:00	<b>REGISTRATION OPENING</b> (hall of the Department of Chemistry, main entrance)	
<b>OPENING CEREMONY (A2)</b>		
10:30 - 11:15	<b>PLENARY LECTURE (A2)</b> chair: Nela Rapinac	<b>Marina Tišma</b> (Faculty of Food Technology Osijek, Josip Juraj Strossmayer University of Osijek): THE ROLE OF CHEMISTS IN BIOECONOMY
11:15 - 11:30 short break		
11:30 - 12:15	<b>PLENARY LECTURE (A2)</b> chair: Nela Rapinac	<b>Gabriela Ambrožić</b> (Faculty of Physics, University of Rijeka): ATOMIC LAYER DEPOSITION: A POWERFUL TECHNIQUE FOR THE SYNTHESIS OF SEMICONDUCTOR THIN FILMS AND FUNCTIONAL HYBRID MATERIALS
12:15 - 13:30 lunch break		
13:30 - 15:00	PANEL DISCUSSION (A2) <b>SCIENCE and/vs INDUSTRY</b>	<b>Ernest Meštrović</b> (chair), <b>Marijana Đaković</b> , <b>Martina Hrkovac</b> , <b>Ivica Komočar</b> , <b>Marina Martinić Kavur</b> , <b>Stribor Marković</b>
15:00 - 15:15 short break		
SECTION LECTURES (A2) chair: Ivan Raič		SECTION LECTURES (P1) chair: Karla Remar
15:15 - 15:30	● <b>Tamara Papić:</b> ADSORPTION OF POLY(ACRYLIC ACID) ON CALCIUM FLUORIDE NANOPARTICLES	● <b>Mislav Vorkapić:</b> INVESTIGATION OF THE SOLUBILITY OF ● ORTHOPHENYLPHENOL IN MEAT WITH DIFFERENT FAT CONTENTS
15:30 - 15:45	● <b>Stjepan Dolić:</b> UNDERSTANDING THE STRUCTURAL PROPERTIES OF PEROVSKITE SOLAR CELLS	● <b>Katarina Čačić:</b> NON-COVALENT INTERACTIONS IN CONTROLLED ALKYLATION OF UNPROTECTED INDOLES
15:45 - 16:00	● <b>Emilija Petrović Hađar, Antun Habajec:</b> PATH OF NO RETURN	● <b>Lovro Vučetić:</b> CHEMO- AND REGIOSELECTIVE ALKYLATION OF PHENOLS INDUCED BY BLUE LIGHT
16:00 - 16:30 coffee break		
16:30 - 17:00	<b>INVITED LECTURES (A2)</b> chair: Magda Topić	<b>Adrijana Vinter</b> (Selvita): AI IN DRUG DISCOVERY
17:00 - 17:30		<b>Filip Topić</b> (IQM Quantum Computers): NOT A QUANTUM CHEMIST – CHEMIST IN A QUANTUM COMPUTING COMPANY
17:30 - 17:45 short break		
17:45 - 18:30	<b>PLENARY LECTURE (A2)</b> chair: Ema Begović	<b>Jasna Adamov</b> (School of Sciences, University of Novi Sad): AUGMENTED REALITY AND VIRTUAL REALITY IN LEARNING CHEMISTRY
18:30 - 18:45 <b>ANNOUNCEMENTS (A2)</b>		
18:45 - 21:00 <b>Chemistry on Tap: A Molecular Mixer</b> (ground level of the Department of Chemistry, -1)		

**PROGRAMME LEGEND**

- biochemistry
- education
- engineering
- inorganic chemistry
- organic chemistry
- physical chemistry

**SATURDAY**  
12th of October 2024

<b>ANNOUNCEMENTS (A2)</b>	
10:00 - 10:10	<b>PLENARY LECTURE (A2)</b> chair: Antonio Magnabosco
10:10 - 10:55	<b>Tomislav Friščić</b> (School of Chemistry, University of Birmingham): Surprise Lecture
10:55 - 11:10 short break	
11:10 - 11:55	<b>PLENARY LECTURE (A2)</b> chair: Antonio Magnabosco
11:55 - 12:05 <b>Serbian Young Chemists' Club: Short Presentation (A2)</b>	
12:05 - 13:15 <b>Posters Over Coffee</b> <b>POSTER SECTION</b> (1st floor of the Department of Chemistry)	
SECTION LECTURES (A2) chair: Emanuel Pištan	
SECTION LECTURES (P1) chair: Sara Macan	
13:15 - 13:30	<ul style="list-style-type: none"> <li>● <b>Dora Hećimović:</b> STUDY ON THE GROWTH OF MARINE MICROORGANISMS</li> </ul>
13:30 - 13:45	<ul style="list-style-type: none"> <li>● <b>Karlo Grgurević:</b> PRODUCTION OF ECO-FRIENDLY</li> <li>● <b>POLYHYDROXYALKANOATES USING WASTE STARCH</b></li> </ul>
13:45 - 14:00	<ul style="list-style-type: none"> <li>● <b>Mina Stamenković:</b> IMPROVEMENT OF THE PROTEIN PRODUCTION</li> <li>● <b>FROM BY-PRODUCTS OF THE OIL INDUSTRY</b></li> </ul>
13:15 - 13:30	<ul style="list-style-type: none"> <li>● <b>Filip Margetić:</b> ADSORPTION OF POLY(4-STYRENESULFONATE) ON CALCIUM FLUORIDE NANOPARTICLES IN DIFFERENT IONIC STRENGTHS</li> </ul>
13:30 - 13:45	<ul style="list-style-type: none"> <li>● <b>Ivor Vavra Plavšić:</b> DISSOLUTION OF FLUORITE COLLOID PARTICLES COATED WITH SODIUM POLY(4-STYRENESULPHONATE)</li> </ul>
13:45 - 14:00	<ul style="list-style-type: none"> <li>● <b>Dario Šušnić:</b> SALT SCREENING AND CHARACTERIZATION OF PYRIDINECARBOHYDRAZIDE ISOMERS</li> </ul>
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14:15 - 15:30 lunch break	
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16:30 - 16:45 short break	
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19:15 - ... <b>Explosive Conclusions by PO Entropy</b> <b>CLOSING CEREMONY (A2)</b>	
SYMPOSIUM AFTERPARTY (ground level of the Department of Chemistry, -1)	

**PROGRAMME LEGEND**

- biochemistry
- education
- engineering
- inorganic chemistry
- organic chemistry
- physical chemistry



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# PLENARY LECTURES



# THE ROLE OF CHEMISTS IN BIOECONOMY

Marina Tišma

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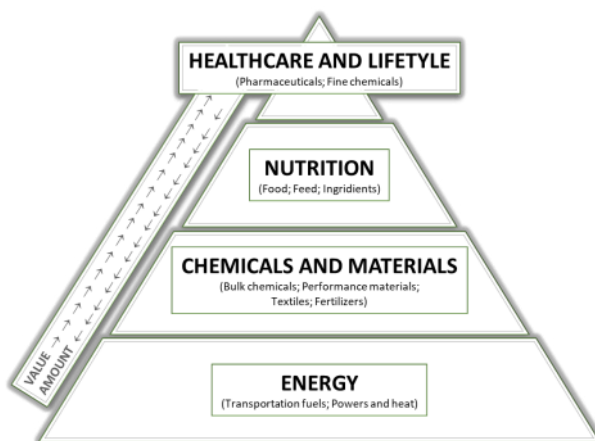
The prevailing linear economic system was based on the “take-make-waste” concept with the processing of fossil raw materials into variety of products. Today, Europe is transforming its economy into circular and sustainable with a focus on the bioeconomy. The concept of bioeconomy encompasses the production, development and use of biological resources, processes and systems to provide products, processes and services.<sup>1</sup>

One of the most important biological resources is biomass, especially lignocellulosic residual biomass. Biorefining is the sustainable processing of biomass into a range of marketable products such as food and feed, chemicals and materials, and bioenergy (electricity, heating/cooling, fuels). Lignocellulosic biorefineries are not yet fully commercialised, many of them are operated at pilot scale, and there are many challenges that need to be addressed.<sup>2</sup>

Chemistry can generally be considered as a central science underpinning fundamental aspects in many of established and emerging sciences.<sup>3</sup>

There is no doubt that chemists can find their place in the development and operation of lignocellulosic biorefineries contributing bioeconomy in general. This presentation will discuss the general aspects of a sustainable and circular bioeconomy and the development of lignocellulosic biorefineries emphasising the role of chemists.

## Bio-based value pyramid



[1] Updated Bioeconomy Strategy 2018, *European Commission*.

[2] M. Tišma, A. Bucić-Kojić, M. Planinić, *Chem Biochem Eng Q* **3** (2021): 139-156.

[3] S. Matlin, G. Mehta, H. Hopf, *et al. Nature Chem* **7** (2015) 941–943.



# ATOMIC LAYER DEPOSITION: A POWERFUL TECHNIQUE FOR THE SYNTHESIS OF SEMICONDUCTOR THIN FILMS AND FUNCTIONAL HYBRID MATERIALS

Gabriela Ambrožić<sup>1,2</sup>, Robert Peter<sup>1,2</sup>, Maria Kolympadi Marković<sup>1,2</sup>, Iva Šarić<sup>1,2</sup>, Ivana Jelovica Badovinac<sup>1,2</sup>, Ivna Kavre Piltaver<sup>1,2</sup>, Silvester Mežnarić<sup>3</sup>, Rafaela Radičić<sup>4</sup>, Petra Linić<sup>5</sup>, Ivana Gobin<sup>3</sup>, Mato Knez<sup>6</sup>

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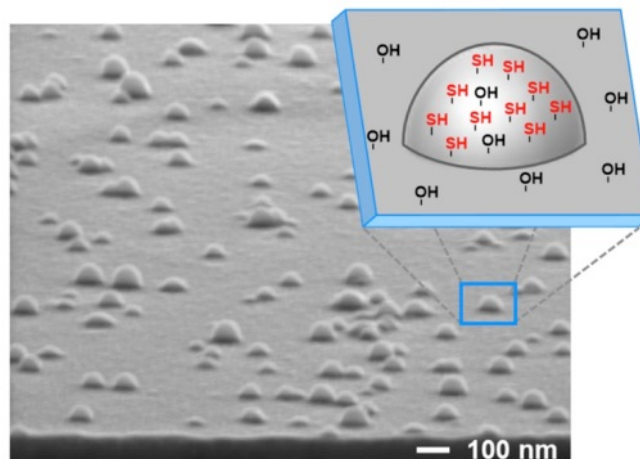
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Atomic layer deposition (ALD)<sup>1</sup> has emerged as the method of choice for innovation in thin film technology, as it enables the highly controlled deposition of inorganic and, more recently, organic layers on a nano or Angstrom scale on inorganic, organic or even biological materials. Such thin films can optimize the physicochemical properties of the material and/or create new properties, such as selective bio-recognition or biocompatibility, stimuli-responsiveness, enhanced catalytic activity, etc.

This presentation will cover the introduction and fundamentals of ALD from a chemistry perspective. The results of our research activities on different strategies for the synthesis of semiconductor thin films and hybrid materials will be presented, focusing on the advantages of ALD for surface functionalization and modification of metal oxides and polymers in the gas phase.<sup>2,3</sup>



*Organosilica hybrid nanohemispheres on alumina thin films deposited by ALD<sup>4</sup>*

[1] P. Gomez-Romero et al., *Chem. Mater.* **36** (2024) 8.

[2] I. Šarić et al., *Chem. Commun.* **55** (2019) 3109.

[3] S. Mežnarić et al., *J. Environ. Chem. Eng.* **10** (2022) 108095.

[4] G. Ambrožić et al., *J. Colloid Interface Sci.* **560** (2020) 303.

## AUGMENTED REALITY AND VIRTUAL REALITY IN LEARNING CHEMISTRY

Jasna Adamov

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Among all the school courses, chemistry is one of the least popular. Students often consider chemical content difficult to understand and complicated to learn. Most chemical concepts are complex and abstract, since chemical particles are too small to be seen even under the most powerful microscope. To explain atomic and molecular structure, the nature of chemical bonding, hybridization, mechanisms of chemical reactions, etc., chemists use complex mathematical models and different visual representations, which are always two-dimensional in textbooks and other printed media or computer screens. To be able to create 3D mental pictures and to understand and manipulate them, students need a well-developed set of visual skills, which exists in only 16% of population. At Chemistry Department of the University of Novi Sad, we use modern educational technology as a powerful tool for both teachers and students in overcoming difficulties with visualization of chemical models, especially augmented reality (AR) and virtual reality (VR) tools. AR technology enables 3D representation of atomic and molecular models and their spatial manipulation. For example, using cell phones and QR codes students evoke 3D models of atoms and molecules and place them anywhere in space. They manipulate these objects (rotate and translate them along all three axes) and observe them from any angle. Holograms can be used to see the models of atoms, molecules, or atomic and molecular orbitals, but also to represent the dynamics of chemical processes, such as bond formation, the change of configuration of organic molecules during substitution and addition, or to determine the R/S optical isomerism in molecules. Using VR goggles students are completely immersed into the 3D surroundings: they hold and move atomic and molecular models, or perform virtual chemical experiments. They also attend virtual tours, “see” technological processes in industrial plants, meet and talk to famous scientists and learn about their life and discoveries, or they visit thematic museums, such as Museum of atoms. Digital virtual escape rooms are used for gamification of learning, both in learning and reviewing chemical content, thus making studying chemistry more interesting and motivating. There are many open-source programs that can be used to create holograms, virtual tours, virtual laboratories and virtual escape rooms with interactive problems for students, such as WebAR, ThingLink or LearningApps. This software is user-friendly, and students learn how to create holograms, spatial 3D objects and VR objects and VR tours themselves.



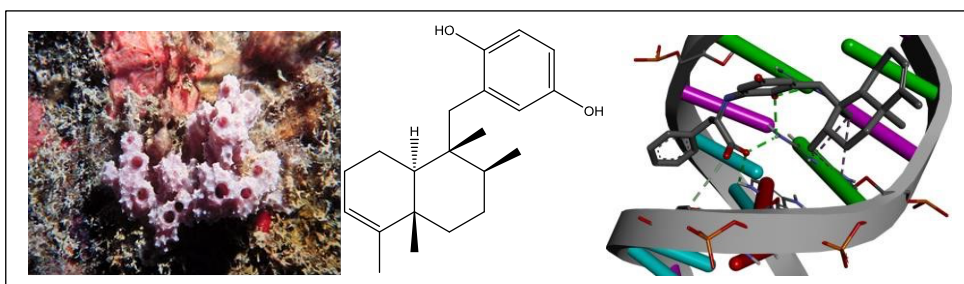


## DNA AS A TARGET: FROM MARINE INVERTEBRATES AND METAL SALTS TO POTENTIAL THERAPEUTICS

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Interactions with DNA of two types of compounds: metal complexes and marine natural products with hydroquinone/quinone moiety, their derivatives and mimetic compounds, will be presented, as well as the resulting biological activity, in particular cytotoxicity to tumor cell lines, including multi-drug resistant cell lines. Among the metal complexes, the focus will be on DNA binding and damage, cell cycle phase distribution, apoptosis and autophagy induction by d-metal complexes with ligands of hydrazone type containing additional heteroatoms, both in the aldehyde and hydrazine building blocks. DNA-targeting natural product-based compounds, whose effects will be presented, include marine meroterpene avarone, its derivatives, bioconjugates with proteins and simple mimetic compounds. Some of the compounds showed a very good selectivity towards multi-drug resistant tumor cell lines.





## METHODOLOGY OF TEACHING CHEMISTRY

### (What's it all about and does anyone needs it?)

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What is chemistry and what does it mean to teach it? This seems to be a simple question but in its essence it is definitely not.

What are one's benefits when thinking about teaching chemistry? Generally, what does it mean to teach at all? What is the best way to teach something (anything)? Maybe an example would be fine? How is teaching related to learning? What are the goals of teaching and how do we define them? Is it hard to define a set of teaching goals? What is a learning outcome or achievement? How are teaching and learning related? Are those terms in any connection? What about communication?

And so many more questions...





**INVITED LECTURES** 



## AI IN DRUG DISCOVERY

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Artificial intelligence (AI) is revolutionizing drug discovery, making the process faster, more affordable, and more efficient. This lecture will give an overview of the current market situation and how AI is being used in chemistry to develop new medicines. It will also discuss how companies like Selvita are at the forefront of this transformation.

Traditional drug discovery is often slow, expensive, and prone to failure. AI provides a powerful solution by quickly analyzing large data sets, predicting how molecules will behave, and identifying promising drug candidates with greater accuracy. Case studies will be presented, including also on how AI, although a powerful tool, is not almighty in the drug discovery process.

We will discuss how Selvita applies these AI technologies in drug discovery by optimizing the properties of potential drugs and predicting possible side effects.

This lecture will emphasize the crucial role of collaboration between AI experts and chemists, showing how Selvita's interdisciplinary approach is leading to groundbreaking discoveries. By the end of the session, participants should understand how their expertise, combined with AI, is transforming drug discovery and what the future might hold for this exciting field



## NOT A QUANTUM CHEMIST – CHEMIST IN A QUANTUM COMPUTING COMPANY

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Quantum computing brings a new paradigm for the future of computing, and a powerful tool to solve difficult computational problems over diverse areas of human activity. IQM Quantum Computers is a full-stack quantum computing company, building and providing quantum computers available on-premises or through cloud access. At the heart of the quantum computer is the quantum processing unit (QPU), produced using known microfabrication methods [1] adapted to the specific requirements of the QPU technology. In this talk, the role of the equipment engineer in enabling key processes in QPU production will be highlighted. Moreover, different aspects of chemical usage in a microfabrication facility – cleanroom – will be presented, including the types of process chemicals used and chemical safety.

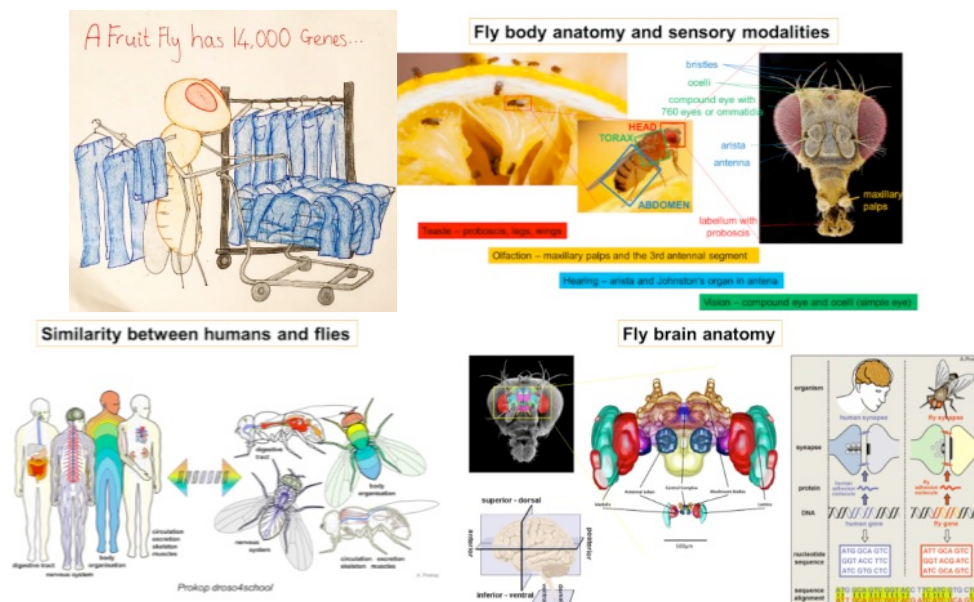
[1] S. Franssila, *Introduction to Microfabrication*, 2<sup>nd</sup> ed., John Wiley & Sons, Ltd., Chichester, 2010.

# UNRAVELING THE GENETIC BLUEPRINT OF BEHAVIOR: INSIGHTS FROM *DROSOPHILA MELANOGASTER*

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The study of behavior and genetics in *Drosophila melanogaster*, commonly known as the fruit fly, provides crucial insights into the genetic and neurological mechanisms underlying behavior. As a widely used model organism, *Drosophila* shares many genetic similarities with humans, making it an invaluable tool for exploring how genes influence behaviors such as courtship, sleep, learning, and social interactions. Recent research has expanded the use of *Drosophila* to model more complex phenomena, such as drug addiction, where fruit flies exhibit behaviors that mimic addiction responses to substances like alcohol and cocaine. These studies provide a clearer understanding of the genetic foundations of addiction and their parallels in human behavior. Additionally, the study of social interaction networks in *Drosophila*, including group dynamics and communication, has shed light on the genetic regulation of social behavior. Importantly, *Drosophila* is also emerging as a powerful model for studying psychiatric disorders, such as depression, anxiety, and schizophrenia. By altering specific genes linked to these conditions, scientists can observe changes in the flies' behavior, allowing them to investigate the genetic and neurological underpinnings of psychiatric disorders. This presentation introduces fundamental concepts in behavioral genetics, exploring how *Drosophila* research helps untangle the complex relationship between genes and the environment. Key techniques like gene knockouts and neurogenetics are outlined, highlighting how these tools reveal the roles of specific genes in shaping behavior. Finally, the broader implications of *Drosophila* research are discussed, from understanding psychiatric disorders and drug addiction to advancing treatments for neurological diseases, demonstrating how this small insect contributes significantly to breakthroughs in genetics, neuroscience, and mental health.



[1] B. Samardžija et al., *Current Issues in Molecular Biology* **46(8)** (2024) 8526.

[2] A. Filošević Vujnović, et al., *BioTech* **13(3)** (2024) 23.

[3] A. Filošević Vujnović, et al., *Future Pharmacology* **4(1)** (2024) 115-138.

[4] A. Filošević Vujnović, et al., *Pharmaceuticals* **16** (2023) 1489.





## SECTION LECTURES



## INVESTIGATION OF THE SOLUBILITY OF ORTHOPHENYLPHENOL IN MEAT WITH DIFFERENT FAT CONTENTS

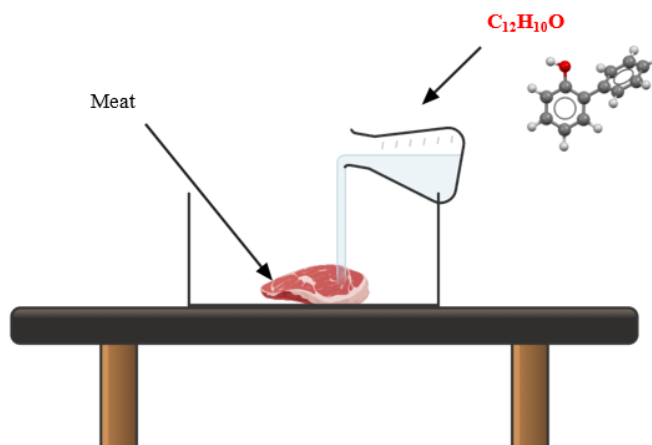
Mislav Vorkapić<sup>1</sup>, Jakov Babić<sup>1</sup>, Ivana Jelavić<sup>2</sup>, Elvira Kovač-Andrić<sup>2</sup>,  
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Orthophenylphenol (E231, C<sub>12</sub>H<sub>10</sub>O) is a fungicide that should only be used for agricultural purposes. Nevertheless, it was used in the food industry as a preservative for the preservation of meat and meat products (often the use of the compound is related to the smoking of meat samples). Its use is banned in some countries. As it is a harmful additive, a significantly higher amount of orthophenylphenol than the permitted amount of 0.01 mg per kilogram of meat was detected in the analysis of various meat samples in this study. High-performance liquid chromatography (HPLC) was used to determine which type of meat contained the highest concentration of the tested compound and its correlation with chemical and physical properties [1,2]. In order to prove the hypothesis that the compound binds best to meat with a higher fat content, industrial conditions were simulated in this study (the average amount of orthophenylphenol in smoke is 0.12 mg per kilogramme of smoke) and samples of different types of meat were treated with an orthophenylphenol solution in the concentration that is also used in the industry for smoking meat products. When evaluating the data from the analyses carried out, it was found that meat samples with a higher fat content actually bind orthophenylphenol better. The research leads to the conclusion that the presence of orthophenylphenol in meat subjected to the industrial smoking process is exclusively due to the meat smoking process in which the investigated compound is present.



[1] L. Votavová, K. Hanušová, L. Vápenka, J. Dobiáš, F. Kvasnička, *Open Chem* **12** (2014) 1162-1167.

[2] M. K. St John 1, L.L. Arnold, T. Anderson, M. Cano, S. L. Johansson, S. M. Cohen *Toxicol Sci* **59** (2001) 346-351.



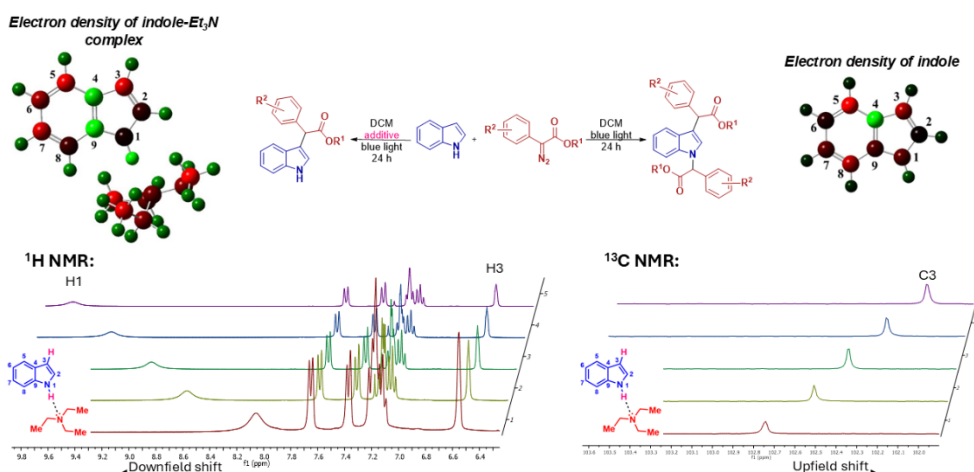
# NON-COVALENT INTERACTIONS IN CONTROLLED ALKYLATION OF UNPROTECTED INDOLES

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The indole's C3 position is known for its high electron density, making it the most nucleophilic site for electrophilic substitution. Despite this, the N-H position can also undergo functionalization.<sup>[1]</sup> To address the competitive regioselectivity between the C3 and N-H positions, the N-H group is typically protected using standard protective groups, which directs functionalization to the C3 position or leads to cyclopropanation of the double bond, depending on the electronic properties of the protecting groups. Research has demonstrated that electron-donating groups attached to the nitrogen atom enhance the nucleophilicity of the C3 position, favoring C3 alkylation. Conversely, electron-withdrawing groups tend to promote cyclopropanation. However, this conventional approach involves at least two extra synthetic steps (protection and deprotection), resulting in increased material usage and lower overall yield. This study proposes an alternative strategy to overcome these limitations by using a masked protective-group approach. The nucleophilicity of different positions on the indole ring was assessed using <sup>1</sup>H and <sup>13</sup>C NMR spectroscopy. The interaction of indole with specific additives influences the NMR chemical shifts, which reflect the electronic environment and nucleophilicity of the relevant atoms. For example, the addition of triethylamine (Et<sub>3</sub>N) causes a downfield shift in the N-H proton signal and an upfield shift in the C3 carbon signal, indicating alongside with DFT calculations an increase in the nucleophilicity at the C3 position. This suggests that certain additives could promote regio- and chemoselective alkylation. To test this hypothesis, a model reaction between indole and a diazoester under blue light irradiation was conducted. Although previous efforts to functionalize unprotected indole under similar conditions were unsuccessful,<sup>[2]</sup> our results showed both C-H and N-H insertion in the reaction, with exclusive formation of C3-monosubstituted indole when an additive was present.



[1] N. Chadha, O. Silakari, *Eur. J. Med. Chem.* **134** (2017) 159-184.

[2] X. Zhang, C. Du, H. Zhang, X. Li, Y. Wang, J. Niu, M. Song, *Synth.* **50** (2018) 889-898.

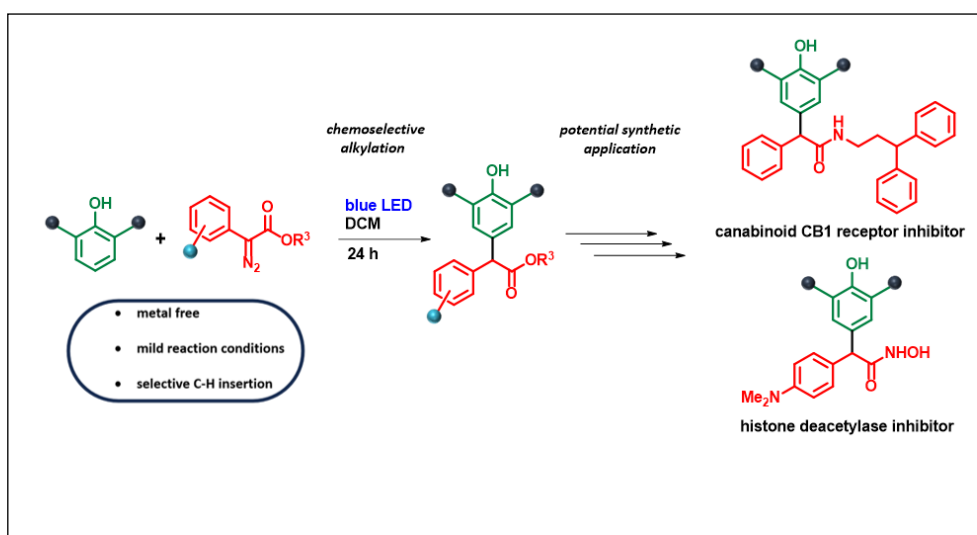
## CHEMO- AND REGIOSELECTIVE ALKYLATION OF PHENOLS INDUCED BY BLUE LIGHT

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Because of the significance of phenyl motifs in natural compounds and pharmaceuticals, the transformation of readily available phenols into structurally more complex homologs is of great interest. Although significant progress has been made in metal-carbenoid induced C-H functionalization of arenes, the direct C-H functionalization of free phenols with diazo compounds remains particularly challenging and surprisingly uncommon. This rarity is likely attributed to the tendency of carbenoids to preferentially undergo O-H bond insertion rather than C-H functionalization.<sup>[1]</sup> Reactive diazoester carbenoid intermediates can be generated through various methods: thermally (impractical due to harsh conditions), via transition metal catalysts, or more recently, photochemically with blue light. Last approach enables reactions to take place under mild, room temperature conditions without the need for catalyst, overcoming the challenges of high energy UV-light which compromised chemoselectivity.<sup>[2]</sup> This work aims to achieve chemo- and regioselective functionalization of phenol and its derivatives by using blue light to induce C-H alkylation with diazoesters at the *para*-position. This methodology is environmentally friendly and cost-effective. The *para*-C-alkylated phenol produced can be further transformed into molecules of great interest. One potential synthetic application is in the synthesis of cannabinoid receptor (CB1) antagonists, which have therapeutic effects against drug abuse and addiction. Another potential application is in synthesis of histone deacetylase inhibitors, which have shown great potential as a treatment option for various cancerous and non-cancerous diseases.<sup>[3]</sup>



[1] Y. Yang, B. Lu, G. Xu, X. Wang, *ACS Central Science* **8** (2022) 581-589.

[2] Ł. W. Ciszewski, K. Rybicka-Jasińska, D. Gryko, *Org. Biomol. Chem.* **17** (2019) 432-448.

[3] Z. Yu, B. Ma, M. Chen, H.-H. Wu, L. Liu, J. Zhang, *Journal of the American Chemical Society* **136** (2014) 6904-6907.

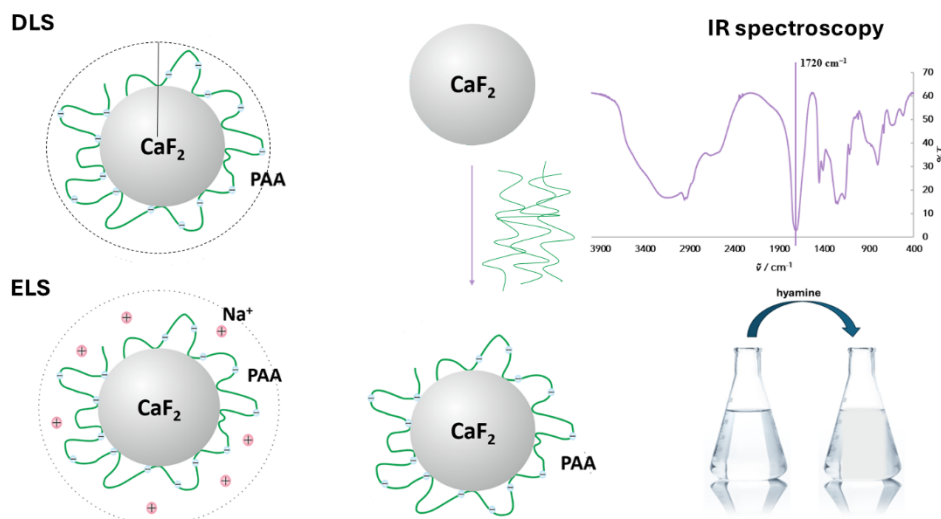


# ADSORPTION OF POLY(ACRYLIC ACID) ON CALCIUM FLUORIDE NANOPARTICLES

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Calcium fluoride, known as fluorite, is the primary natural source of fluoride ions. [1] Therefore, it finds wide application in metallurgy, the cosmetics industry, and dentistry. In dentistry, due to its favorable extremely low solubility, CaF<sub>2</sub> nanoparticles are incorporated into various dental materials. Their very slow dissolution serves as a source of calcium and fluoride ions, which promote tooth regeneration. One way to further modify the properties of calcium fluoride nanoparticles and materials in general is by coating them with various substances, for which polyelectrolytes can be used. [2] Polyelectrolytes are macromolecules that contain a significant portion of ionic and/or easily ionizable groups in their structure, allowing them to adsorb onto oppositely charged material surfaces. The polyelectrolyte used in this study is poly(acrylic acid). Poly(acrylic acid), PAA, is a weak polyanion that is soluble in water. As a synthetic biocompatible material, it has numerous applications. It is used in industry, medicine, and dentistry, where it is applied in the manufacturing of crowns, bridges, and dentures. [3] In this study, the adsorption of PAA onto calcium fluoride nanoparticles was observed under controlled pH, ionic strength, and temperature. The particle size after PAA adsorption onto calcium fluoride was determined by dynamic light scattering (DLS) and the  $\zeta$ -potential by electrophoretic light scattering (ELS). The outcome of adsorption and the quantification of PAA adsorbed onto CaF<sub>2</sub> were further examined by IR spectroscopy of the resulting particles, as well as by analyzing the PAA solution remaining after adsorption. For this purpose, a method that involves the reaction of PAA with hyamine and observing the scattered light with UV/VIS spectrophotometer was used.



[1] Housecroft, C. E. & Sharpe A. G. *Inorganic Chemistry*, Pearson, Harlow, 2012. str. 149

[2] Z. Amjad, *Langmuir* **7** (1991) 2405-2408.

[3] H. Arkaban, M. Barani, M. R. Akbarizadeh, N. P. Singh Chauhan, S. Jadoun, M. Dehghani Soltani, P. Zarrintaj, *Polymers* vol. **14** (2022) 1259

This research was conducted as part of the project by Croatian Science Foundation “Physical chemistry of processes at mineral/(poly)electrolyte solution interface “(IP-2020-02-9571).

## UNDERSTANDING THE STRUCTURAL PROPERTIES OF PEROVSKITE SOLAR CELLS

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Perovskite solar technology has seen a rapid growth in terms of energy conversion efficiency, reaching 26,1% in 2023.[1] The unique properties of hybrid perovskite materials (Figure 1. b)) enable high light absorption in a wide wavelength spectrum and efficient charge transportation. It results in gaining higher electrical performance of perovskite solar cells (PSC) (Figure 1. a)) when compared to its silicon-based counterparts.[2]

The goal of this work is to study how the structure and composition of perovskite materials result in excellent photovoltaic properties of PSC. Some common methods of thin layer deposition used in this study will be explained. The great effects of layer morphology on both the efficiency and the operational lifetime of the acquired solar cells will be discussed.

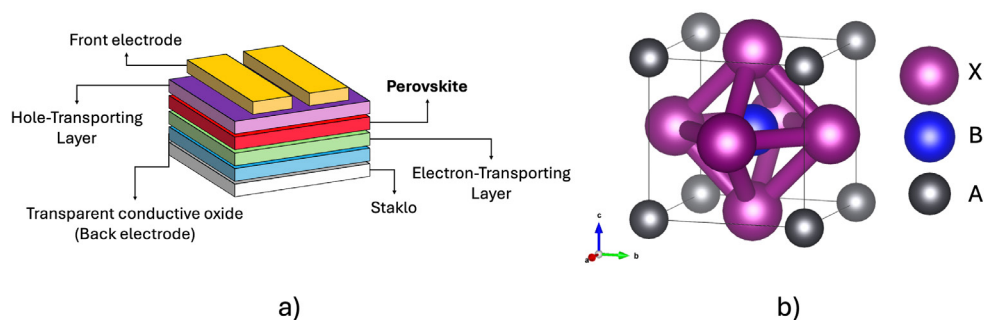


Figure 1. a) Thin layers in perovskite solar cell, b) Hybrid perovskite crystal structure.

ACKNOWLEDGEMENTS: We would like to thank prof. Željko Skoko for performing grazing incidence X-ray diffraction measurements and Laboratory for energy conversion materials and sensors, Division of Material Physics, Ruđer Bošković Institute for used resources including chemicals and instrumentation.

[1] <https://www.nrel.gov/pv/cell-efficiency.html> (accessed 7<sup>th</sup> July 2024)

[2] M. T. Bhatt, J. S. Lee, *New. J. Chem.* **41** (2017) 10508–10527.



## PATH OF NO RETURN

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To spread the interest towards science within society, scientific concepts should be presented in engaging and easily accessible ways. It is also important to consider the target audience and tailor the content according to their interests and prior knowledge. Escape rooms have recently become increasingly popular, making them an appropriate and innovative format for science workshops.

“Path of no return” is an interactive workshop designed in the style of an escape room. It was created with the aim of introducing chemistry and related branches of science to elementary and high school students in a fun, interesting, and novel way. The participants were required to solve a series of 15 puzzles within 45 minutes to successfully finish the workshop. To solve the puzzles participants themselves conducted experiments, except for a few experiments where assistance was provided for safety reasons. To connect the puzzles into a cohesive unit, the story of Flogi from Ston, a fictional alchemist, and the “elixir of life” was stretched throughout the workshop.

In April and May 2024, a total of 11 workshops were held with a total of 85 participants which all gave positive feedback on the format of the workshop. The workshop successfully familiarised elementary and high school students with concepts in chemistry and related fields. This shows that the escape room format is viable for science popularization in a novel, interactive, and engaging way.



Figure 1. Ground plan of library with marked puzzles and clues participants could find while solving the Escape Room “Path of no Return”.

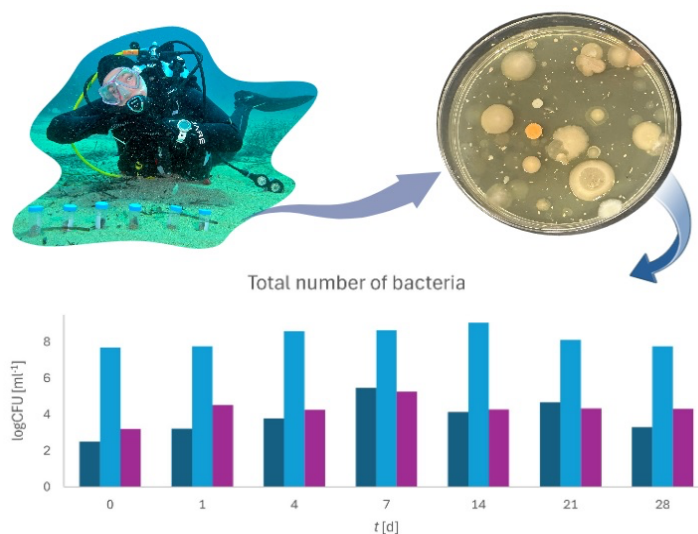


## STUDY ON THE GROWTH OF MARINE MICROORGANISMS

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Human health is severely affected by environmental pollution. The quality of life of the world's population depends on the development of new technologies. Bioremediation is an inventive and optimistic technology suitable for the recovery and reduction of numerous pollutants through the use of microorganisms [1]. With the aim of finding a new way to neutralize the impact of humans on the environment, scientists are constantly expanding the screening of microorganisms for bioremediation in less explored environments such as the marine environment [2]. Knowing the abundance of microorganisms under different environmental conditions is crucial for their cultivation. In this work, the abundance of marine microorganisms from seawater was monitored over a period of 28 days in a batch submerged conditions at 28 °C. The samples for this experiment were collected in the southern Adriatic Sea and DO, pH, CFU and OD were determined. During the experiment, DO decreased by 12 % and did not vary significantly. The average pH value was  $8.18 \pm 1.71$ . The maximum values of CFU and OD of  $1.15 \cdot 10^9 \text{ mL}^{-1}$  and 8.23 were determined on the 8th and 7th day of the experiment. A nutrient-rich environment leads to increased growth of marine microorganisms without a significant decrease in biomass during the study period.



[1] S. Verma, A. Kuila, *Bioremediation of Heavy Metals by Microbial Process* **14** (2019) 100369.

[2] F. Ameen, S. AlNadhari, A. A. Al-Homaidan, *Marine Microorganisms as an Untapped Source of Bioactive Compounds* **28** (2021) 224–231.



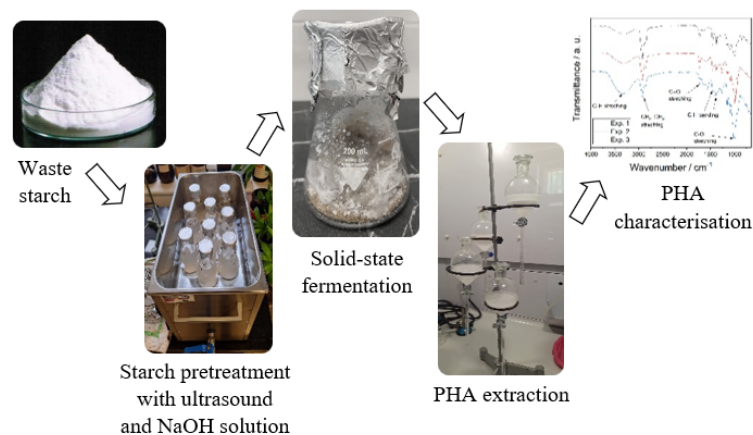
# PRODUCTION OF ECO-FRIENDLY POLYHYDROXYALKANOATES USING WASTE STARCH

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Plastics made from crude oil are among the most commonly used materials in people's daily lives. However, due to increasing production, the problem of toxicity, appropriate disposal and accumulation in the environment arises. For this reason, intensive research is being carried out into the development of new alternative types of plastic that are characterized by rapid biodegradability. One of these types is polyhydroxyalkanoates (PHA), which are specific for their synthesis method and their completely biodegradable properties. It can only be produced by metabolic processes of microorganisms if they feed on a substrate with a lack of nitrogen and a large surplus of carbon. PHA is ultimately produced as a reserve energy source. Agro-industrial waste has been considered as a potentially usable substrate for these purposes. However, agro-industrial wastes require a suitable pretreatment method to become a favorable substrate for PHA production. In this work, ultrasonic pretreatment of waste starch was investigated by changing the duration of ultrasonic treatment (30, 60 and 90 min), ultrasonic power (1, 2 and 3 W mL<sup>-1</sup>) and concentration of NaOH solution (0.01, 0.05 and 0.10 mol L<sup>-1</sup>). Seven PHA-producing microorganisms were isolated from starch: *Leukonostoc* sp., *Citrobacter freundii*, *Staphilococcus lentus*, *Bacillus licheniformis*, *Cryptococcus humicola*, *Geotrichum klebahnii* and *Candida krusei*. These microorganisms were used in solid-state fermentation (SSF) to produce PHA. The results showed the highest value of PHA accumulation of 0.5572% under starch pretreatment conditions of 30 min, 2 W mL<sup>-1</sup> and 0.01 mol L<sup>-1</sup>. According to results, stronger starch pretreatment conditions (longer pretreatment, higher ultrasonic power and higher concentration of NaOH solution) resulted in lower PHA accumulation. FTIR, TGA and DSC analyses indicated the presence of PHB and PHV homopolymers, PHBV copolymers with different HB and HV contents or copolymers of short- and medium-chain PHAs.



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-II .04.0059) funded by National Recovery and Resilience Plan (funded by the European Union, NextGenerationEU).

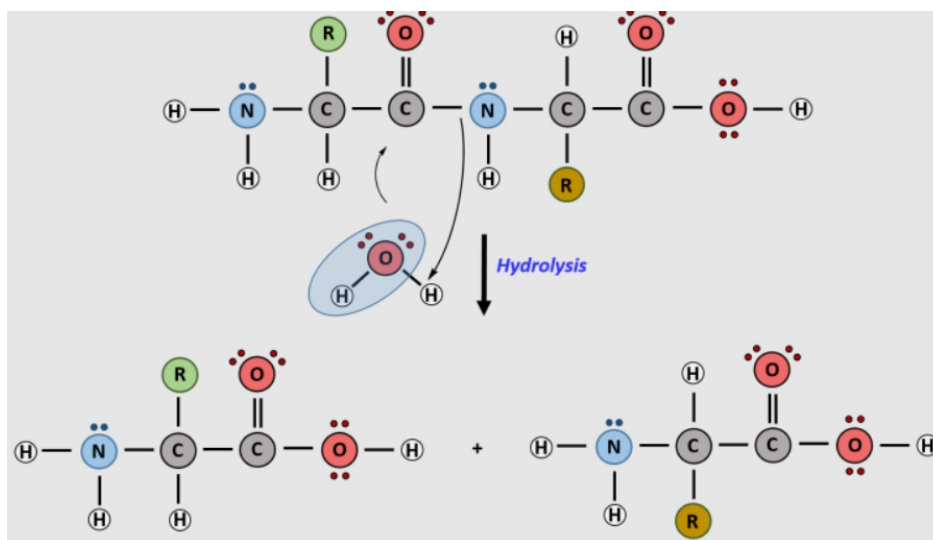
## IMPROVEMENT OF THE PROTEIN PRODUCTION FROM BY-PRODUCTS OF THE OIL INDUSTRY

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Finding renewable and ecologically acceptable high-nutrient food leads to alternative protein sources like plant-based proteins. Importance and use of plant-based proteins grows, with the growth of human population, and those numbers are getting bigger year by year. Also, consumer preferences like religious beliefs, vegan and vegetarian diet. The oil industry is very developed, and with its high production of oil comes a large quantity of by-products, that need to be utilized in a way that also generates economic benefits. As a potential protein source, because of its simple way of cultivation and protein-rich oil cake, rapeseed could be used. [1] The tested rapeseed cake sample was subjected to hydrolysis without prior treatment to produce protein isolates. The advantage of direct hydrolysis lies in simpler industrial production process. Hydrolysis was performed under alkaline and acidic conditions, resulting in the formation of peptides with different solubilities. Antioxidant activity was determined using the DPPH and ABTS tests to evaluate their antioxidant capacity. [2]



[1] J. Crnobarac, R. Marinković, A. Marjanović-Jeromela, i N. Marinković-Dušanić, "Unapređenje tehnologije proizvodnje uljane repice," Acta Agriculturae Serbica, vol. 7, br. 1, str. 34-42, ISSN 0354-9496, 2002.

[2] T. Sedlar, "Nusproizvod agroindustrije – zeleno lišće: Novi izvor proteina i bioaktivnih jedinjenja," Tehnološki fakultet, Farmaceutsko inženjerstvo, Univerzitet u Novom Sadu, Novi Sad, 2022.

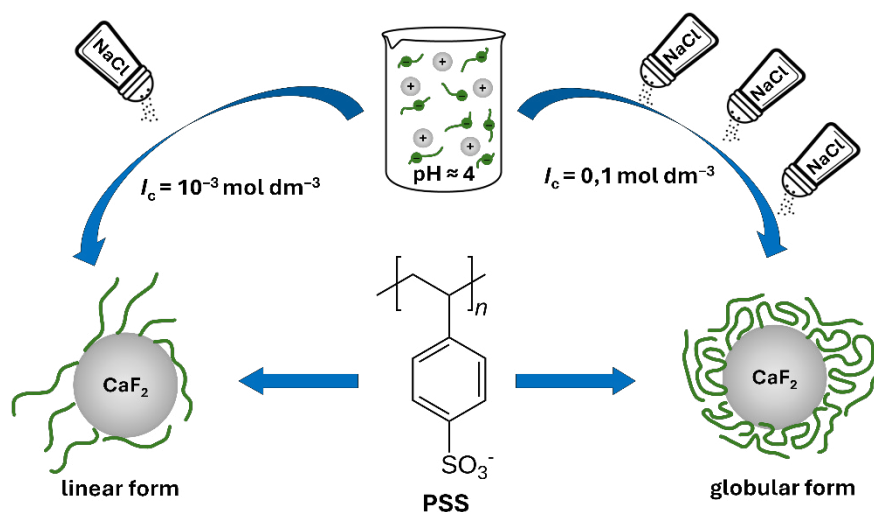


# ADSORPTION OF POLY(4-STYRENESULFONATE) ON CALCIUM FLUORIDE NANOPARTICLES IN DIFFERENT IONIC STRENGTHS

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Polyelectrolytes are long chained macromolecules with monomer units containing functional groups that can be ionized. The adsorption process of polyelectrolytes on different types of surfaces has yielded a variety of industrial and technological applications due to the ability to change the surface charge or protect a material from its surroundings after the adsorption process. Poly(4-styrenesulfonate) (PSS) is a strong polyanion, carrying a negative charge when dissolved in water, meaning it can readily adsorb onto positive surfaces. It is often used as a chemical agent which can make stable complexes with alkali and earth alkaline ions.[1] Additionally, adsorption of a polyelectrolyte to a surface can be tuned by varying the ionic strength of the polyelectrolyte deposition solution. When ionic strength of the solution is high, the polyelectrolyte will be in a globular form due to the ions from the solution screening the repulsive forces between like-charged segments of the molecule. Conversely, when ionic strength of the solution is low, polyelectrolytes form more linear structures. Calcium fluoride ( $\text{CaF}_2$ ) nanoparticle surface can adsorb polyelectrolytes such as PSS because of their relatively inert chemical properties. It is mostly used in dental and general medicine for its antibacterial properties and in glass or ceramics manufacturing.[2] The results of this study provide insights into PSS- $\text{CaF}_2$  interactions at different ionic strengths. To understand the adsorption of PSS to  $\text{CaF}_2$  it is necessary to determine the amount of PSS adsorbed to  $\text{CaF}_2$ , size and charge of the particles interacting with PSS. The amount of PSS adsorbed was determined by UV-VIS spectrophotometry, while the size and charge were determined by dynamic light scattering (DLS) and electrophoretic light scattering (ELS).



- [1] M. Chen, K. Shafer-Peltier, S. J. Randtke, E. Peltier, *Chem. Eng. J.* **344** (2018) 155-164.  
[2] W. A. Bala, V. S. Benitha, K. Jeyasubramanian, G. S. Hikku, P. Sankar, S. V. Kumar, *J. Fluor. Chem.* **193** (2017) 38-44.

This research was carried out as part of the Croatian Science Foundation project “Physical chemistry of processes at mineral/(poly)electrolyte solution interface” (IP-2020-02-9571).

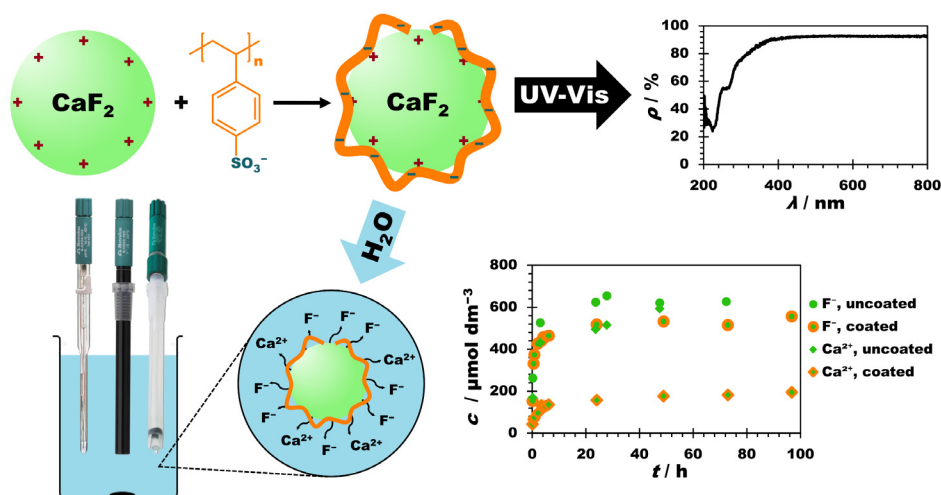
# DISSOLUTION OF FLUORITE COLLOID PARTICLES COATED WITH SODIUM POLY(4-STYRENESULPHONATE)

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Fluorite is a poorly soluble, naturally-occurring mineral of calcium fluoride ( $\text{CaF}_2$ ). It has many industrial uses, including the production of hydrofluoric acid and manufacture of various optical elements. [1] Purifying raw fluorite is achieved through flotation, a process where hydrophobic fluorite particles bind to air bubbles and rise to the surface. Flotation is strongly influenced by surface properties of fluorite and its dissolution in water so understanding these factors could be useful for optimizing the flotation process. [2] Adsorption of polyelectrolytes, macromolecules which contain ionic or ionizable groups like poly(4-styrenesulfonate) (PSS) onto surfaces of materials plays a crucial role in various industrial and technological applications. [3] Adsorbing these substances onto a material can significantly change its surface properties and dissolution behaviour by creating a protective layer that shields the material from external factors. [4] In this study, fluorite colloid particles coated with PSS were prepared and the presence of PSS on the surface of particles was confirmed with UV-Vis spectrophotometry and electrophoretic light scattering. Dissolution kinetics of fluorite particles in water were investigated before and after coating with PSS at different pH values using a fluoride ion-selective electrode and a calcium ion-selective electrode. Ion-selective electrode measurements showed that coated particles dissolve more slowly than uncoated ones, with the fastest dissolution observed at pH = 4 and no significant difference between pH = 6 and pH = 8.



[1] M. J. Janicki et. al., *Physicochem. Probl. Miner. Process.* **52** (2016) 451–458.

[2] Z. Gao et al., *Adv. Colloid Interface Sci.* **290** (2021) 102382–102396.

[3] M. Chen et. al., *Chem. Eng. J.* **344** (2018) 155–164.

[4] M. M. Thomas et. al., *Chem. Geol.* **109** (1993) 227–237.

This research was conducted as part of the project by the Croatian Science Foundation "Physical chemistry of processes at mineral/(poly)electrolyte solution interface" (IP-2020-02-9571).



# SALT SCREENING AND CHARACTERIZATION OF PYRIDINECARBOHYDRAZIDE ISOMERS

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Different molecular conformations, intermolecular interactions, and packing arrangements can result in significant differences in the physical, chemical, morphological, and biopharmaceutical properties of solid forms of the same active substance. [1] Therefore, to ensure the optimal stability and efficacy of a drug, it is often necessary to investigate various solid forms of the active substance, such as polymorphs, salts, cocrystals, or amorphous forms. [2] By converting the active substance, in the form of a free base or acid, into a salt, key properties such as crystal structure, thermal stability, melting point, solubility, and dissolution rate are altered, which can improve the stability and bioavailability of the substance. [1] Although salt synthesis often presents synthetic and analytical challenges, such modifications play a key role in enhancing the pharmaceutical properties of drugs. In this study, the synthesis, structure, and properties of salts of pyridylcarbohydrazide isomers, including pyridine-4-carbohydrazide (better known as isoniazid), an antibiotic commonly applied in the form of a free base, were investigated. Chloride, bromide, nitrate, perchlorate, hydrogensulfate, sulfate, and dihydrogen phosphate salts of these carbohydrazides were prepared and characterized, and the conditions of their synthesis and crystallization were examined. Empirical relationships between the structure and properties of the prepared salts were established.

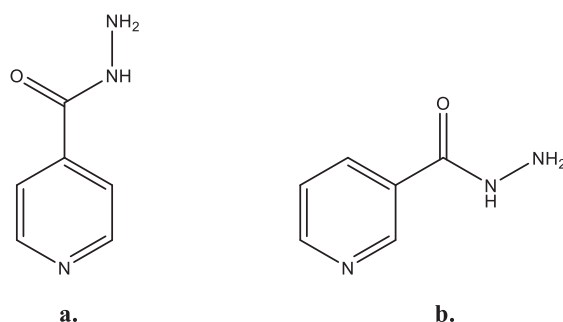


Figure 1. Molecular structures of pyridine-4-carbohydrazide (a.) and pyridine-3-carbohydrazide (b.), substances whose salts were researched

[1] Y. Qui, G. G. Z. Zhang, R. V. Mantri, Y. Chen, L. Yu, *Developing Solid Oral Dosage Forms*, Academic Press, Cambridge, 2017, 85–112.

[2] A. Karagianni, M. Malamatari, K. Kachrimanis, *Pharmaceutics* **10** (2018) 18.







**POSTER PRESENTATIONS** 



# THE EFFECT OF A NEW COPPER(II) COMPOUND ON THE SUPPRESSION OF THE GROWTH OF MALIGNANT LIVER CELLS

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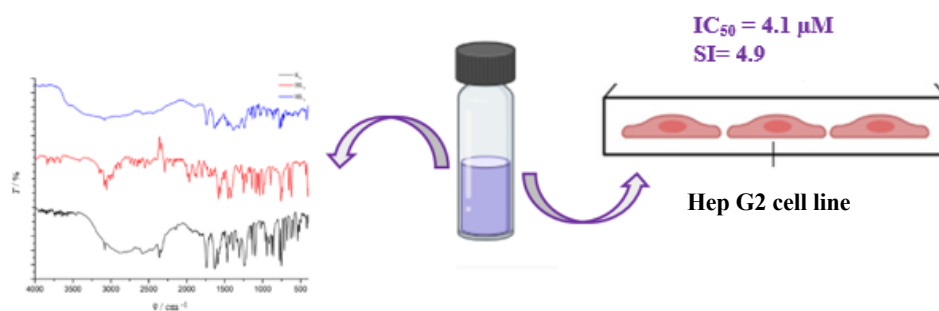
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Many copper complexes with chromone ligands have been screened for antitumor activity, and most of the synthesized compounds have shown increased cytotoxicity against various phenotypes of tumor cell lines. To further modulate the biological activity of the complex, the incorporation of secondary ligands (hydrophobic/hydrophilic, e.g. 2,2'-bipyridine) is often considered a desirable option. In addition, the extended aromatic ring systems in 1,10-phenanthroline and 2,2'-bipyridine can facilitate intercalation between neighboring nitrogen bases of nucleic acids (DNA; RNA) [1,2]. In this study, a copper(II) compound was prepared with chromone-2-carboxylic acid and 2,2'-bipyridine. This mixture of the two ligands yielded a compound that is highly specific for the Hep G2 cell line and exhibits an inhibitory effect of 79.7% at the highest concentration tested ( $10^{-5}$  mol dm<sup>-3</sup>). The compound showed no inhibitory effect on a healthy cell line (MRC-5) at any concentration. To confirm the biological activity of the compound, the values of IC<sub>50</sub> (inhibitory concentration; 4.1 μM) and selectivity index (SI = 4.9) were calculated, indicating significant cytotoxicity of the compound. The knowledge gained from this research may contribute to the development of new, highly selective compounds.



[1] F.Arjmand, Z.Afsan, T.Roisnel, *RSC Adv.* 8(2018) 37375.

[2] N.,K., Duggirala, M.L., Perry, Ö Almarsson, M.J. Zaworotko, *Chem. Commun.*, 52(2016). 640–655.

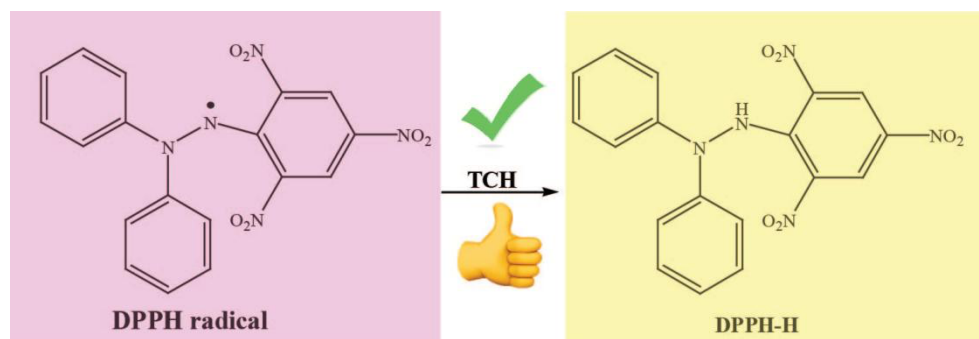
## STUDY OF ANTIOXIDATIVE PROPERTIES OF SELECTED ASYMMETRIC THIOCARBOHYDRAZONE DERIVATIVES

Ema Begović, Nevena Jokić, Suzana Apostolov, Đeđi Vaštag, Dragana Mekić, Borko Matijević, Gorana Mrđan\*

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Thiocarbohydrazone derivatives belong to the class of organic compounds obtained by a condensation process. In the reaction of thiocarbohydrazide with various aldehydes or ketones, monosubstituted and bisubstituted derivatives can be formed. Bisubstituted compounds can be symmetric and asymmetric, where asymmetric thiocarbohydrazones are far less investigated due to the more complicated process of their synthesis. Overall, thiocarbohydrazone derivatives have attracted great attention from scientists due to their wide biological activity. Many compounds investigated so far have proven to be good antioxidant [1], antimicrobial [2], antitumor [3], anticancer [4], and antidiabetic [5] agents. In this study, antioxidant properties of eight newly synthesized asymmetric thiocarbohydrazones have been tested. Evaluation of their efficacy as radical scavengers was examined using a DPPH assay. Based on the obtained results, it was concluded that the structure of the investigated compounds has a great influence on their activity.



- [1] H. Muglu, et al., *Journal of Physics and Chemistry of Solids*, **164** (2022) 110618.  
 [2] H. Yakan, et al., *Journal of Molecular Structure*, **1277** (2023) 134799.  
 [3] M. P. Sathisha, et al., *Metal-Based Drugs*, **2008** (2008) 362105.  
 [4] I. N. Cvijetic, et al., *Pharmaceuticals*, **16** (2023) 341.  
 [5] L. Srividya, et al., *Asian Journal of Biological Sciences*, **10** (2017) 126–129.



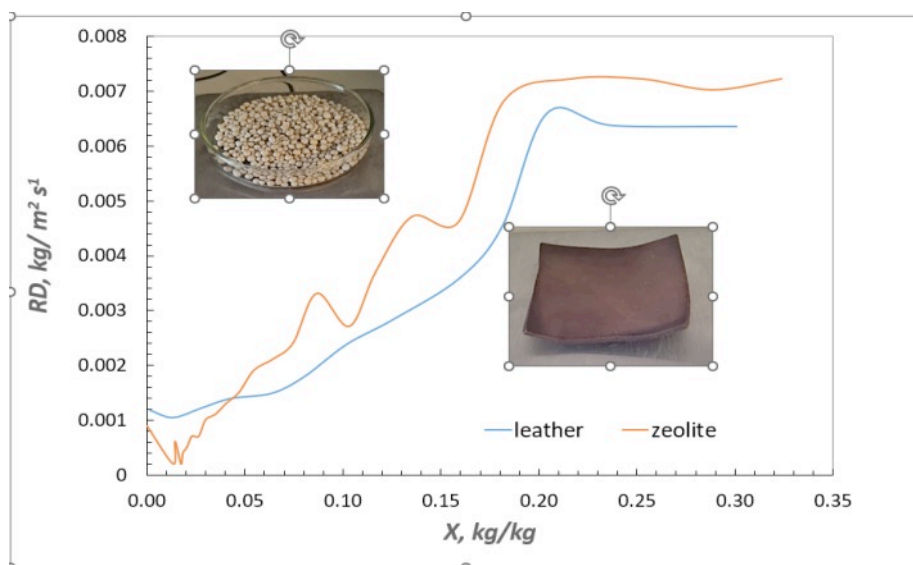
## COMPARISON OF ZEOLITE AND LEATHER DRYING IN A LABORATORY TRAY DRYER

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When drying solids, small amounts of water or other liquids are removed to reduce the residual liquid content to an acceptable level. This is considered a complicated process as it involves a simultaneous heat exchange and mass transfer that is accompanied by physicochemical changes in treated samples. On a laboratory scale, the most commonly used device is a tray dryer, in which heated air circulates over the wet material on the tray. The mechanism of drying depends on many factors that influence the rate of heat exchange and mass transfer. By measuring the evaporation rate ( $E=k \cdot A \cdot (P_s - P_a)$ ) of liquids over time per unit surface area, the solids drying process can be analysed through two distinct drying zones; zone of the constant-rate period and the falling-rate zone. The two zones are demarcated by a breakpoint, corresponding the critical moisture content.<sup>1</sup>

The aim of this work was to analyse and compare the drying behaviour of two different solid materials: wet leather and wet zeolite particles exposed to the same drying conditions. Drying was carried out in a convective tray dryer in a batch laboratory with air heated to 70 °C. During the drying process, the mass of the leather and zeolite samples was measured at specific times and the samples were photographed. Based on the results obtained, the changes in water content during the process were calculated and displayed graphically. In addition, the drying rate curves for both materials were plotted to analyse and compare the constant-rate zone and the falling-rate zone and to determine the critical moisture content of both materials. The results show that the water content and the drying rate were higher in the zeolite throughout the entire process duration, as well as the drying rate. The duration of the constant rate period of the zeolite particles was longer and the critical moisture content is lower. Based on the appearance of the sample surfaces and the drying behaviour of the material, changes in the drying conditions of the materials were suggested.



<sup>1</sup> W. McCabe, J. Smith, P. Harriott (2001) *Unit Operations of Chemical Engineering* (6th ed.) McGraw Hill, Boston, pp. 773-811.

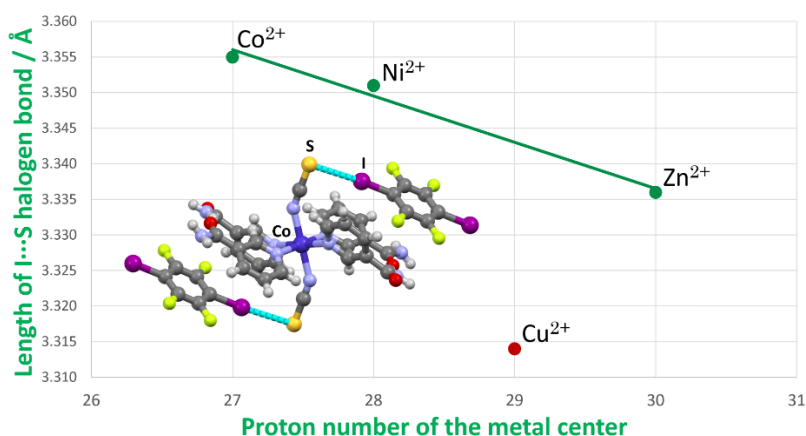
# ISOSTRUCTURAL HALOGEN-BONDED COCRYSTALS ACHIVED BY USING EQUIVALENT COORDINATION COMPOUNDS OF Co(II), Ni(II), Cu(II) AND Zn(II)

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In this work we explore the halogen bond acceptor potential of isothiocyanate sulfur atom in the synthesis of cocrystals involving metal-organic building blocks [1,2], by using coordination compounds whose pendant isothiocyanate groups enable halogen bonding. For this purpose, we have prepared four novel octahedral  $M(L)_4(NCS)_2$  coordination compounds ( $M = Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}$ ;  $L =$  nicotinamide) [3] and cocrystallized them with the classical halogen bond donor 1,4-diiodotetrafluorobenzene both by crystallization from solution and liquid-assisted grinding. Our results demonstrate the effectiveness of this strategy by the assembly of four isostructural cocrystals involving equivalent metal-organic building blocks. Single crystal X-ray diffraction experiments revealed that the carbonyl oxygen atoms of nicotinamide ligands do not act as halogen bond acceptors, but instead connect metal-organic units into 2D networks by  $N-H \cdots O$  hydrogen bonds. Each isothiocyanate ligand is connected to one halogen bond donor by  $S \cdots I$  halogen bonds, which bridge between 2D networks of metal-organic units. Furthermore, the synthesis of isostructural cocrystals also made possible an interesting insight into the effect that variation of the central atom of a coordination compound have on the length of the halogen bond. By plotting bond lengths against proton numbers of the metal centers, a negative linear correlation has been observed, with copper cocrystal deviating from the trend. Hirshfeld surfaces and the corresponding diagrams of dependence of  $d_e$  on  $d_i$  were also calculated, confirming the barely noticeable trend in the change of intermolecular distances. Moreover, the  $C-S \cdots I$  angle was also compared amongst the prepared cocrystals, but no significant trend has been observed, as when comparing the various hydrogen bond lengths.



[1] V. Nemeć, K. Lisac, N. Bedeković, L. Fotović, V. Stilinović, D. Cinčić, *CrystEngComm* **23** (2021) 3063–3083

[2] L. Posavec, D. Cinčić, *Cryst. Growth Des.* **24** (2024) 7514–7523

[3] F.A. Mautner, P.V. Jantscher, R.C. Fischer *et al.*, *Transit. Met. Chem.* **46** (2021) 191–200



# OPTIMIZING OLIGONUCLEOTIDE LIBRARY FOR DNA DATA STORAGE WITH MOLECULAR DYNAMICS (ONGOING RESEARCH)

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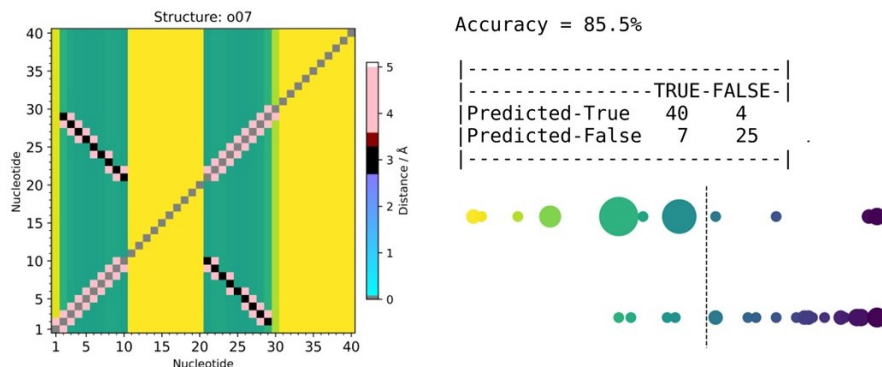
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Information for known life is encoded in DNA molecules. Optimized through two billion years of evolution, DNA is an attractive target for modern data storage solutions. As such, it is a subject of interest in a wide area of research for this specific purpose (among many others). For companies to be able to cold-store massive amounts of data for e.g. disaster recovery, archiving, etc, DNA data storage system would have to be optimized (among other things) in terms of cost, efficiency, and stability. For that reason, a predetermined set of oligonucleotides with desired properties, an “oligolibrary”, would be defined. Each oligonucleotide would map onto a packet of information (e.g. one byte), and oligonucleotides would have specific complements so that they assemble into a long strand of DNA that then encodes desired information. However, besides the desired interactions, oligonucleotides could bind in all other undesired ways. To optimize the selection of oligonucleotides that would constitute an oligolibrary, it is necessary to estimate the affinity of intended and unintended matches. In this research molecular dynamics (MD) is employed for the goal of assessing intended and unintended bindings between oligonucleotides from an oligolibrary. A structure is derived from sequences using AlphaFold3[1], and molecular dynamics using Gromacs[2] are run to research dynamical properties of pairs of oligonucleotides. A modified contact map depicting stable base pairings during the three 5 ns simulations, for a total of 15 ns simulation time, is used to predict if an oligonucleotide pair belongs to intended or unintended binding group. The model based off that is used to analyse the whole set of 77 structures with 3 simulation replicas, for a total of 231 MD simulations. The modified map, called “Base Pairing Plot”, is also discussed as a useful tool for batch analysis of DNA molecular dynamics simulations.



[1] J. Abramson *et al.*, *Nature* **630** (2024), 493 – 500.

[2] H. Bekker *et al.* *Physics computing* **92** (1993), 252 – 256.

## THE ROLE OF COMPOSTING IN SUSTAINABLE ORGANIC WASTE MANAGEMENT

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The production of organic waste is increasing worldwide. Composting has proven its worth in the sustainable management of solid waste rich in organic matter and can bring numerous environmental benefits [1]. It is an aerobic process that converts organic waste into a stable material that reduces greenhouse gas emissions, improves soil quality and conserves water. Good management of the composting process, from feedstock to finished compost, is associated with optimal conditions [1,2]. In this work, the characterization of the substrate in the different stages of composting was carried out. The analyses were carried out for samples in the thermophilic phase (A) and in the maturing phase (B). The results of the physical and chemical analyses show that the values for chemical oxygen demand (COD), pH, electrical conductivity (EC) and volatile solids (VS)/total solids (TS) ratio are 4428 and 1280 mg O<sub>2</sub>/L, 7.8 and 8.2, 2.39 and 1.87 mS/cm and 0.633 and 0.513 for samples A and B, respectively. Composting of organic waste is an essential part of sustainable waste management as it is a valuable process for recycling organic matter.



[1] S. Biyada, M. Merzouki, H. Imtara, MF. Alajmi, K. Elkarrach, H. Mechchate, R. Conte, M. Benlemlih, *Processes* 9 (2021) 1364.

[2] EE. Manea, C. Bumbac, LR. Dinu, M. Bumbac, CM. Nicolescu, *Sustainability* 16 (2024) 6329.

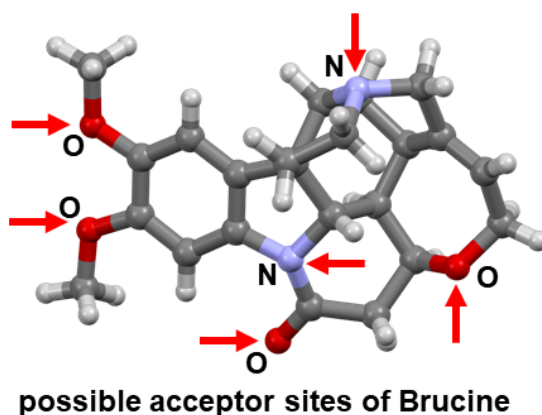


## COCRYSTALLIZATION OF BRUCINE WITH PERFLUORINATED IODOBENZENES

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Halogen bonding can be achieved with a wide range of potential acceptor atoms (N, O, S, halogenide, P, As, Sb etc.), the majority of halogen bonded crystal structures to date include nitrogen and oxygen as the halogen bond acceptor. [1] Polycyclic alkaloids often have multiple inequivalent nitrogen and oxygen atoms that can act as potential halogen bond acceptor sites making them interesting potentially polytopic halogen bond acceptors. However, almost no studies of halogen bonding of polycyclic alkaloids have been reported to date. [2] In this work, we have examined halogen bonding proclivities of brucine (**bruc**), a heavier analogue of highly toxic alkaloid strychnine. Using **bruc** and two perhalogenated halogen bond donors, two halogen-bonded cocrystals were prepared by crystallization from solution. Molecular and crystal structures of the two cocrystals were determined by single crystal X-ray diffraction. Observed structures have shown that in the cocrystal with tetrafluoro-1,2-diiodobenzene, the amine N atom and amide O atom of **bruc** act as acceptors. In cocrystal with tetrafluoro-1,4-diiodobenzene only the amine N atom acts as halogen bond acceptor. Furthermore, structural analysis revealed that both  $I\cdots N$  and  $I\cdots O$  halogen bonds are mostly linear and short with relative shortening in the 21.2 % – 24.4 % range and angles in the  $165.4^\circ$  –  $178.8^\circ$  range for  $I\cdots N$  contacts, and 14.8 % – 18.8 % with angles of  $164.4^\circ$  –  $170.1^\circ$  for  $I\cdots O$  contact respectively.



[1] G. Cavallo, P. Metrangolo, R. Milani, T. Pilati, A. Priimagi, G. Resnati, G. Terraneo, *Chem.Rev.* **116** (2016) 2478.

[2] C. R. Groom, I. J. Bruno, M. P. Lightfoot, S. C. Ward, *Acta Cryst.* **B72** (2016) 171.



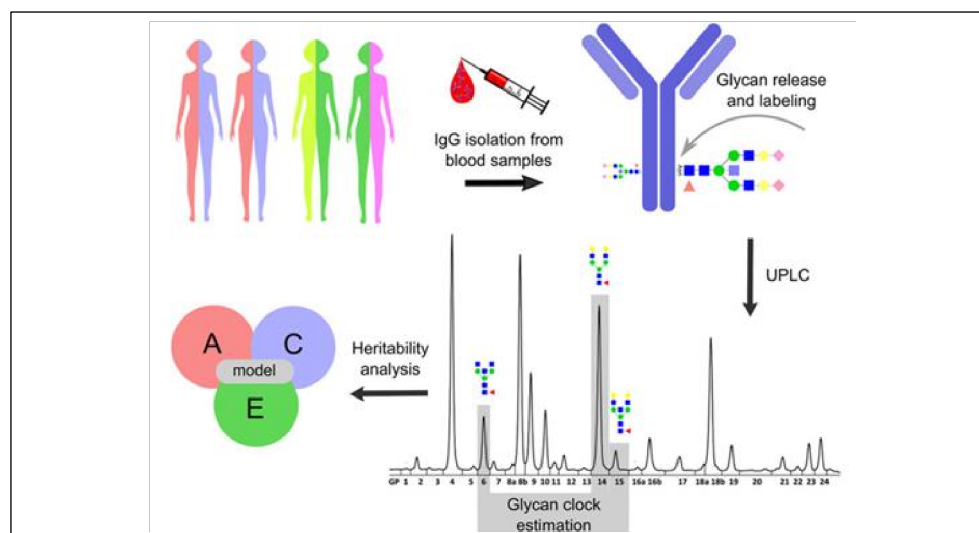
## METHOD DEVELOPMENT FOR CONSECUTIVE ANALYSIS OF *N*-GLYCOMES OF IMMUNOGLOBULINS A AND G FROM THE SAME INITIAL SAMPLE OF HUMAN BLOOD PLASMA

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A method was developed for the analysis of *N*-glycans from immunoglobulin A (IgA) and G (IgG) from the same human plasma sample. The aim of the study was to optimize the isolation of both immunoglobulins using affinity chromatography and to examine their glycosylation profiles. IgA and IgG were isolated using protein G plate for IgG and CaptureSelect™ IgA affinity beads for IgA.<sup>1</sup> After isolation, the *N*-glycans were labeled with a fluorescent tag (procainamide) and analyzed by hydrophilic interaction liquid chromatography coupled with ultra-high-performance liquid chromatography and fluorescence detection (HILIC-UHPLC-FLR), which enabled highly sensitive tracking of glycosylation patterns.<sup>2</sup> The results showed distinct glycosylation patterns between IgA and IgG, with IgA exhibiting more complex and diverse glycan structures. This method allows for the simultaneous analysis of both immunoglobulins from the same sample, reducing the need for larger quantities of biological material and increasing the precision of the analysis.



[1] G. Lauc, M. Pezer, J. Rudan, H. Campbell, *Glycobiology* **26** (2016) 929-939.

[2] I. Gudelj, G. Lauc, M. Pezer, *Cell. Immunol.* **333** (2018) 65-79.



# EXPLORING HYDRATE AND SOLVATE PATTERNS OF AZITHROMYCIN USING THE COFFEE RING EFFECT

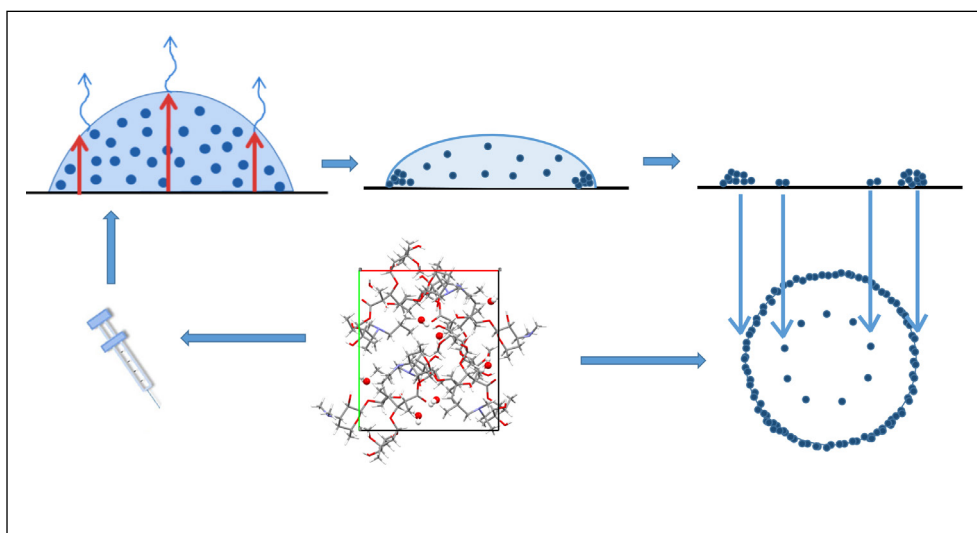
Tihana Mlinarić, Ernest Meštrović

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The study of hydrates and solvates is crucial in understanding the stability, solubility, and bioavailability of pharmaceutical compounds. Azithromycin, a widely used antibiotic, forms hydrates and solvates which show different properties relevant for preparation of final dosage forms. Traditional methods for studying these forms can be time-consuming and may not provide detailed spatial distribution information.

In this work, we explore the innovative application of the coffee ring effect—a phenomenon typically observed in drying colloidal suspensions—to investigate the formation of hydrates and solvates of azithromycin [1]. By analysing the deposition patterns formed as solvent evaporates from azithromycin solutions, we gain insight into the crystallization behaviour and the spatial arrangement of different hydrate and solvate forms.

Our findings demonstrate that the coffee ring effect can be effectively utilized to distinguish between various hydrates and solvates based on their unique deposition patterns. The method provides a rapid, low-cost, and visually intuitive approach to studying these forms, offering potential advantages over conventional techniques. This approach could be extended to other pharmaceutical compounds, opening new avenues for the study of polymorphism in drug development. The results of this study highlight the potential of the coffee ring effect as a powerful tool in the pharmaceutical sciences, particularly in the field of drug formulation and stability testing.



[1] T. Mlinarić, I. Rezić, & E. Meštrović, *AMSE* 2024 89.

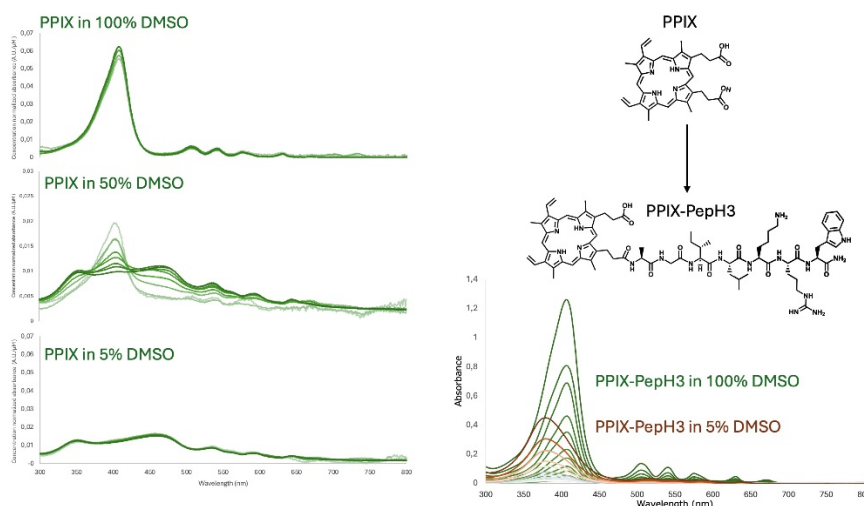
# STUDYING AGGREGATION OF PROTOPORPHYRIN IX, MESOPORPHYRIN IX AND THEIR PEPTIDE CONJUGATES BY MOLECULAR DYNAMICS AND UV/VIS SPECTROSCOPY

Andrej Nikolić<sup>1</sup>, Marko Babić<sup>1</sup>, Daniela Kalafatović<sup>1</sup>, Toni Todorovski<sup>1</sup>,  
Patrizia Janković<sup>1</sup>

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Porphyrins, a class of macrocyclic compounds, are crucial in biological processes and are applied in catalysis, solar energy conversion, and photodynamic therapy (PDT) due to their ability to produce reactive oxygen species (ROS), which is an effective treatment for some cancer types<sup>1</sup>. With the increasing problem of multidrug-resistant microbes and viral infection outbreaks, porphyrins' antimicrobial properties are receiving renewed interest<sup>2</sup>. However, their therapeutic potential is challenged by aggregation issues. Aggregation behavior of antimicrobial porphyrins, specifically protoporphyrin IX (PPIX) and mesoporphyrin IX (MPIX), and their conjugates with cell-penetrating peptide PepH3 (AGILKRW) was investigated. The study employed all-atom molecular dynamics simulations to elucidate the aggregation mechanisms and the effects of peptide conjugation. UV/Vis spectroscopy goals included determining the spectral changes indicative of aggregation. The peptide AGILKRW was synthesized using solid-phase peptide synthesis (SPPS) and its conjugation with PPIX was performed while still anchored on the solid support. Successful synthesis of the PPIX-PepH3 conjugate was confirmed by MALDI-TOF-MS and LC-MS. Spectroscopic studies of PPIX in dimethyl sulfoxide showed a Soret band at 408 nm, which split and broadened with increasing water content, indicative of aggregation. Notably, peptide conjugation reduced these changes to a slight blueshift which suggests that peptide conjugation can mitigate extensive aggregation. In silico simulations revealed that porphyrins primarily aggregate through  $\pi$ - $\pi$  interactions, forming dimers and larger aggregates. The peptide's presence altered this behavior, leading to the formation of globular structures stabilized by additional electrostatic and hydrogen bonding interactions.



[1] J. Kou, D. Dou and L. Yang, *Oncotarget* **8** (2017) 81591–81603.

[2] T. Todorovski, D. A. Mendonça, L. O., Fernandes-Siqueira, C. Cruz-Oliveira, G. Guida, J. Valle, M. Cavaco, F. I. V. Limas, V. Neves, Í. Cadima-Couto, S. Defaus, A. S. Veiga, A. T. Da Poian, M. A. R. B. Castanho and D. Andreu, *Pharmaceutics* **14** (2022) 738.

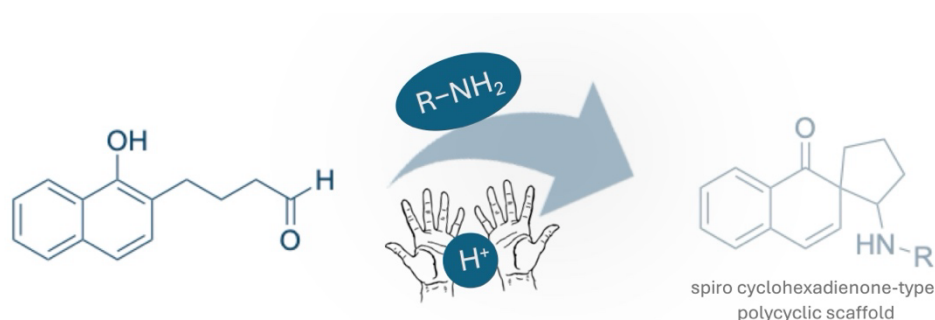


# SYNTHESIS OF NAPHTHOL PRECURSORS FOR THE DEVELOPMENT OF INTRAMOLECULAR SPIROCYCLIZATIONS

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This research investigates synthesis of a precursor, 4-(1-hydroxynaphthalen-2-yl)butanal (**1**), for the development of organocatalytic asymmetric dearomative (OCADA) intramolecular spirocyclizations [1]. The synthesis of compound **1** was attempted through three different synthetic routes. The initial route involved the synthesis via succinic acid ester, where the desired naphthol derivative was generated through Fries rearrangement. This approach was ultimately abandoned due to unsuccessful deprotection steps. The second route involved the elongation of substituted naphthylacetaldehyde with two carbon atoms, which also failed due to deprotonation of the undesirable carbon atom during the Wittig reaction. The desired aldehyde **1** was successfully synthesized by elongating substituted naphthaldehyde with three carbon atoms using the Wittig reaction. The intramolecular spirocyclization with the obtained compound **1** was unsuccessful due to the free *para*-position relative to the phenol, which interfered with the reaction and led to undesired condensation. In future research, derivatives of compound **1** that incorporate a phenyl group in the *para*-position will be synthesized and their reactivity in OCADA intramolecular spirocyclization will be investigated.



[1] T. Dohi, A. Maruyama, N. Takenaga, K. Senami, Y. Minamitsuji, H. Fujioka, S.B. Caemmerer, Y. Kita, *Angewandte Chemie International Edition* **47** (2008) 3787-3790.

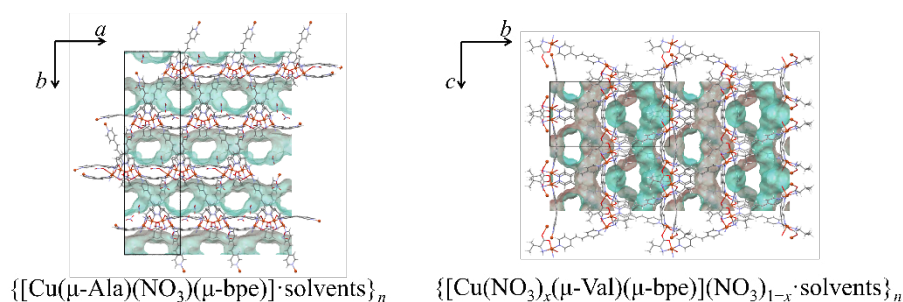
## 2D PORES IN 3D METAL-ORGANIC FRAMEWORKS WITH CHIRAL AMINOACIDATES: SYNTHESIS AND CRYSTAL STRUCTURE ANALYSIS

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Metal-organic frameworks (MOFs) are porous coordination polymers that exhibit diverse functions due to their tuneable structure and properties, like pore size and the nature of non-covalent interactions [1]. MOFs can be used as adsorbents, heterogeneous catalysts, and in chiral recognition and separation [2]. The adsorption of gases like H<sub>2</sub>, N<sub>2</sub>, CH<sub>4</sub> or CO<sub>2</sub> has been studied much more compared to the adsorption of water or other solvent vapours. Given that estimates indicate over half of the world's population lacks access to safe drinking water [3], investigation of water harvesters becomes increasingly important.

Our goal is to optimize the structural properties of MOFs to design compounds with tailored adsorption properties. For this purpose, we synthesized a series of MOFs containing essential metals and biocompatible ligands [4,5]. In this work, two 3D coordination polymers of copper(II) with L-alanine (**HAla**), L-valine (**HVal**) and (*E*)-1,2-bis(pyridin-4-yl)ethene (**bpe**) were synthesized by solution-based method: {[Cu(μ-Ala)(NO<sub>3</sub>)(μ-bpe)]·solvents}<sub>n</sub> (**1**) and {[Cu(NO<sub>3</sub>)<sub>x</sub>(μ-Val)(μ-bpe)](NO<sub>3</sub>)<sub>1-x</sub>·solvents}<sub>n</sub> (**2**). Compounds were characterized by single-crystal X-ray diffraction method. Both **1** and **2** contain octahedral and square-pyramidal coordination of copper(II) ions, where **Ala** or **Val** and **bpe** are bridging two copper(II) ions, and form two 3D interpenetrated frameworks. Solvent molecules are disordered and are arranged in 2D layers, occupying 35.0% and 38.6% of the unit cell volume of **1** and **2** (including disordered nitrate ions), respectively.



**Figure 1.** Backbones of **1** and **2** with solvent and nitrate contact surface areas

- [1] M. J. Kalmutzki, C. S. Diercks, O. M. Yaghi, *Adv. Mater.* **30** (2018) e1704304.  
 [2] G. Wei, C. Zhijie, J. Dong, Y. Liu, Y. Cui, *Chem. Rev.* **122** (2022) 9078–9144.  
 [3] J. Wolf, R. B. Johnston, A. Ambelu, B. F. Arnold, R. Bain, M. Brauer, J. Brown, B. A. Caruso, T. Clasen, J. M. Colford Jr., J. Esteves Mills, B. Evans, M. C. Freeman, B. Gordon, G. Kang, C. F. Lanata, K. O. Medlicott, A. Prüss-Ustün, C. Troeger, S. Boisson, O. Cumming, *The Lancet* (2023) 401: 2060–2071.  
 [4] D. Vušak, Z. Lemaić, M. Z. Mišković, B. Prugovečki, *Synthesis and Structural Study of Three-Component Chiral Metal-Organic Frameworks*, Solid-State Science & Research Meeting, Zagreb, 2023  
 [5] M. Jurković, K. Ležaić, *Synthesis and Structural Characterization of Copper(II) Metal-Organic Frameworks with N-Alkyl Glycinates and Heterocyclic Bases*, Rector's award thesis, Faculty of Science, University of Zagreb, 2022



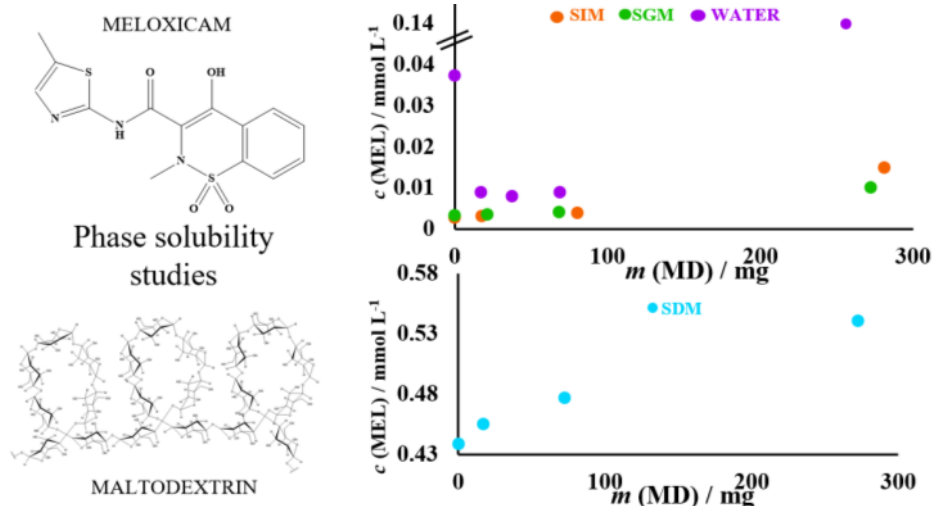
# INFLUENCE OF MALTODEXTRIN ON MELOXICAM SOLUBILITY IN WATER AND BIORELEVANT MEDIA

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Poorly soluble drugs are characterized by their limited solubility in aqueous media which affects their bioavailability, absorption efficiency, and ultimately their therapeutic potential. More than 70 % of molecules that are candidates for new drugs exhibit low water solubility, while 40 % of orally administered drugs with immediate release are categorized as insoluble. Consequently, traditional approaches to drug formulation need to be modified to overcome these limitations and unlock the full therapeutic potential of poorly soluble drugs. One of the most prominent ways to increase the solubility of drugs is the formation of inclusion complexes with cyclic oligosaccharides-cyclodextrins (CD) [1]. Meloxicam (MEL) is a non-steroidal anti-inflammatory drug (NSAID), classified as BCS II drug due to its low solubility and high permeability [2]. Although the formation of the inclusion complexes between meloxicam and cyclodextrins has been studied [3], there has not been any published research regarding the impact of maltodextrin (MD), a linear oligosaccharide, on the solubility of meloxicam. In this study, the effect of maltodextrin on the solubility of meloxicam in water, simulated gastric media (SGM pH= 1.2), simulated intestinal media (SDM pH = 4.5) and simulated duodenal media (SIM pH = 6.8) was investigated. Phase solubility studies were performed according to the method presented by Higuchi and Connors, and the concentration of meloxicam was determined by UV-Vis spectrophotometry. The associated diagrams were constructed along with the calculation of the solubility potential (increase in concentration of MEL in the presence of MD,  $S_{\max}/S_0$ ). The research shows that MD negatively affects the solubility of MEL in water while it has the opposite effect in SDM. Additionally, the greatest solubility potential was observed in SDM (5.39), while the smallest was in SIM (1.23). Comparing the effects of maltodextrin and cyclodextrins on the solubility of meloxicam, cyclodextrins are still the better choice because of greater solubility potentials [3].



[1] Y. Kawabata, K. Wada et al., *Int. J. Pharm.* **420** (2011) 1-10.

[2] P. Luger, K. Daneck et al., *Eur. J. Pharm. Sci.* **4** (1996) 175-187.

[3] B.N. Nalluri, K.P.R. Chpwdary et al., *J. Incl. Phenom. Macrocycl. Chem* **53** (2005) 103-110.

ACKNOWLEDGEMENTS: This work was supported by Croatian Science Foundation (project IP-2022-10-6033).

## NMR SPECTROSCOPY IN THE ANALYSIS OF SLOVENIAN AND CROATIAN SPARKLING WINES

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Wines have a very complex chemical composition with hundreds of different compounds in varying concentrations. Determining the chemical composition of wine is important for establishing the quality and value of wine, as well as detecting counterfeits and frauds.<sup>[1]</sup> Among various spectroscopic methods used in wine analysis, NMR spectroscopy has gained more popularity due to its simpler and non-destructive sample preparation as well as application in both targeted and non-targeted analysis. DOSY NMR spectroscopy is an NMR technique with significant potential, since it separates components according to their translational properties and diffusion coefficient without physical separation. The DOSY NMR spectrum is therefore a pseudo-two-dimensional spectrum where proton chemical shifts represent one dimension, while the other dimension displays translational diffusion coefficients. It can be used for analyzing complex chemical mixtures<sup>[2]</sup> and determining wine origin, authenticity, cultivar, as well as grape variety.<sup>[3]</sup> In this work NMR spectroscopy was used to characterize Croatian and Slovenian sparkling wines. The wine samples originated from different vintages and grape varieties. <sup>1</sup>H and DOSY NMR spectra provided information on different compounds present in the sparkling wines.<sup>[2]</sup> Furthermore, quantitative inverse-gated <sup>13</sup>C NMR spectra were also recorded to determine percentages of particular chemical components present in the complex wine samples such as aliphatics, aromatics, alcohols, carboxylic acids etc. Data so obtained will further be used for classification of wines by applying deep learning analysis.<sup>[3]</sup>

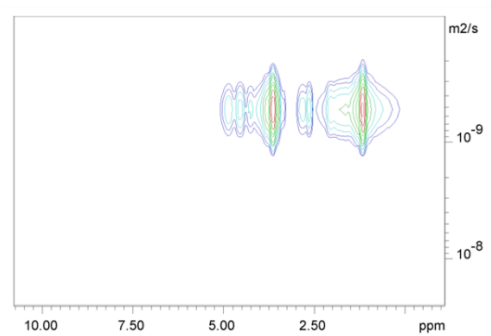


Figure 1. Typical <sup>1</sup>H DOSY NMR spectrum of a wine sample

- [1] J. V. Fonayet, G. Loupit, T. Richard, *Adv. Bot. Res.* **98** (2021) 297–357.
- [2] D. Rašević, J. Parlov Vuković, V. Smrečki, Lj. Marinić Pajc, P. Novak, T. Hrenar, T. Jednačak, L. Konjević, B. Pinević, T. Gašparac, *Fuel.* **305** (2021) 121561.
- [3] A. Jagatić Korenika, A. Jeromel, I. Tomaz, T. Jednačak, S. Rončević, I. Nemet, I. Primožič, T. Hrenar, P. Novak, *Food Chemistry: X* **21** (2024) 101162.



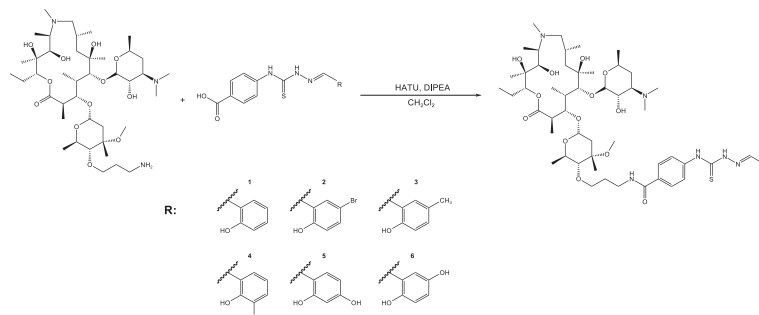
# ISOLATION AND CHARACTERIZATION OF NOVEL MACROZONE DERIVATIVES USING HPLC-SPE-NMR

Danijela Šimić,<sup>1</sup> Katarina Smetko,<sup>1</sup> Iva Habinovec,<sup>1</sup> Leda Divjak,<sup>1</sup> Kristina Smokrović,<sup>2</sup> Predrag Novak<sup>1</sup>

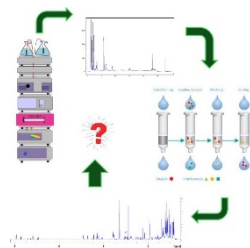
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Macrozones are novel compounds prepared by conjugating azithromycin and thiosemicarbazones. Azithromycin, a 15-membered macrolide and a top-selling antibiotic, is favored for its excellent pharmacokinetics, including high cellular accumulation and stability. However, widespread misuse of antibiotics globally has led to the development of bacterial resistance to existing antibiotics, including macrolides, which now poses a significant threat to human health. Consequently, it is imperative to discover new macrolide scaffolds to restore and enhance their antibacterial efficacy. In this study, we successfully prepared 2-hydroxyphenyl thiosemicarbazone 4''-macrozone derivatives and analyzed the reaction mixtures components. A hyphenated HPLC-SPE/NMR system has become an indispensable tool for complex mixture characterization and was used here to analyze macrozone reactions outcomes. The 2-hydroxyphenyl thiosemicarbazone 4''-macrozone derivatives were prepared by coupling 4''-( $\gamma$ -aminopropyl) azithromycin with six thiosemicarbazones (Scheme 1). HPLC was employed for separation of the reaction mixtures components, while post-column trapping of the selected compounds on SPE cartridges enhanced sensitivity for detecting analytes at low concentration. The results of NMR studies provide detailed insights into the molecular structure of the newly synthesized 4''-macrozone derivatives.



**Scheme 1.** The final step in the synthesis of 4''-macrozone derivatives.



- [1] I. Grgičević, I. Mikulandra, M. Bukvić, M. Banjanac, V. Radovanović, I. Habinovec, B. Bertoša, P. Novak, *Int. J. Antimicrob. Agents* **56** (2020) 106147.
- [2] I. Habinovec, I. Mikulandra, L. E. Sekula, J. Gašparov, S. Kazazić, P. Novak, *Molecules* **26** (2021) 6316.
- [3] A. Firth, P. Prapathan, *Eur. J. Med. Chem.* **207** (2020) 112739.



## APPLICATION OF NMR SPECTROSCOPY FOR EDIBLE OIL CHARACTERIZATION

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Vegetable oils are high-quality products that play an essential role in the human body. They are an indispensable part of the human diet providing essential fatty acids and valuable sources of micronutrients and bioactive substances such as carotenoids, polyphenols and alkaloids. Olive oils are responsible for many health benefits associated to “Mediterranean diet” that is one of healthiest diets in the world. They are a complex mixture consisting of different molecules generally divided in saponifiable fraction, which includes mono-, di- and triglycerides and unsaponifiable fraction, which include aliphatic alcohols, hydrocarbons, sterols, pigments, tocopherols, phenolic and volatile compounds. It is considered that the intake of 25-50 ml of extra virgin olive oil per day is sufficient to achieve a positive effect on health. The great interest in the quality of oils is also linked to the rapidly growing awareness of consumers who want to use safe and nutritious products with positive effects on health.<sup>[1]</sup>

Croatia is a growing market for extra virgin olive oil and there is a great need for the establishment of an olive oil bank. Understanding of vegetable oils is of particular interest for the research and development of production processes, production control and the determination of product quality. Edible oils, especially olive oils, are also susceptible to various types of adulteration.<sup>[2]</sup> Over the last decades, nuclear magnetic resonance spectroscopy (NMR) has proven to be a powerful tool for studying the composition and properties of vegetable oils.<sup>[3,4]</sup> Here we report NMR study of three different olive oil samples (Istria 1, Istria 2, Dalmatia 1) and one sunflower oil sample. We characterized these oils by using different one-dimensional NMR techniques (<sup>1</sup>H and <sup>13</sup>C) and then compared them by special areas of each spectra. The results can help us to remove suspicion of adulteration.

[1] D. Ancora, J. Milavec, A. Gradišek, M. Cifelli, A. Sepe, T. Apih, B. Zalar, V. Domenici, *J. Agric. Food Chem.* **2021**, 69, 12081–12088

[2] G. Vigli, A. Philippidis, A. Spyros, P. Dais, *J Agric Food Chem.* **2003**, 10, 5715-22.

[3] M. E. Di Pietro, A. Mannu, A. Mele, *Processes.* **2020**, 8, 410.

[4] V. Maestrello, P. Solovyev, L. Bontempo, L. Mannina, F. Camin F. *Compr Rev Food Sci Food Saf.* **2022**, 21, 4056-4075.

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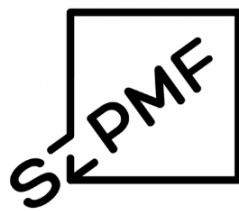


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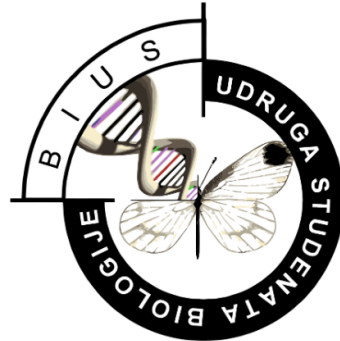
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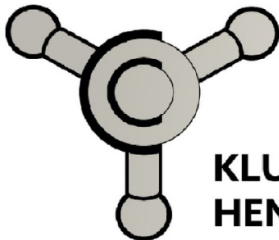
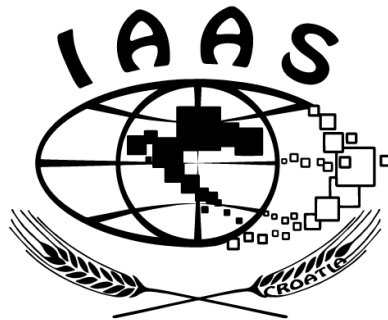
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