

Book of Abstracts

SiSK¹¹



BOOK OF ABSTRACTS

11th Symposium of Chemistry Students

9th and 10th of October 2026

Department of Chemistry, University of Zagreb, Faculty of Science

Zagreb, Croatia



SiSK¹¹

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PREFACE BY THE PRESIDENT OF THE ORGANIZING COMMITTEE

Dear colleagues, mentors and all those whose eyes grace these pages,

it is truly an honor to welcome you all to the 11th Symposium of Chemistry Students on behalf of the entire Organizing Committee.

As youngsters (*is that what the kids call themselves these days?*), we aren't well known for following tradition, but one tradition that we feel is our responsibility to follow is the tradition of SiSK. Since its beginnings, SiSK has had students at the forefront in such a way that it allows students to gain new and otherwise hard to obtain experiences which have the potential to be life changing. What we've tried to do this year is put the focus on learning whilst having fun, as we believe that "childish" curiosity is a characteristic which makes us better scientists, more engaging colleagues, more approachable speakers. With that in mind, we've decided to spice things up a bit by adding a new format, more about which you can read on the following page (See: Preface by the Head of the Student Section of CCS). Apart from the workshops, which we hope you enjoy, we've decided to shine a spotlight and give attention to a topic (and community) we've found to often be underrepresented which is the art of teaching. To discuss such an important topic, we've opted for a round table discussion because we believe that we should all be a part of this discourse and we hope that you'll decide to join us.

I would like to take this opportunity to thank CCS and especially its president, Professor Ernest Meštrović, who has showed us again and again how far he's willing to go for us, answering calls as soon as he's able, giving us advice and support throughout every step of the process. We would also like to thank the Department of Chemistry, headed by Professor Višnja Vrdoljak, which has allowed us to host the Symposium on *the hill* once again, enabling us to gain new experiences and make new acquaintances on familiar grounds; familiar for most students, but welcoming enough even for those of us who don't attend the Faculty of Science. Additionally, we would like to thank all our sponsors, donors and partners, without the support of which we wouldn't have been able to organize the Symposium.

Last, but certainly not least, I am extremely grateful for being given the chance to participate in yet another SiSK and to have been surrounded by such an amazing group of people without whom many of these ideas never would've become a reality. We did it, you guys :) (ok, technically not yet, but we will).

Dear all, I hope you enjoy the 11th Symposium of Chemistry Students and stay curious!

Vedrana Stantić

President of the Organizing Committee of the 11th SiSK

TLDR: SiSK is the best, we thank you all (especially some), curiosity did NOT kill the cat





PREFACE BY THE HEAD OF STUDENT SECTION OF CCS

Hi SiSKers, welcome back!

What a privilege it is to greet you all at another Symposium edition, a year has passed and we've been cooking up lots (pun intended)! SiSK is yet again establishing itself as a no. 1 event for chemistry students of Croatia – at least according to testimonies of our fellow colleagues after each Symposium edition. With such a legacy left for us to uphold, we can only set one goal: *make it even better*.

Thus, let me properly introduce our new conference activity – SiSK Workshops! During the first year of our mandate, a surprisingly strong but positive impression was left on me that chemistry students want to learn *more*. Learn more about topics not available to them through their university courses and learn more practical skills they can further build upon. So, to deliver on my last year's promise, we listened. We enriched this year's SiSK programme with two fun, relevant and non-standard workshops through which students can, with their own hands, explore all the fascinating ways chemistry impacts our lives.

Although we're implementing a new programme segment, the core of the Symposium stays the same: *students*. This year's Organizing Committee was ecstatic once we saw the number of student presentations registered. The everlasting trend of a high number of active student participants is probably the best proof there is to show that what we are doing matters. Providing such a platform matters, especially to younger students just starting their research internships, thesis work and/or similar occupancies. Very few conferences target undergraduate and graduate students, and it is a pleasure to organize a unique conference tailored exclusively to them. Our greatest intention is to show the world that chemistry students of Croatia can indeed offer very high quality research and be viewed head-to-head with students of other respected universities.

Organizing an event of these proportions is no easy task. Luckily, the people who do it make all the difference. I thank Vedrana for her brave commitment and initiative to lead this year's SiSK; Vice for always being a helping hand whenever we needed it (whether we knew it or not); Tonka for her sharp leadership and delegation; Luka K and Nina for their great attention to detail and resourcefulness; Viktor, Nika, Luka L and Nikola for lots of resilience and patience; Paula and Lucija Š for their limitless creativity and ingenuity; Lovre and Lucija M for their skill and effort.

I thank all the wonderful sponsors, donors, and other partners who share this passion of shining light on bright young minds. With your help, we can continue the legacy and showcase all of this year's talent pooling at the Chemistry Department. Thank you for being an example of what it means to support younger generations, we will never forget it.

And for the sake of sounding cliché, thank you for coming to our Symposium and I wish you all an unforgettable conference experience!

Josip Mikulić

Head of the Student Section of the Croatian Chemical Society







PROGRAMME





FRIDAY

9th of October, 2026

11:30	REGISTRATION OPENING (hall of the Department of Chemistry, main entrance)	
13:30 – 14:00	OPENING CEREMONY (A1, chair: Vice Limov)	
14:00 – 14:45	PLENARY LECTURE (A1, chair: Vice Limov)	Burkhard König (University of Regensburg): BETTER CHEMICAL SYNTHESIS WITH LIGHT!
14:45 – 15:00	SHORT BREAK	
15:00 – 15:30	INVITED LECTURE (A1, chair: Viktor Delač)	Domagoj Vrsaljko (University of Zagreb): 3D PRINTING OF MICROFLUIDIC MODULES FOR ADVANCED FLOW CHEMISTRY
15:30 – 16:00	COFFEE BREAK	
16:00 – 16:45	WORKSHOP (A1, chair: Tonka Musić)	Edi Topić (University of Zagreb) DEMISTIFYING AI: HOW TO USE THE NEWEST TECH TO YOUR ADVANTAGE
16:45 – 17:15	INVITED LECTURE (A1, chair: Tonka Musić)	Marta Popović (Ruder Bošković Institute) MECHANISMS OF DNA-PROTEIN CROSSLINK REPAIR: DEVELOPING NEW DISEASE MODELS AND IDENTIFYING MOLECULAR CAUSES OF HUMAN DISEASES
17:15 – 19:45	POSTER SECTION (levels 1 and 2 of the Department of Chemistry)	
19:45 – 21:15	SISQuiz – a SISK Pub Quiz (–1 level of the Department of Chemistry, chair: Luka Klemen)	

SATURDAY

10th of October, 2026

9:00	REGISTRATION OPENING (hall of the Department of Chemistry, main entrance)	
10:00 – 10:45	PLENARY LECTURE (A2, chair: Luka Klemen)	Aleksandra Djurišić (Ruder Bošković Institute): PHOTO/ELECTROCHEMICAL STABILITY OF ORGANIC LEAD HALIDE PEROVSKITES
10:45 – 11:15	BREAK	
	STUDENT ORAL PRESENTATIONS	
	SECTION I (A2, chair: Tonka Musić)	SECTION II (A1, chair: Vice Limov)
11:15 – 11:30	Josip Mikulić: UTILIZING HYDROGEN BONDING FOR REACTIVITY SUPPRESSION: A STUDY OF SYNTHETICALLY USEFUL VISIBLE-LIGHT-GENERATED CARBENES	Viktor Delač: HALOGEN-BONDED COCRYSTALS OF TWO-DIMENSIONAL Mn(II), Fe(II), Co(II), Ni(II), Cu(II) AND Zn(II) METAL-ORGANIC FRAMEWORKS
11:30 – 11:45	Marko Pečina: PHOTOPHYSICAL CHARACTERIZATION OF QUINAZOLINE-DERIVED ESIPT EMITTERS	Emanuel Novak: THE INFLUENCE OF THE STRUCTURE OF VANADIUM(V) COORDINATION COMPLEXES WITH A HYDRAZONE LIGAND ON THE CATALYTIC OXIDATION OF AROMATIC ALCOHOLS
11:45 – 12:00	Roko Budiselić: THE INFLUENCE OF THE DYNAMIC BOND POSITION IN AMPHIPHILE STRUCTURE ON THE pH-STABILITY OF NONIONIC SUPRAMOLECULAR AGGREGATES	Vilim Pavlović: HALOGEN-BONDED COCRYSTALS OF NITROGEN-CONTAINING ACCEPTORS AND IMINES DERIVED FROM PERHALOGENATED ANILINES
12:00 – 12:15	Luka Sumić: SYNTHESIS OF NOVEL MANNOSYLATED TRIAZOLE CONTAINING DESMURAMYL PEPTIDES	Tomislav Bunjevčević: FROM MECHANOCHEMISTRY TO CATALYSIS: MOLYBDENUM(VI) SCHIFF-BASE COMPLEXES FOR SELECTIVE ALCOHOL OXIDATION
12:15 – 12:30	SHORT BREAK	
12:30 – 13:15	WORKSHOP (A2, chair: Josip Mikulić)	Jana Pisk (University of Zagreb): EAT LIKE A SCIENTIST, NOT A CHEF
13:15 – 13:45	INVITED LECTURE (A2, chair: Josip Mikulić)	Marina Tranfić Bakić (University of Split): MOLECULAR MACHINES: CONTROLLED MOTION AT NANOSCALE



13:45 – 14:00	GROUP PHOTO	
14:00 – 15:30	LUNCH BREAK	
15:30 – 17:00	ROUNDTABLE DISCUSSION (A2)	<i>Teaching Chemistry: Finding the Right Formula</i> Luka Sumić (chair), Tajana Begović, Lana Šojat, Nenad Raos
17:00 – 17:45	Coffee & Chemistry PARTNERS' AND SPONSORS' STANDS (level 0 of the Department of Chemistry)	
	STUDENT ORAL PRESENTATIONS	
	SECTION III (A2, chair: Luka Klemen)	SECTION IV (A1, chair: Lucija Šolić)
17:45 – 18:00	Bruno Mršić: THE LEVEL OF NITRIC (II) OXIDE IN PLASMA SAMPLES COLLECTED FROM HEALTHY RESIDENTS FROM ZAGREB AND VINKOVCI IN TWO SEASONS	Tino Lonza: MECHANO-CHEMICAL SYNTHESIS OF ZEOLITIC IMIDAZOLATE FRAMEWORKS USING STRUCTURE-DIRECTING LIQUID ADDITIVES AND THEIR ACTIVATION
18:00 – 18:15	Nina Cankar: DEOXYFLUORINATION OF CARBOXYLIC ACIDS ENABLES SYNTHESIS OF AMIDES AND SHORT PEPTIDES	Andrej Nikolić: STRUCTURAL DYNAMICS AND MEMBRANE INTERACTION OF NOVEL PEPTIDE-PORPHYRIN CONJUGATES WITH ANTIMICROBIAL POTENTIAL
18:15 – 18:30	Nicoleta Stoian: EXPLORING PHARMACOLOGICAL SPACE THROUGH SELF-ORGANIZING MAPS (SOMS)	Saša Bulović: ADSORPTION OF INDOMETHACIN AND CHITOSAN ON MESOPOROUS SILICA PARTICLES
18:30 – 18:45	Hrvojka Lukac: AMIDE DERIVATIVES FOR FUNCTIONAL AND STRUCTURAL STUDIES OF CE15 GLUCURONYL ESTERASES	
18:45 – 19:00	SHORT BREAK	
19:00 – 19:20	SHORT PARTNER PRESENTATIONS (A2, chair: Viktor Delač)	Institute for Medical Research and Occupational Health, Serbian Young Chemists' Club
19:20 – 19:50	INVITED LECTURE (A2, chair: Viktor Delač)	Ivana Brekalo (Ruder Bošković Institute): BUILDING CASTLES IN THE SKY: THE SYNTHESIS OF POROUS MATERIALS THROUGH MECHANOCHEMISTRY
19:50 – ∞	CLOSING CEREMONY	
	SYMPOSIUM AFTERPARTY (level –1 of the Department of Chemistry, chair: <i>you</i>)	





CONTENTS

PLENARY LECTURES

- PL1 BETTER CHEMICAL SYNTHESIS WITH LIGHT!..... 23**
Burkhard König
- PL2 PHOTO/ELECTROCHEMICAL STABILITY OF ORGANIC LEAD HALIDE PEROVSKITES 25**
Aleksandra B. Djurišić

INVITED LECTURES

- IL1 3D PRINTING OF MICROFLUIDIC MODULES FOR ADVANCED FLOW CHEMISTRY 29**
Domagoj Vrsaljko, Ivan Karlo Cingesar, Elizabeta Forjan, Lara Štorga, Marijan-Pere Marković
- IL2 MECHANISMS OF DNA-PROTEIN CROSSLINK REPAIR: DEVELOPING NEW DISEASE MODELS AND IDENTIFYING MOLECULAR CAUSES OF HUMAN DISEASES 30**
Marta Popović, Cecile Otten, Marin Kutnjak, Marija Pranjić, Leona Verasto
- IL3 MOLECULAR MACHINES: CONTROLLED MOTION AT NANOSCALE 31**
Marina Tranfić Bakić
- IL4 BUILDING CASTLES IN THE SKY: THE SYNTHESIS OF POROUS MATERIALS THROUGH MECHANOCHEMISTRY 32**
Ivana Brekalo

SECTION LECTURES

- SL1 CHOLINESTERASE INHIBITION BY 2-(ACYLAMINO)ACETAMIDES: INSIGHTS FROM QUANTUM CHEMICAL DOCKING 37**
Roko Budiselić, Aleks Logožar, Anamarija Knežević
- SL2 ADSORPTION OF INDOMETHACIN AND CHITOSAN ON MESOPOROUS SILICA PARTICLES 38**
Saša Bulović, Ivor Vavra Plavšić, Tajana Begović
- SL3 FROM MECHANOCHEMISTRY TO CATALYSIS: MOLYBDENUM(VI) SCHIFF-BASE COMPLEXES FOR SELECTIVE ALCOHOL OXIDATION 39**
Tomislav Bunjevčević, Josipa Sarjanović, Jana Pisk
- SL4 DEOXYFLUORINATION OF CARBOXYLIC ACIDS ENABLES SYNTHESIS OF AMIDES AND SHORT PEPTIDES 40**
Nina Cankar, Jan Jelen, Gašper Tavčar





SL5	HALOGEN-BONDED COCRYSTALS OF TWO-DIMENSIONAL Mn(II), Fe(II), Co(II), Ni(II), Cu(II) AND Zn(II) METAL-ORGANIC FRAMEWORKS.....	41
	Viktor Delač, Jogirdas Vainauskas, Vinko Nemec, Tomislav Friščić, Dominik Cinčić	
SL6	MECHANOCHEMICAL SYNTHESIS OF ZEOLITIC IMIDAZOLATE FRAMEWORKS USING STRUCTURE-DIRECTING LIQUID ADDITIVES AND THEIR ACTIVATION	42
	Tino Lonza, Katarina Lisac, Ivana Brekalo	
SL7	AMIDE DERIVATIVES FOR FUNCTIONAL AND STRUCTURAL STUDIES OF CE15 GLUCURONOYL ESTERASES.....	43
	Hrvojka Lukac, Ali Wang, Junjun Tan, Scott Mazurkewich, Johan Larsbrink, Leila Lo Leggio	
SL8	UTILIZING HYDROGEN BONDING FOR REACTIVITY SUPPRESSION: A STUDY OF SYNTHETICALLY USEFUL VISIBLE-LIGHT-GENERATED CARBENES	44
	Josip Mikulić, Marko Purić, Nikola Topolovčan	
SL9	THE LEVEL OF NITRIC(II) OXIDE IN PLASMA SAMPLES COLLECTED FROM HEALTHY RESIDENTS FROM ZAGREB AND VINKOVCI IN TWO SEASONS	45
	Bruno Mršić, Ana-Marija Domijan, Goran Gajski, Marko Gerić, Katarina Matković, Luka Kazensky, Mandica Sanković, Antun Šumanovac	
SL10	STRUCTURAL DYNAMICS AND MEMBRANE INTERACTION OF NOVEL PEPTIDE-PORPHYRIN CONJUGATES WITH ANTIMICROBIAL POTENTIAL.....	46
	Andrej Nikolić, Toni Todorovski	
SL11	THE INFLUENCE OF THE STRUCTURE OF VANADIUM(V) COORDINATION COMPLEXES WITH A HYDRAZONE LIGAND ON THE CATALYTIC OXIDATION OF AROMATIC ALCOHOLS	47
	Emanuel Novak, Josipa Sarjanović, Jana Pisk	
SL12	HALOGEN-BONDED COCRYSTALS OF NITROGEN-CONTAINING ACCEPTORS AND IMINES DERIVED FROM PERHALOGENATED ANILINES	48
	Vilim Pavlović, Nea Baus Topić, Vinko Nemec, Dominik Cinčić	
SL13	PHOTOPHYSICAL CHARACTERIZATION OF QUINAZOLINE-DERIVED ESIPT EMITTERS	49
	Marko Pećina, Đani Škalamera, Ivan Ljubić, Iva Džeba	
SL14	EXPLORING PHARMACOLOGICAL SPACE THROUGH SELF-ORGANIZING MAPS (SOMs)	50
	Nicoleta Stoian, Liliana Halip	



- SL15 SYNTHESIS OF NOVEL MANNOSYLATED TRIAZOLE-CONTAINING DESMURAMYL PEPTIDES.....51**
 Luka Sumić, Vesna Petrović Peroković, Željka Car, Rosana Ribić

POSTER PRESENTATIONS

- P1 ADVANCED COMPOSITE PLASTERS WITH EMBEDDED PHASE CHANGE MATERIALS..... 55**
 Barbara Absec, Tina Skalar, Petra Štukovnik, Nataša Čelan Korošin
- P2 EFFECTS OF DISPERSANTS AND CALENDERING ON NMC CATHODE PERFORMANCE 56**
 Nika Arambašić, Iva Kulušić, Rahela Bilić, Hrvoje Tašner, Grgur Mihalinec, Zoran Mandić
- P3 EFFECT OF Pr CONCENTRATION ON THE STRUCTURAL EVOLUTION OF CERIA-BASED HIGH-ENTROPY OXIDES 57**
 Jakov Babić, Stjepan Šarić, Dalibor Tatar, Jelena Kojčinović, Petra Šušak, Igor Djerdj
- P4 QUANTUM CHEMICAL DOCKING OF PYRIDINE UGI DERIVATIVES AS CHOLINESTERASE INHIBITORS..... 58**
 Bruna Bakota, Jakov Borovec, Toni Divjak, Alma Ramić, Ines Primožič, Tomica Hrenar
- P5 SYNTHESIS, CRYSTAL STRUCTURE AND DNA-BINDING PROPERTIES OF A TERNARY COPPER(II) COMPLEX WITH GLYCINE AND PYRAZINO[2,3-f][1,10]PHENANTHROLINE 59**
 Mihael Belas, Ivana Kekez, Darko Vušak, Biserka Prugovečki
- P6 APPLICATION OF ARTIFICIAL INTELLIGENCE FOR THE OPTIMIZATION OF PYROLYSIS PROCESSES IN INDUSTRIAL WASTE VALORIZATION AND CHEMICAL FEEDSTOCK PRODUCTION60**
 Amina Bjelić, Sara Baždalić
- P7 SOLID DISPERSIONS OF DRUG AND BIOACTIVE COMPOUNDS: SYNTHESIS, CHARACTERIZATION AND PHARMACEUTICAL POTENTIAL.....61**
 Sanja Blek, Katarina Sokač Pogrmilović, Krunoslav Žižek
- P8 SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF A NEW COPPER(II) METAL-ORGANIC FRAMEWORK WITH L-ASPARAGINE AND 4,4'-BIPYRIDINE 62**
 Roko Budiselić, Darko Vušak, Biserka Prugovečki
- P9 SUBSTITUENT EFFECTS IN CHLORINATION OF C₅-SUBSTITUTED URACILS: A HAMMETT-TYPE DFT AND NMR STUDY..... 63**
 Emma Činčurak, Lucija Špiljak, Antonio Ljulj, Davor Šakić, Valerije Vrček





- P10 SYNTHESIS AND CRYSTAL STRUCTURES OF MULTICOMPONENT COPPER(II) MOFS WITH L-ALANINE AND (E)-1,2-DI(PYRIDIN-4-YL)DIAZENE.....64**
Leonarda Čutura, Darko Vušak, Biserka Prugovečki
- P11 NUTRITIONAL POTENTIAL OF COMMON SOWTHISTLE (*Sonchus oleraceus* L.): INFLUENCE OF GREEN EXTRACTION METHODS .. 65**
Lana Galetović, Antonija Rezić, Dea Amber Radić, Lara Vukšić, Ivana Anđelić
- P12 DIASTEREOSELECTIVE SYNTHESIS OF PHENYL-SUBSTITUTED ALDONOLACTONE DERIVATIVES VIA DOUBLE GRIGNARD ADDITION66**
Martin Husinec, Marija Alešković, Mario Oraić, Katarina Pičuljan, Nikola Cindro
- P13 LOW-DIMENSIONAL HYBRID HALOCUPRATES(II) BASED ON PARA-SUBSTITUTED BENZYLAMINES..... 67**
Marko Ivanišević, Edi Topić, Marko Bochniček, Mirta Rubčić
- P14 ENVIRONMENTAL FATE AND RISK ASSESSMENT OF CONTAMINANTS OF EMERGING CONCERN IN WASTEWATER: A COMPARATIVE STUDY OF SLOVENIAN AND PORTUGUESE TREATMENT SYSTEMS68**
Martina Ivanova, Andreja Žgajnar Gotvajn, Helena Prosen, Aleksander Kravos, Rita Maurício
- P15 BIODEGRADATION OF THE ANTIVIRAL DRUGS RITONAVIR, FAVIPRAVIR AND DACLATASVIR AND DETERMINATION OF OPTIMAL PROCESS CONDITIONS.....69**
Tijana Jezerčić, Dora Lastovčić, Luka Večenaj, Anja Rakas, Matija Cvetnić, Marinko Markić, Tomislav Bolanča, Dajana Kučić Grgić, Šime Ukić†
- P16 REMOVAL OF THE PESTICIDE ATRAZINE FROM GROUNDWATER AND DETERMINATION OF ITS ECOTOXICITY BY *Vibrio fischeri* . 70**
Barbara Jezerčić, Bruna Babić Visković, Anica Pavlinović, Iva Ćurić, Danijela Ašperger, Davor Dolar
- P17 AMMONIUM SALTS AND ALKOXIDE DERIVATES OF VANADIUM(V) COMPLEXES WITH THE ⁴OMESIH LIGAND71**
Ana Jurčević, Dino Kuzman, Juraj Toplak, Višnja Vrdoljak
- P18 VALORIZATION OF ANTIOXIDANT COMPOUNDS FROM CHAMOMILE HERBAL DUST USING DIFFERENT EXTRACTION APPROACHES..... 72**
Helena Jurić, Magdalena Mikić, Mario Komar, Maja Molnar, Martina Jakovljević Kovač



- P19 CHLORINATION OF CYCLOPHOSPHAMIDE AND IFOSFAMIDE IN AQUEOUS ENVIRONMENTS: A QUANTUM-CHEMICAL STUDY.. 73**
Anamarija Jurjević, Elena Erlić, Antonio Ljulić, Valerije Vrčec
- P20 EXPLORING METAL CATION COMPLEXATION USING THE INTRINSIC FLUORESCENCE OF CALIX[6]ARENE..... 74**
Luka Klemen, Andrea Usenik, Franka Sunjka, Karla Kukina Gradečak, Katarina Leko, Nikola Cindro, Gordan Horvat, Ivo Piantanida, Vladislav Tomišić
- P21 SORPTION OF LANTHANOID IONS FROM MULTICOMPONENT SOLUTIONS USING NEUTRAL AND FUNCTIONALIZED IRON NANOPARTICLES 75**
Petra Kovačić, Ivan Nemet, Nikolina Ilić
- P22 HALOGEN-BONDED COCRYSTALS OF $M(NCS)_2(3\text{-XPYRIDINE})_4$ COORDINATION COMPOUNDS ($M = \text{Co, Ni, Fe, Mn}$; $X = \text{Cl, Br, I}$) 76**
Tom Kovačić, Vinko Nemec, Dominik Cinčić
- P23 SYNTHESIS AND CHARACTERISATION OF ZINC(II) COMPLEXES WITH COUMALIC ACID 77**
Tea Kozić, Tomislav Balić, Nikolina Filipović, Anamarija Stanković
- P24 SYNTHESIS AND PHOTOPHYSICS OF AN AZOBENZENE PHENYLBORONIC ACID DERIVATIVE..... 78**
Petra Labrović, Marina Tranfić Bakić
- P25 COMPARISON OF THE ANTIOXIDANT POTENTIAL OF MULTIFLORAL AND LINDEN HONEY FROM CROATIA: PERSPECTIVES FOR HONEY VALORISATION 79**
Marina Kranjac, Marina Lončar, Saša Prdun, Carlo I.G. Tuberoso, Jelena Puzić
- P26 MECHANOCHEMICAL SYNTHESIS OF COPPER(II) SCHIFF BASE COMPLEXES BY STEPWISE AND ONE-POT ROUTES80**
Hrvojka Lukac, Vinko Nemec, Dominik Cinčić
- P27 SOLVENT INCLUSION IN CALIX[4]ARENE: A COMPREHENSIVE EXPERIMENTAL, THERMODYNAMIC, AND COMPUTATIONAL STUDY.....81**
Sven Marinac, Andrea Usenik, Matija Modrušan, Jakov Borovec, Katarina Pičuljan, Katarina Leko, Gordan Horvat, Josip Požar, Nikola Cindro, Tomica Hrenar, Vladislav Tomišić
- P28 COMPLETE NMR ASSIGNMENT OF PINGUISANIN AND DEOXYPINGUISONE.....82**
Katarina Nejić, Miljana Đorđević Zlatković, Dragan Zlatković, Niko Radulović





- P29 TOWARDS ZERO WASTE CONCEPT – PLANT SECONDARY WASTE AS PROMISING SOURCE OF HEMICELLULOSE 83**
Luka Niković, Milica Perović, Jelena Vukosavljević, Branimir Pavlić, Mirjana Antov
- P30 TERNARY COPPER(II) COORDINATION COMPOUND WITH L-PHENYLALANINE: SYNTHESIS, CHARACTERIZATION AND INTERACTIONS WITH DNA.....84**
Ema Novak, Darko Vušak, Ivana Kekez, Biserka Prugovečki
- P31 THE USE OF TEMPLATED ZINC IMIDAZOLATE ($ZnIm_2$) FRAMEWORKS IN THE SEPARATION OF SOLID MIXTURES 85**
Danea Obratov, Emilija Petrović Hađar, Ivana Brekalo
- P32 TOWARD THE TOTAL SYNTHESIS OF DENTITHECAMIDE A86**
Nino Perković, Mirko Duvnjak, Marta Rotar, Ilias Timotheidis, Nikola Cindro
- P33 SYNTHESIS AND CHARACTERIZATION OF NOVEL UGI PRODUCTS 87**
Leon Prša, Alma Ramić, Ines Primožič
- P34 SYNTHESIS OF HYBRID HALIDE PEROVSKITES WITH *p*-HALOGENATED BEZYLAMINES.....88**
Jana Salajec, Dino Kuzman, Edi Topić, Mirta Rubčić
- P35 DIFFERENTIATION OF "GRAŠEVINA" AND "PLAVAC MALI" WINES USING ICP-MS AND NMR METHODS89**
Kora Sertić, Ivan Nemet, Nikolina Ilić, Predrag Novak, Tomislav Jednačak, Ana Badenić, Petra Vuković, Ana-Marija Jagatić Korenika
- P36 THERMODYNAMIC AND STRUCTURAL INSIGHTS INTO CATION COMPLEXATION BY A THIOAMIDE CALIX[4]ARENE DERIVATIVE90**
Bruno Šijić, Katarina Leko, Nikola Cindro, Andrea Usenik, Vladimir Stilinović, Gregor Talajić, Vladislav Tomišić
- P37 TOTAL PHENOLIC CONTENT AND BIOACTIVITY OF SLOVENIAN HONEY SAMPLES OF DIFFERENT ORIGIN91**
Katica Stevanović, Katarina Žarko, Sonja Smole Možina
- P38 STABILITY ASSESSMENT OF 3D-PRINTED MBBR BIOMASS CARRIERS IN MUNICIPAL WASTEWATER 92**
Patricija Tisaj, Maša Legan, Andreja Žgajnar Gotvajn
- P39 MECHANOCHEMICAL SYNTHESIS OF EXPANDED MOF-74 93**
Nina Torma, Emilija Petrović Hađar, Nikola Jakupec, Krunoslav Užarević
- P40 UV-C INDUCED OXIDATION OF REMDESIVIR AND RITONAVIR ..94**
Leonarda Zovko, Luka Večenaj, Dora Lastovčić, Kristina Bule Možar, Lidija Furač, Marinko Markić, Dajana Kučić Grgić, Matija Cvetnić, Tomislav Bolanča







PLENARY LECTURES





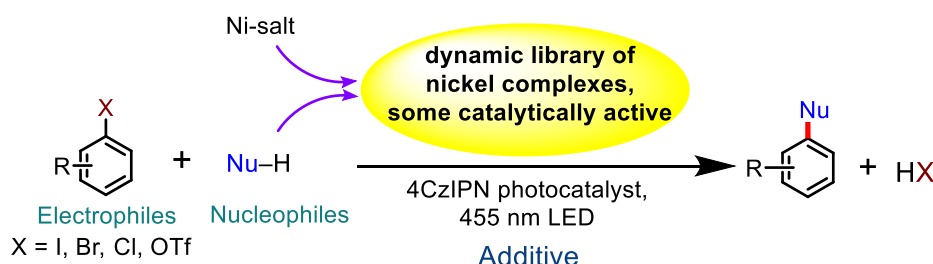
BETTER CHEMICAL SYNTHESIS WITH LIGHT!

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Light is a form of energy and an ideal reagent for many chemical reactions. It enables transformations under ambient conditions and even drives endergonic reactions that are impossible under thermal conditions [1]. We discuss the key principles of the technology, some applications in organic synthesis, and the opportunities photocatalysis offers for more energy-efficient chemical production in the future. Light energy promotes redox-neutral reactions with ideal atom economy and excellent energy efficiency, making them ideal candidates for large-scale synthesis [2,3]. Photochemical carbonyl Umpolung reactions represent another class of light-promoted synthesis that yields higher-energy products [4,5]. Cross-coupling reactions are among the most important in organic synthesis, both in industry and academia. Photochemistry can enhance the performance of this reaction class. The new concept of adaptive dynamic homogeneous catalysis (AD-HoC; see Figure) uses light to control the redox state of catalytically active species, enabling rapid, predictable cross-coupling of all classes of nucleophiles with halogenated arenes and heteroarenes [6,7]. Alternatively, photochemical reactions “on water” provide simple conditions for cross-coupling reactions within electron donor-acceptor complexes [8].



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- [6] I. Ghosh *et al.*, *Nature* **619** (2023) 87.
- [7] K. Das *et al.*, *Angew. Chem. Int. Ed.* **64** (2025) e202510715526.
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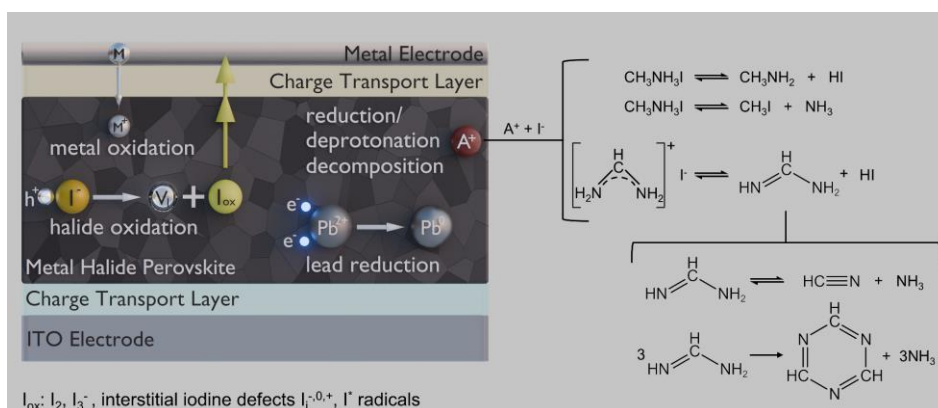


PHOTO/ELECTROCHEMICAL STABILITY OF ORGANIC LEAD HALIDE PEROVSKITES

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Metal halide perovskites have attracted significant attention for their application in photovoltaic cells due to their exceptionally high efficiency, outperforming conventional silicon cells. However, they also exhibit instability upon exposure to oxygen, moisture, elevated temperature, bias voltage, and illumination, which are expected operational stressors for solar cells. Therefore, it is critical to understand the mechanisms leading to performance deterioration during operation. In this talk, photo/electrochemical reactions which occur in perovskite materials under illumination and bias, with particular emphasis on the reactions affecting organic cations [1], will be discussed.



[1] Z. L. Ren *et al.*, *Nat. Energy* **11** (2026) 662–670.





INVITED LECTURES





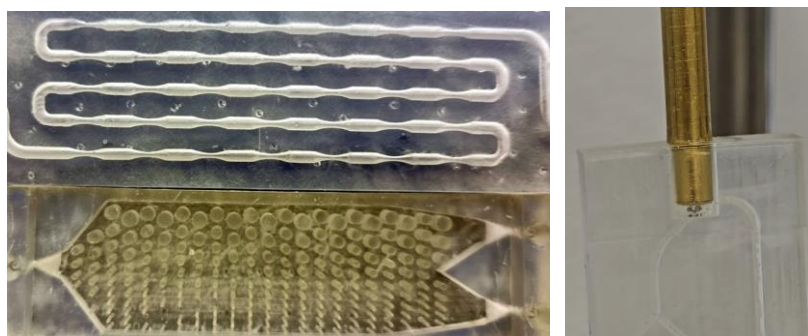
3D PRINTING OF MICROFLUIDIC MODULES FOR ADVANCED FLOW CHEMISTRY

Domagoj Vrsaljko¹, Ivan Karlo Cingesar², Elizabeta Forjan¹, Lara Štorga¹,
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Additive manufacturing has emerged as a powerful tool for the development of microfluidic systems in flow chemistry, enabling the fabrication of complex and highly customizable devices with reduced production time and cost. Compared with conventional manufacturing methods, such as soft lithography and micromachining, which often require specialized equipment and multi-step fabrication procedures, additive manufacturing offers greater design flexibility and easier integration of functional components, including sensors and catalysts. In particular, stereolithography (SLA) and digital light processing (DLP) enable the fabrication of transparent micro- and milliscale reactionware with complex geometries and tailored properties. Previous studies demonstrated that printing parameters and post-curing conditions significantly influence the mechanical, thermal, and chemical resistance of photocurable resins, highlighting the importance of process optimization for the production of robust microfluidic devices. This research is part of the HRZZ INDIGO project, which focuses on the development of advanced 3D-printing approaches for the fabrication of microfluidic systems, including microreactors and separators, intended for flow chemistry applications. As continuous processes increasingly replace conventional batch operations, the need for real-time process monitoring through on-line *in situ* measurements is becoming increasingly important. This study focuses on the design, fabrication, and optimization of pH sensors, surface coatings, and reactor channels to enable the integration of FTIR probes and other analytical tools into 3D-printed microfluidic systems. By optimizing digital light processing (DLP) and fused filament fabrication (FFF) processes, the project aims to enhance the mechanical performance, chemical resistance, and functional properties of printed devices. Newly developed microfluidic platforms with integrated sensors will provide real-time on-line *in situ* monitoring and improved control of flow chemistry processes. The ultimate goal is to establish robust and versatile systems suitable for both research and industrial applications [1–3].



ACKNOWLEDGEMENTS This work has been supported by the Croatian Science Foundation under the projects: HRZZ-IP-2022-10-8004, HRZZ-DOK-2021-02-5999, HRZZ-DOK-NPOO-2023-10-1144 and HRZZ-DOK-2025-02-4318.

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[2] E. Forjan, M.P. Marković, P. Kassal, D. Vrsaljko, *J Sol-Gel Sci Technol* **115** (2025) 1–16.

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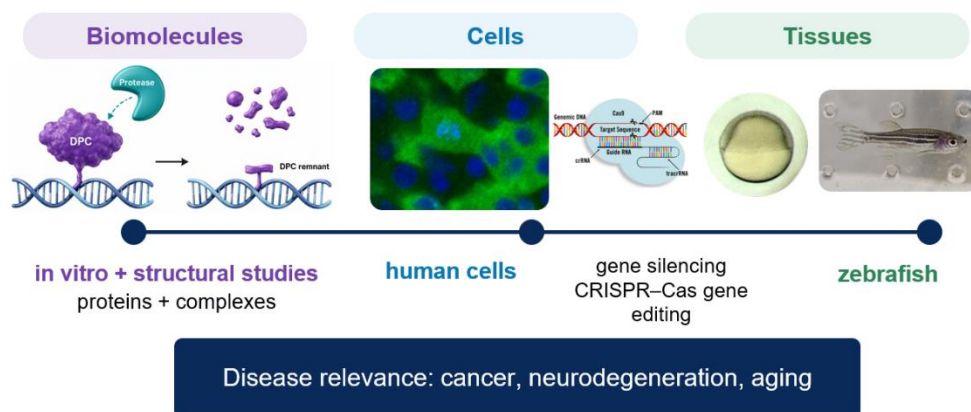
MECHANISMS OF DNA-PROTEIN CROSSLINK REPAIR: DEVELOPING NEW DISEASE MODELS AND IDENTIFYING MOLECULAR CAUSES OF HUMAN DISEASES

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DNA–protein crosslinks (DPCs) are the second most common type of DNA lesion and can obstruct replication and transcription. Defective repair of these toxic lesions is associated with cancer, neurodegeneration, and ageing. DPC-inducing agents are used clinically to treat several cancers; therefore, understanding DPC repair could support the development of new drugs and combination therapies. Moreover, the accumulation of DPCs contributes to ageing and neurological disorders, underscoring the importance of elucidating the mechanisms of DPC repair. In recent years, our group and others have gained important mechanistic insights into DNA–protein crosslink repair (DPCR) factors [1,2]. We use *in vitro* approaches, human cell lines, and zebrafish models to investigate the structure and function of DPC-repair proteins and protein complexes. The structures of large protein complexes and proteins containing intrinsically disordered regions are partially resolved using cryo-electron microscopy (cryo-EM). The functions of individual proteins and/or protein complexes are investigated using gene silencing and CRISPR–Cas gene editing in stable cell lines, zebrafish embryos, and adult zebrafish. We found that ACRC is an essential protease during vertebrate development: a catalytic mutation causes early embryonic lethality, associated with the accumulation of specific DPCs, including histones, topoisomerases, and PARP1. We also show that SPRTN cannot compensate for ACRC function during early development. In addition, we will present unpublished data on the structure and function of the SPRTN–p97 protein complex and on the role of tyrosyl-DNA phosphodiesterases in DPC repair. Our results provide insight into the complex pathways of DPCR and their implications for human disease and cancer treatment.

DNA–PROTEIN CROSSLINK REPAIR



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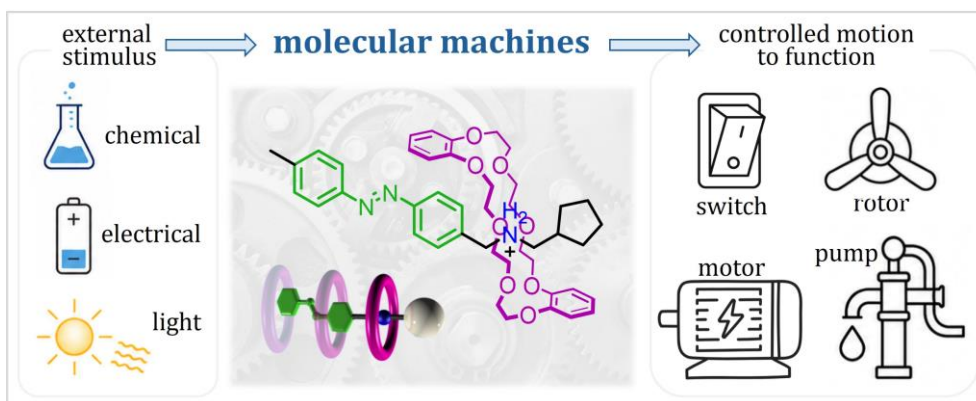


MOLECULAR MACHINES: CONTROLLED MOTION AT NANOSCALE

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Molecular machines are complex systems composed of one or more molecules that undergo controlled motion in response to an external stimulus and perform a specific function [1]. Inspired by natural molecular machines, which carry out a wide range of highly specialized tasks in living organisms, scientists have sought to design, synthesize, and investigate their artificial counterparts [2]. Considering the complexity of these systems, however, their development and characterization remain highly challenging. This lecture will introduce the fundamental principles underlying the operation of molecular machines, including the conversion of chemical, light, or electrical energy into controlled directional motion at the molecular level. A brief historical overview will trace the development of this relatively young yet rapidly advancing field at the interface of supramolecular chemistry and nanotechnology, from early concepts of manipulating matter at the nanoscale to the synthesis of molecular switches, rotors, motors, pumps, and other functional systems. Finally, experimental approach to the characterization of artificial molecular machines will be demonstrated [3].



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- [2] A. Warschel, *Angew. Chem. Int. Ed.* **38** (2014) 10020–10031.
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BUILDING CASTLES IN THE SKY: THE SYNTHESIS OF POROUS MATERIALS THROUGH MECHANOCHEMISTRY

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Zeolitic Imidazolate Frameworks (ZIFs) - a class of MOFs built from tetrahedral metal centers and imidazolate linkers - appear in many different solid forms, some of which have potential for applications such as separations, gas capture, and catalysis [1]. Unfortunately, the solvothermal synthesis of ZIFs is energy intensive, low-yielding and often gives mixtures of products. Many of these drawbacks can be addressed by using mechanochemistry. Mechanochemical ZIF syntheses are fast, conducted at room temperature, quantitative in yield, independent of solubility, and create little to no waste [2]. Furthermore, the use of different additives can influence the solid form obtained in the mechanochemical reaction, presumably through templating and/or pore-filling stabilization, providing an avenue for form control [3]. We here demonstrate the use of liquids as structure-directing agents in the mechanochemical screening for solid forms of the simplest ZIF, unsubstituted zinc imidazolate (ZnIm_2). We show that multiple ZnIm_2 forms can be prepared using LAG screening, including new forms of the **crb** topology, and use previously validated periodic DFT modeling to explain the observed synthetic results [4]. This approach can then be expanded to many different functional directing agents, as well as different types of porous materials.

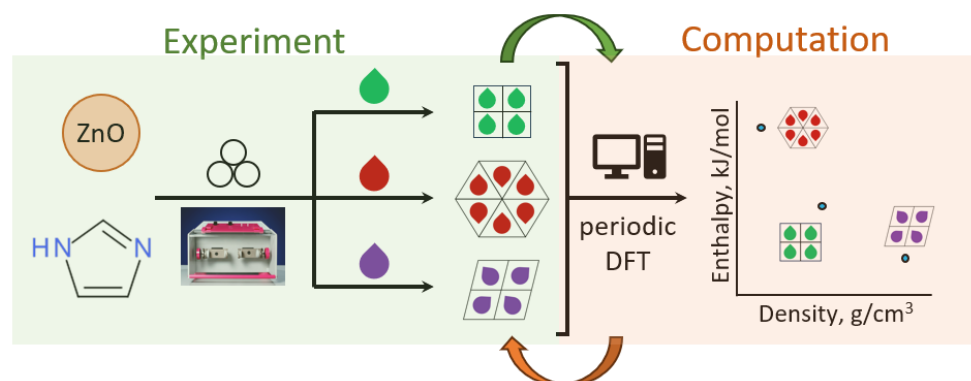


Figure 1: Schematic representation of the dependence of form outcome of the mechanochemical synthesis of ZnIm_2 on liquid additives, and the interplay of computation and experiment.

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- [4] I. Brekalo *et al.*, *J. Am. Chem. Soc.* **147** (2025) 27413–27430.







SECTION LECTURES





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

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Self-assembly of amphiphilic molecules in aqueous media provides access to a wide range of supramolecular nanostructures, including micelles, vesicles, fibers, wormlike aggregates, and others. The self-assembly in aqueous media is driven by the aggregation of hydrophobic segments as they minimize their contact with water, while the hydrophilic segments remain solvated [1]. The incorporation of a dynamic covalent bond into amphiphile structures enables the development of pH-responsive supramolecular materials. Dynamic covalent bond defines the “breaking point” of the molecule and determines its disassembly products [2]. In this work, we investigated the influence of dynamic imine bond position within amphiphile structures on the self-assembly, stability and responsiveness of their non-ionic supramolecular aggregates. Two amphiphilic structural isomers were designed and synthesized containing imine bond at different positions within the molecular framework, as well as other key structural motifs in order to obtain anisotropic aggregates. Naphthalene subunits which promote linear organization through π - π stacking interactions were also incorporated into the molecular structure. The volume ratio of hydrophilic and hydrophobic moieties was considered during the molecular design. Prepared supramolecular assemblies and their stability were characterized by suitable microscopic, thermal, and spectroscopic techniques. The location of the imine bond impacted aggregate stability and pH-responsiveness, in regard to its placement in the hydrophobic environment of the core or being exposed to the aqueous region.

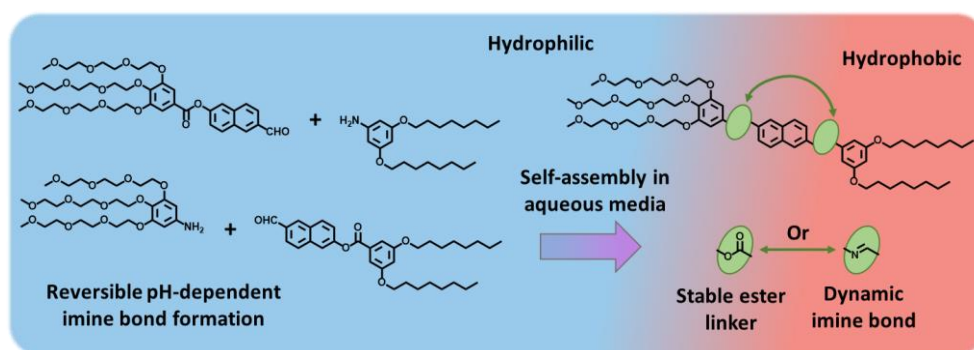


Figure 1. Non-ionic pH-dependent supramolecular assemblies in aqueous media.

ACKNOWLEDGEMENTS This work was financially supported by STARTNOW project (NPOO.C3.2.R2-I1.06.0042) funded by the NextGenerationEU (finalized on 31st of July 2026).

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[2] M. Ikeda, *Polym. J.* **51** (2019) 371.



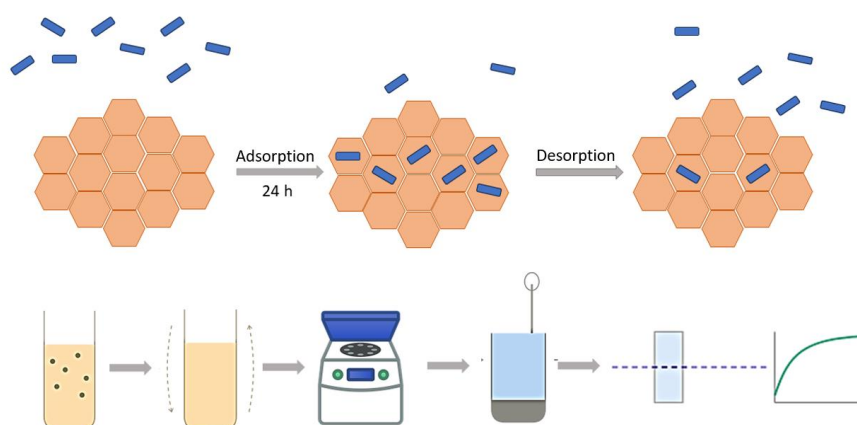


ADSORPTION OF INDOMETHACIN AND CHITOSAN ON MESOPOROUS SILICA PARTICLES

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Indomethacin is a non-steroidal anti-inflammatory drug whose low aqueous solubility limits its absorption and complicates the prediction of its behavior in the organism. Mesoporous silica particles (MSP) are highly ordered nanostructured materials characterised by a large specific surface area and pore volume, which make them excellent carriers for pharmacologically active substances, capable of improving drug solubility, enabling controlled release and reducing dosing frequency. Chitosan, a natural cationic polysaccharide obtained by partial deacetylation of chitin, is commonly used to modify the MSP surface and further improve their efficiency as carriers of active pharmaceutical ingredients, for example as an agent limiting premature drug release. In the present study, mesoporous silica particles (MSP) were investigated as potential carriers for indomethacin. The adsorption of chitosan onto MSP was investigated as a first step towards MSP modification for improvement of controlled drug release. The adsorption of indomethacin on MSP from acetone and ethanol solutions was examined by means of adsorption isotherms. The adsorption of chitosan on MSP was studied in water containing HCl (pH = 2). The particle size and ζ -potential of MSP were determined by dynamic and electrophoretic light scattering, and the desorption of indomethacin was followed *in vitro* by determining the amount of indomethacin released from MSP surface in phosphate buffer. The adsorption of indomethacin was more pronounced from acetone than from ethanol, owing to the higher solubility of the drug in this solvent. The adsorption of indomethacin onto MSP particles follows the Langmuir model, yielding the equilibrium adsorption constants and maximum surface concentrations. Desorption of indomethacin occurred almost completely within the first 24 hours, indicating a rapid release profile favourable for the application of MSP as carriers for controlled drug delivery. The adsorption of chitosan on MSP was likewise best described by the Langmuir isotherm, in accordance with monolayer formation on a homogeneous surface [1,2].



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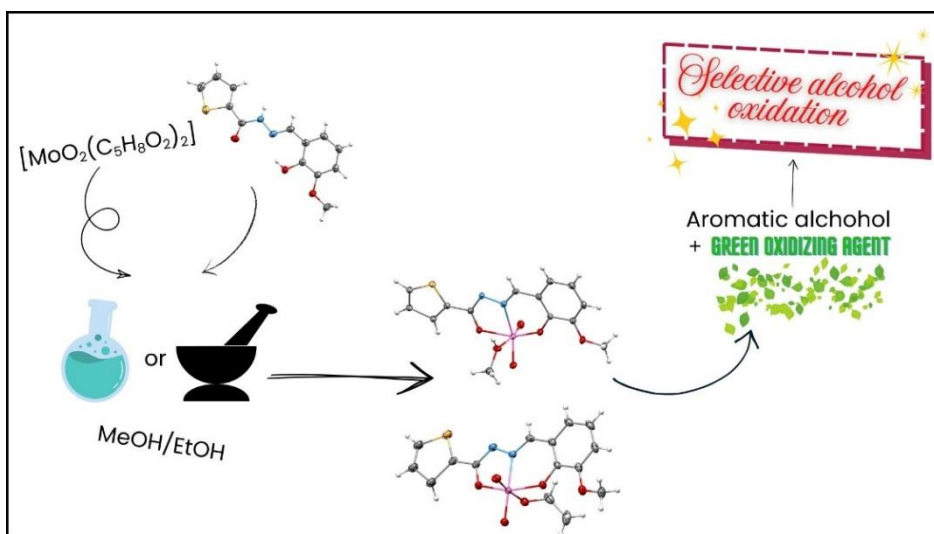
FROM MECHANOCHEMISTRY TO CATALYSIS: MOLYBDENUM(VI) SCHIFF-BASE COMPLEXES FOR SELECTIVE ALCOHOL OXIDATION

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Selective oxidation of alcohols to the corresponding aldehydes and ketones is a fundamental transformation in both fine-chemical synthesis and industrial manufacturing. However, conventional procedures frequently rely on stoichiometric quantities of hazardous oxidants and generate substantial amounts of waste, creating a demand for more selective and environmentally sustainable catalytic systems [1]. In this context, *cis*-dioxomolybdenum(VI) complexes bearing Schiff-base ligands have emerged as promising oxidation catalysts because they efficiently work with environmentally preferable oxidants, including hydrogen peroxide and *tert*-butyl hydroperoxide [1–3]. Recent studies demonstrate that their catalytic performance is governed not only by the presence of the $\{\text{MoO}_2\}^{2+}$ core but also by ligand electronics and reaction medium. Rational modification of these structural and reaction parameters can therefore provide highly active and tunable catalysts for selective alcohol oxidation under comparatively mild conditions [1–3]. The catalysts were prepared by reacting the Mo(VI) precursor $[\text{MoO}_2(\text{acac})_2]$ with a tridentate Schiff-base ligand derived from 2-hydroxy-3-methoxybenzaldehyde and thiophene-2-carboxylic acid hydrazide. Both the ligand and its Mo(VI) complexes were obtained by conventional solution-based synthesis and mechanochemistry, providing a more sustainable alternative to solvent-intensive synthetic procedures. Complexation in methanol afforded $[\text{MoO}_2(\text{L})(\text{MeOH})]$, whereas the corresponding reaction in ethanol yielded $[\text{MoO}_2(\text{L})(\text{EtOH})]$. The molecular and crystal structures of the ligand and complexes were determined by single-crystal X-ray diffraction, while additional characterisation was performed by ATR-FTIR spectroscopy, thermogravimetric analysis, differential scanning calorimetry and powder X-ray diffraction. The resulting complexes were subsequently evaluated as catalysts for the selective oxidation of aromatic alcohol using environmentally more acceptable oxidants, thereby combining greener catalyst preparation with more sustainable oxidation protocols.



[1] X. Liu *et al.*, *Afinidad* **80** (2023) 35–50.

[2] L. Pavić *et al.*, *RSC Adv.* **15** (2025) 46194–46206.

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DEOXYFLUORINATION OF CARBOXYLIC ACIDS ENABLES SYNTHESIS OF AMIDES AND SHORT PEPTIDES

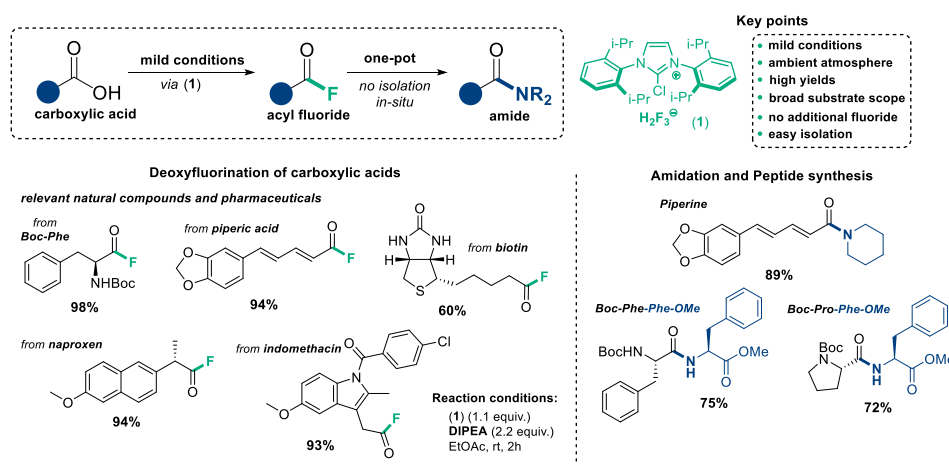
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Acyl fluorides are strategically useful carboxylic acid derivatives that combine the acyl-transfer competence of activated acid derivatives with a stability profile that is uncommon for other carboxylic acid derivatives. This balance is particularly valuable for amide-bond formation; for example, in liquid-phase peptide synthesis. Herein, we report the conversion of carboxylic acids to corresponding acyl fluorides using 1,3-bis(2,6-diisopropylphenyl)-2-chloroimidazolium dihydrogen trifluoride as a deoxyfluorination agent, as established from our previous work [1,2]. Both aliphatic and (hetero)aromatic carboxylic acids were successfully converted into the corresponding acyl fluorides with excellent yields, exhibiting high functional group tolerance, under mild conditions without the need for dry and expensive solvents. Substrates used include biologically and pharmaceutically significant carboxylic acids such as *amino acids*, *piperic acid*, *biotin*, *naproxen* and *indomethacin*, among others. The developed deoxyfluorination method is shown to be comparable to, or even outperforming, existing literature methods. Furthermore, a simple one-pot synthesis of amides via *in situ* generated acyl fluorides is demonstrated on the naturally occurring compound *piperine* and translated to liquid-phase peptide synthesis on two relevant dipeptides, namely Boc-Pro-Phe-OMe and Boc-Phe-Phe-OMe, with high yields and easy isolation without the need for column chromatography. X-Ray crystal structure of the obtained dipeptide after Boc-deprotection showed retention of stereochemistry, further emphasising synthetic applications.



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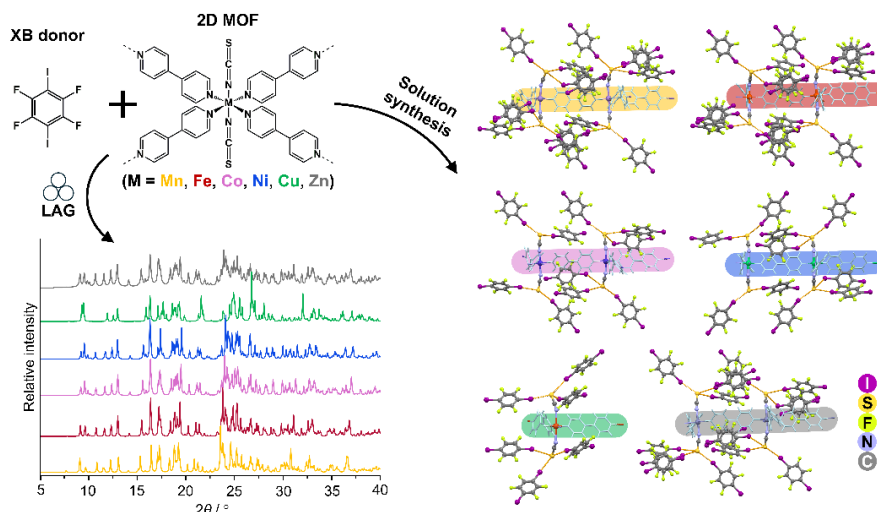
HALOGEN-BONDED COCRYSTALS OF TWO-DIMENSIONAL Mn(II), Fe(II), Co(II), Ni(II), Cu(II) AND Zn(II) METAL-ORGANIC FRAMEWORKS

Viktor Delač¹, Jogirdas Vainauskas², Vinko Nemec¹, Tomislav Friščić²,
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Metal-organic frameworks (MOFs) are among the most extensively studied materials of the 21st century, thanks to their high porosity and interesting magnetic, electrical, and catalytic properties [1,2]. One way of modifying the properties of a compound, commonly employed in crystal engineering, is through cocrystallization [3]. Such an approach has recently gathered significant popularity in the design of metal-organic systems and general strategies have been developed for the design of multi-component crystals based on halogen bonds [4]. However, no examples of halogen-bonded cocrystals in which one of the components is a metal-organic framework have been reported to date. Hence, the aim of this research was to prepare a series of cocrystals comprising a halogen bond donor 1,4-diiodotetrafluorobenzene (**14tfib**) and a 2D metal-organic framework $[M(4,4'\text{-bipyridine})_2(\text{NCS})_2]_n$ ($M = \text{Mn}^{2+}$, Fe^{2+} , Co^{2+} , Ni^{2+} , Cu^{2+} , Zn^{2+}). The X-ray structural analysis revealed that five out of six prepared cocrystals were isostructural, the copper(II) cocrystal being an exception. It is also evident that the dominant supramolecular interactions in all cocrystals are $\text{I}\cdots\text{S}$ halogen bonds between isothiocyanate sulphur and halogen bond donor iodine atoms, through which **14tfib** molecules connect adjacent layers in the framework. Thermogravimetric analysis has shown that the metal centre substitution has a significant effect on the thermal stability of the cocrystals.



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





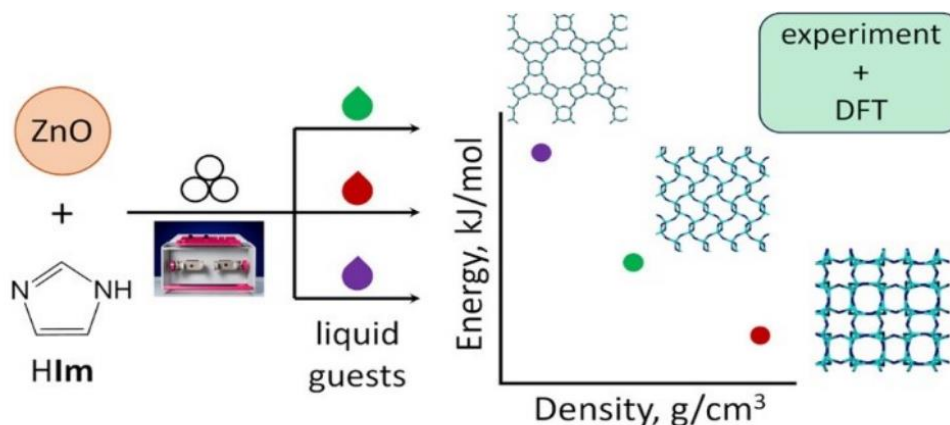
MECHANOCHEMICAL SYNTHESIS OF ZEOLITIC IMIDAZOLATE FRAMEWORKS USING STRUCTURE-DIRECTING LIQUID ADDITIVES AND THEIR ACTIVATION

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



[1] J. M. Marret *et al.*, *Adv. Mater.* **37**(52) (2025) 2418707.

[2] P. J. Beldon *et al.*, *Angew. Chemie Int. Ed.* **49** (2010) 9640.

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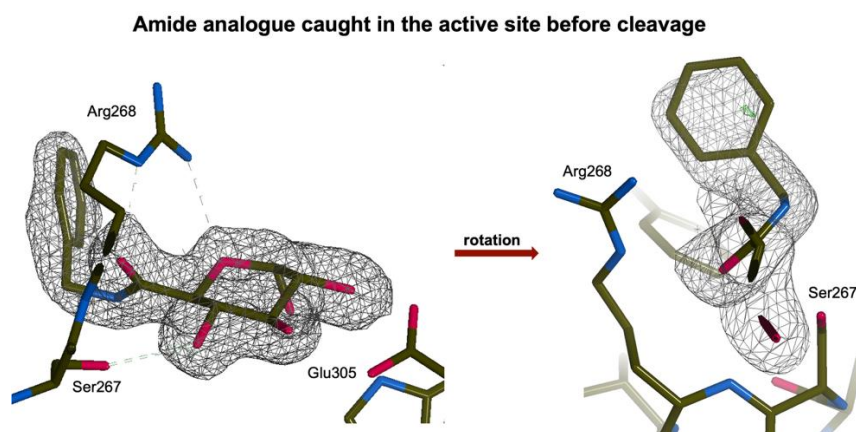
AMIDE DERIVATIVES FOR FUNCTIONAL AND STRUCTURAL STUDIES OF CE15 GLUCURONOYL ESTERASES

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Covalent lignin–carbohydrate complexes (LCCs) are a principal obstacle to the enzymatic deconstruction of lignocellulosic biomass. Of their canonical linkages only the uronic-acid ester between (4-*O*-methyl-)glucuronic acid substituents of xylan and lignin is targeted by a dedicated enzyme family, the glucuronoyl esterases of carbohydrate esterase family 15 (CE15). Despite extensive characterisation of CE15, no pre-reactive Michaelis complex with an intact lignin-like substrate has been crystallised, because soaking experiments, even with catalytically impaired variants, preferentially captures post-reactive states [1]. Here the scissile ester was replaced by an amide and the analogue characterised kinetically and crystallographically using *Ot*CE15A from *Opitutus terrae*. Contrary to expectation, *N*-benzyl-D-glucuronamide — which differs from the ester substrate benzyl D-glucuronate only in the scissile bond — was hydrolysed by the wild type, with $K_m = 6.68 \pm 0.35$ mM, $k_{cat} = 4.99 \pm 0.17$ s⁻¹ and $k_{cat}/K_m = 0.747 \pm 0.047$ s⁻¹ mM⁻¹, approximately sixfold below the value reported for the ester [2,3]; the loss was driven by turnover rather than by binding. D-glucuronamide, another amide analogue, was likewise cleaved, while a screen of CE15 homologues found some that could and some that could not cleave amide bonds. No CE15 enzyme had previously been reported to act on a non-ester substrate. Nevertheless, the analogue was trapped intact in the catalytically impaired H408A variant: two independent structures, refined at 1.4 and 1.9 Å, gave the first crystallographic view of an aromatic substituent in the *Ot*CE15A aglycone subsite. Amide analogues therefore proved useful for capturing an intact ligand in a CE15 active site, and more faithful lignin mimics are the natural next test.



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UTILIZING HYDROGEN BONDING FOR REACTIVITY SUPPRESSION: A STUDY OF SYNTHETICALLY USEFUL VISIBLE-LIGHT-GENERATED CARBENES

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Utilization of carbenes as highly reactive intermediates has proven to be a valuable method for rapid construction of a diverse carbon scaffold. Thus, a number of innovative methods regarding their *in situ* generation were consequently developed. Such a method is the visible-light-induced generation of carbenes from diazoesters – a high-yielding transformation under mild conditions [1]. This method was readily applied in generating substituted norcaradienes, which can further undergo oxidation and ultimately provide synthetically valuable, highly functionalized compounds (Figure 1a) [2]. Although the mentioned carbenes are nowadays easy to generate, directing their reactivity remains a challenge. In this work, we explored means of directing their selectivity in a diversely functionalized system (Figure 1b). With carbazole as a model substrate, a series of organic bases and inorganic salts were utilized to investigate hydrogen bonding as a method of transient non-covalent protection. Furthermore, carbazole's reactivity relative to previously investigated carbene-trapping agents was explored to screen functionalities which can further be selectively reacted upon.

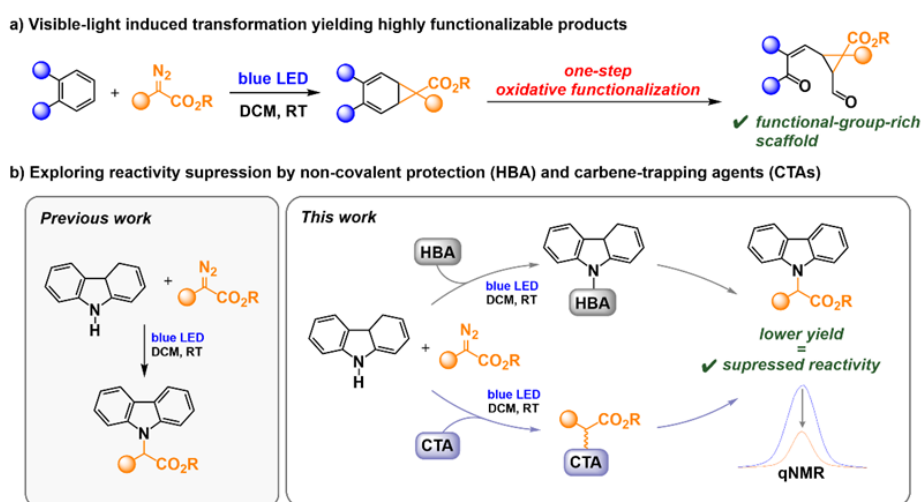


Figure 1. a) Implementing photochemically generated carbenes in constructing highly functionalized synthetic precursors; b) investigating possibilities for carbazole reactivity suppression by applying transient non-covalent protection and carbene-trapping agents.

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THE LEVEL OF NITRIC(II) OXIDE IN PLASMA SAMPLES COLLECTED FROM HEALTHY RESIDENTS FROM ZAGREB AND VINKOVCI IN TWO SEASONS

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Katarina Matković², Luka Kazensky², Mandica Sanković³, Antun
Šumanovac⁴

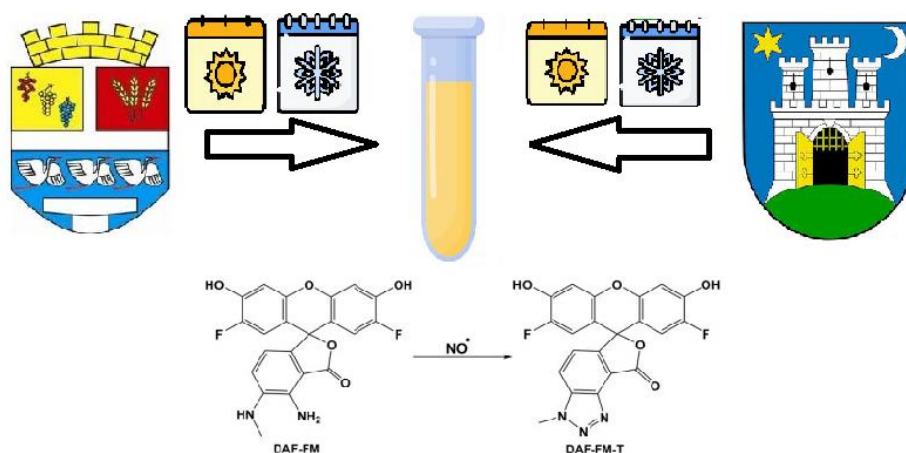
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Nitric oxide (NO) has numerous beneficial effects on the human body, among which is its vasodilatory role. However, excessive amounts of NO contribute to the development of oxidative stress. Therefore, estimating NO levels indicates the level of oxidative stress. The first aim of this study was to optimise method for reliable detection of NO in plasma. In the next step, the method was applied to human plasma samples collected in two cities, Zagreb and Vinkovci, in order to estimate a difference between the NO level of the residents of two cities with different pollution burdens during colder and warmer periods of the year. The plasma NO level was assessed fluorometrically using nonfluorescent probe 4-amino-5-methylamino-2',7'-difluorescein (DAF-FM) that react with NO forming a fluorescent benzotriazole (DAF-FM-T) [1]. The fluorescence of DAF-FM-T was estimated using plate reader set at excitation/emission: 485/525 nm. Obtained results were statistically evaluated applying *t*-test (Excel, MS Office). The NO level in plasma of residents from Zagreb was higher in the colder season (1965267 ± 1319827 RFU) than in the warmer season ($1,34466 \times 10^6 \pm 7,58087 \times 10^5$ RFU; $p = 0,006$). In contrast, plasma NO levels of residents from Vinkovci was higher in the warmer season ($1,081519 \times 10^6 \pm 5,33293 \times 10^5$ RFU) than in the colder season ($9,01366 \times 10^5 \pm 4,02368 \times 10^5$ RFU; $p = 0,046$). Furthermore, higher plasma NO levels were observed in the plasma of residents from Zagreb during both the colder and warmer seasons, compared with those detected in the plasma of residents of Vinkovci during the colder and warmer seasons. The results might suggest that Zagreb residents may be exposed to higher levels of environmental pollutants (e.g. air pollutants) typical of urban areas compared to residents of Vinkovci, who live in a more rural area with a different pollutant profile. It should be emphasised that differences in NO levels can also be influenced by other factors related to the living and working environment, as well as the lifestyle habits of the subjects themselves.



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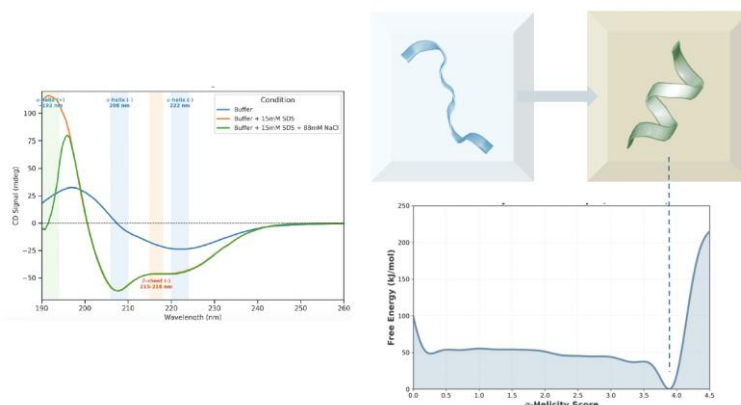


STRUCTURAL DYNAMICS AND MEMBRANE INTERACTION OF NOVEL PEPTIDE-PORPHYRIN CONJUGATES WITH ANTIMICROBIAL POTENTIAL

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Antimicrobial peptides (AMPs) are considered a promising solution to the global concern of growing bacterial antibiotic resistance, as their membrane-targeting mode of action was determined to be energetically costly to repair and less likely to induce resistance [1]. Likewise, porphyrins are recognized as viable therapeutics against bacteria through both light-activated reactive oxygen species production and light-independent membrane disruption [2]. To improve stability and therapeutic profiles of both drug classes, the conjugation of AMPs with porphyrins to form peptide-drug conjugates (PDCs) offers a compelling paradigm to achieve a synergistic effect, solubilize the porphyrin, and shield the peptide from protease-induced degradation. In this study, four AMPs with different modes of action were synthesized and conjugated with one of two studied protoporphyrin-like structures at either C- or N-terminal position. Because the exact biophysical impact of attaching a hydrophobic porphyrin ring on the peptide's structural dynamics and membrane interaction is poorly understood, a combined experimental and computational approach was utilized, integrating Circular Dichroism (CD) spectroscopy, Nuclear Magnetic Resonance (NMR), and Molecular Dynamics (MD) simulations. Spectroscopic measurements revealed environment-dependent differences in peptide structure, with both sequence and porphyrin identity influencing the observed conformational preferences. Porphyrin conjugation was associated with pronounced changes in the observed secondary-structure signatures. Furthermore, NMR measurements revealed residue-specific perturbations consistent with a defined spatial relationship between the peptide backbone and the conjugated porphyrin. Unbiased all-atom MD simulations and metadynamics were subsequently used to resolve the structural and thermodynamic basis of these observations in aqueous and membrane-mimicking environments. Together, the results indicate that porphyrin conjugation can reshape peptide conformational dynamics in a sequence- and environment-dependent manner, with the porphyrin moiety additionally providing a basis for supramolecular organization.



ACKNOWLEDGEMENTS This research was funded by the European Union – NextGenerationEU – PANTERA: "Peptidni Antimikrobni Novi Terapeutici za Eliminaciju Rezistencije Antibiotika" – uniri-iz-25-31.

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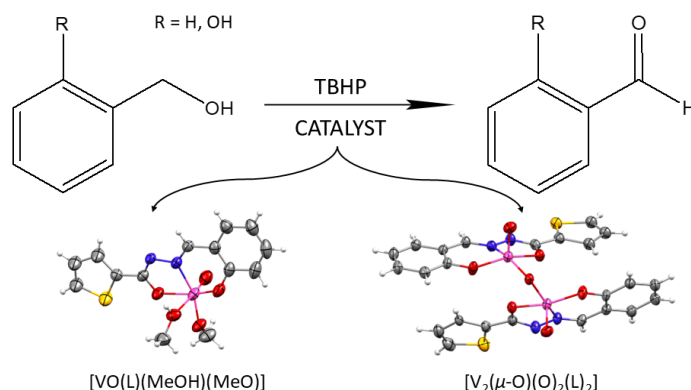


THE INFLUENCE OF THE STRUCTURE OF VANADIUM(V) COORDINATION COMPLEXES WITH A HYDRAZONE LIGAND ON THE CATALYTIC OXIDATION OF AROMATIC ALCOHOLS

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Vanadium(V) complexes have attracted considerable interest as oxidation catalysts because of the metal's variable oxidation states, flexible coordination geometries, pronounced oxophilicity, and Lewis acidity [1]. These properties contribute to the ability of vanadium complexes to promote oxidation reactions using oxidising agents such as hydrogen peroxide and *tert*-butyl hydroperoxide (TBHP) [2]. Their catalytic behaviour is, besides the metal centre, strongly affected by the ligand environment, which influences the stability, redox properties, selectivity, and reactivity of the metal complex [3]. In this work, vanadium(V) complexes containing a hydrazone ligand were prepared, structurally characterised, and evaluated as catalysts for the oxidation of aromatic alcohols. The hydrazone ligand **H₂L** was synthesised by condensation of salicylaldehyde and thiophene-2-carboxylic acid hydrazide using both solution-based and mechanochemical methods. Reaction of the ligand **H₂L** with [VO(C₅H₇O₂)₂] afforded the mononuclear complex [VO(L)(OMe)(MeOH)] in methanol, whereas the dinuclear complex [V₂O₃(L)₂] was obtained from acetone, acetonitrile, and dichloromethane. The molecular and crystal structures of the ligand and complexes were determined by single-crystal X-ray diffraction, while additional characterisation was performed by ATR-FTIR spectroscopy, thermogravimetric analysis, differential scanning calorimetry, and powder X-ray diffraction. Catalytic activity was investigated for the oxidation of benzyl alcohol (both with and without acetonitrile) and salicyl alcohol with acetonitrile, using aqueous TBHP as the oxidising agent. Reactions were monitored by gas chromatography. Both complexes exhibited good activity in the investigated oxidation reactions, while their performance depended on the used substrate and added cosolvent. The mononuclear complex exhibited higher catalytic activity in the oxidation of salicyl alcohol than the dinuclear complex, indicating that catalytic performance was governed not only by the number of vanadium centres but also by their accessibility, coordination environment, and interactions with the substrate and oxidant.



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HALOGEN-BONDED COCRYSTALS OF NITROGEN-CONTAINING ACCEPTORS AND IMINES DERIVED FROM PERHALOGENATED ANILINES

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Halogen bond is a highly directional noncovalent interaction that has been shown as a reliable tool in crystal engineering of multicomponent crystals [1]. The vast majority of research has been focused on studying *classic* organic perhalogenated compounds as halogen bond donors and various organic and metal-organic compounds as halogen bond acceptors [2]. While many of the studied multicomponent systems contain imines as halogen bond acceptors, only a few examples have been reported in which imines act as halogen bond donors [3]. In this research, the halogen bond donor potential of four novel imines with a perhalogenated periphery was investigated. The imines were synthesised from two perhalogenated anilines, 2,3,5,6-tetrafluoro-4-bromoaniline (**btfa**) and 2,3,5,6-tetrafluoro-4-iodoaniline (**itfa**), and two brominated derivatives of salicylaldehyde, 5-bromosalicylaldehyde (**5Brsal**) and 3,5-dibromosalicylaldehyde (**35dBrsal**). To assess their halogen-bond donor potential, cocrystal screening was performed with three selected nitrogen-containing acceptors, (*N,N*-dimethylaminopyridine (**dmap**), 1,4-diazabicyclo[2.2.2]octane (**dabco**) and 4,4'-bipyridine (**bpy**), using a mechanochemical approach and crystallization from solution. The resulting products were characterized by X-ray diffraction methods and thermal analysis. The mechanochemical experiments yielded 10 novel products, whereas solution crystallization afforded five cocrystals, whose crystal structures were determined. The five cocrystals were: (**itfa5Brsal**)(**dmap**), (**itfa5Brsal**)₂(**bpy**), (**itfa5Brsal**)₂(**dabco**), (**btfa35dBrsal**)(**bpy**), and (**itfa35dBrsal**)₂(**dabco**). Crystal structure determination revealed that all five cocrystals feature halogen bonds, either I $\cdots$ N or Br $\cdots$ N. The cocrystals of 2:1 stoichiometry exhibit molecular trimers consisting of two imine molecules and one acceptor molecule interconnected by halogen bonds, whereas the cocrystals of 1:1 stoichiometry exhibit discrete halogen-bonded dimers. The results obtained so far indicate that, among the four studied imines, those derived from **itfa** exhibit a greater halogen bond donor potential than those derived from **btfa**.

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PHOTOPHYSICAL CHARACTERIZATION OF QUINAZOLINE-DERIVED ESIPT EMITTERS

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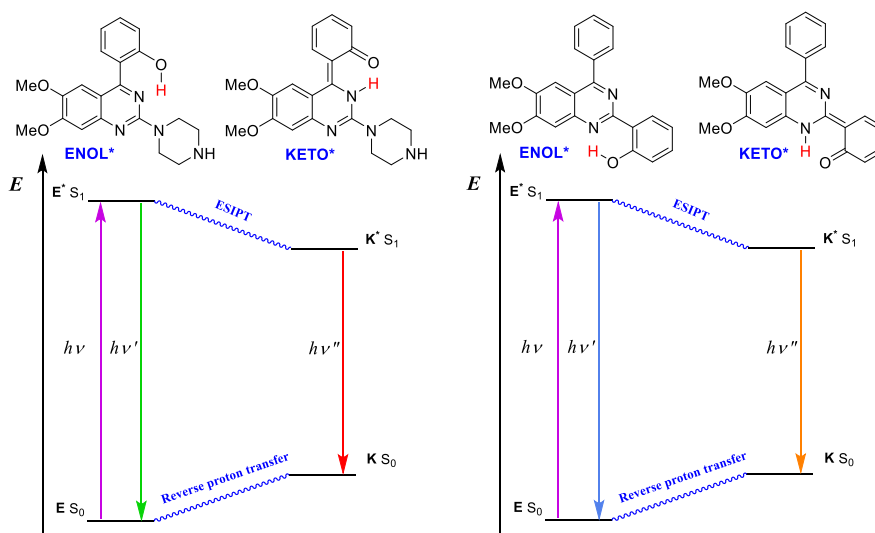
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Excited state intramolecular proton transfer (ESIPT) is a rapid photochemical process in which a molecule absorbs light, becomes electronically excited into an excited singlet state S_n , and transfers a proton between a donor group and an acceptor group within the same molecule. After proton transfer, the electronically excited molecule in its keto form returns to the ground state S_0 , emitting a red-shifted fluorescence band, followed by a reverse proton transfer that regenerates the enol form. ESIPT depends on various factors, such as solvent polarity, viscosity, proticity, intramolecular hydrogen bond strength, molecular conformation and pH [1]. The development of ESIPT-based emitters has been the subject of thorough investigation due to their potential applications as molecular sensors and lighting materials [2]. In this work, an overview of the photophysical properties of ESIPT-based emitters with a quinazoline backbone is given. The derivatives were characterised using steady-state and time-resolved absorption and emission spectroscopy in both solution and the solid state, along with computational support. Furthermore, the impact of solvent properties on fluorescence was analysed giving insights into the factors governing the emissive behaviour of the investigated quinazoline derivatives.



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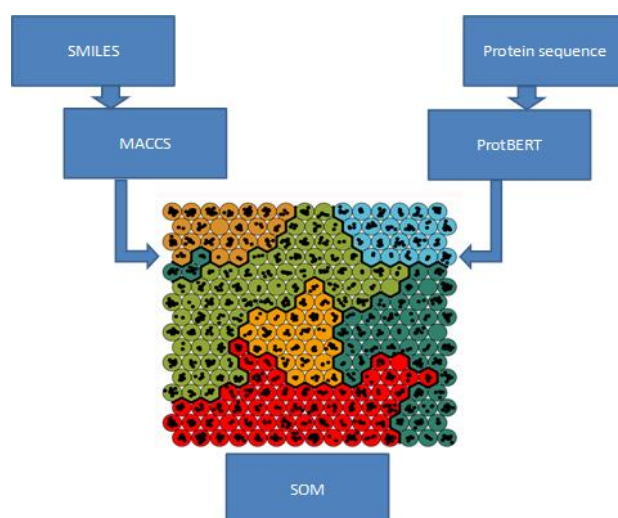


EXPLORING PHARMACOLOGICAL SPACE THROUGH SELF-ORGANIZING MAPS (SOMs)

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Prevalent computational methods used in drug design focus more often than not on well-established structure-activity analysis, with little regard towards target profiling [1]. Starting from the lock-and-key model we assumed target structure could provide relevant information about mechanisms of action. Thus, we developed a bi-layer self-organizing map (SOM) model in which drug molecules are encoded using MACCS fingerprint, while the second layer integrates ProteinBERT-derived (Protein Bidirectional Encoder Representations from Transformer) vectors to capture receptor-level sequence features [2,3]. The dual layer SOM treats the layers equally in weight and preserves the domain-specific topologies, thus allowing structurally different compounds to be associated with similar targets. Model performance was evaluated through two standard SOM metrics: quantization error, which measures how well the map represents the input data, and topographic error which measures how closely the topology of input space is preserved. Analysis of the five regions revealed differentiations based on molecular size, target class and lipophilicity. This model was used post-training on a small number of drugs currently in clinical trials. Mapping new compounds hinted rational data placement either through structural similarity or usage similarity with their neighbours.



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SYNTHESIS OF NOVEL MANNOSYLATED TRIAZOLE-CONTAINING DESMURAMYL PEPTIDES

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Lipophilic mannosylated derivatives of desmuramyl peptide (L-Ala-D-*iso*Gln, DMP) and their adjuvant activity are the subject of our long-term research [1,2]. The mannose subunit is attached to the amino group of L-Ala, while lipophilic subunits, such as adamantyl, cholesteryl or alkyl chains, are introduced to the α - or γ -position of *iso*Gln. Introduction of a triazole moiety as a linker in drug design, in general brings several advantages due to its stability in solution and ability to form specific interactions with various biological targets [3]. Previous studies demonstrated that incorporation of a triazole linker between a lipophilic substituent and the α -position of *iso*Gln can result in compounds with pronounced *in vivo* adjuvant activity. In this work, an alternate positioning of the triazole subunit between the mannose residue and the DMP pharmacophore was explored. A functionalized mannosylated triazole-containing building block containing a terminal carboxyl group was synthesized and coupled with various DMP derivatives containing different lipophilic chains to obtain a new series of mannose-triazole-DMP conjugates whose adjuvant activity is to be evaluated (Figure 1).

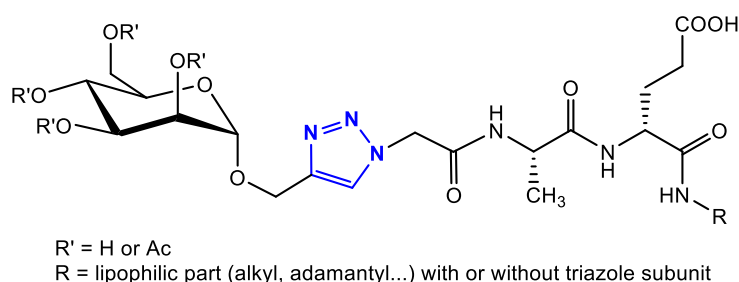


Figure 1. General structure of novel mannosylated triazole-containing desmuramyl peptides

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

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POSTER PRESENTATIONS





ADVANCED COMPOSITE PLASTERS WITH EMBEDDED PHASE CHANGE MATERIALS

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The construction sector accounts for a significant share of global energy consumption. Various studies and data indicate that buildings account for approximately 40% of total greenhouse gas emissions during their lifecycle. This figure is particularly pronounced in older building stock. Given the high energy consumption for heating and cooling, the integration of thermal energy storage systems into building envelopes is one of the key measures to improve energy efficiency and transition toward sustainable construction [1,2]. Energy reduction measures include the use of innovative materials, such as plaster with phase change materials (PCM) [2]. In this study, two different plasters were prepared. The reference sample (R) is traditional plaster made with dolomite sand, white cement and lime (volume ratio A:C:L = 6:2:1). Sample P contains an addition of PCM slurry at 30 vol.% and a partial substitution of sand with Liapor. The properties of both investigated mixtures correspond to commercial plaster. Using an optical microscope, the homogenous integration of PCM microcapsules in sample P was successfully confirmed. The thermal behaviour of the two plasters was determined using differential scanning calorimetry (DSC), with repeated heating and cooling cycles performed to evaluate the stability and reproducibility of the prepared samples. The results demonstrated consistent and reproducible thermal effects, while further testing of decomposition processes using coupled thermogravimetric analysis and quadrupole mass spectrometry (TGA-QMS) – simulating fire exposure – confirmed that no harmful gases were released during heating up to 1200 °C in air.

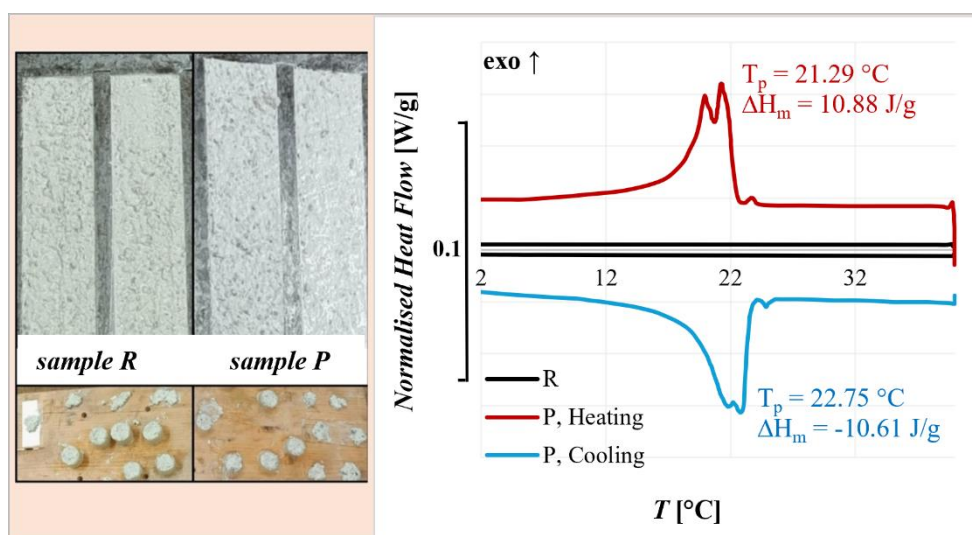


Figure 1. Images of the samples (R and P), and the measurements obtained through differential scanning calorimetry (DSC) with heating and cooling rates at 10 K/min.

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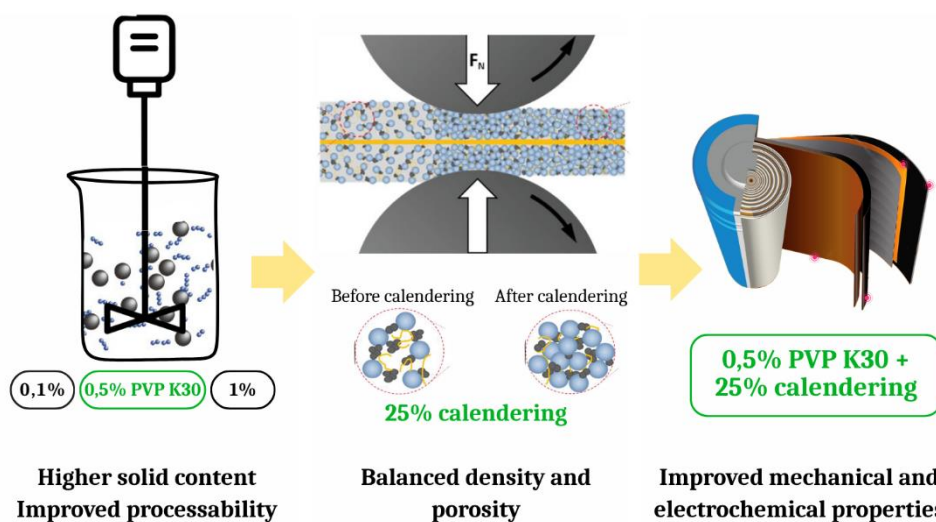


EFFECTS OF DISPERSANTS AND CALENDERING ON NMC CATHODE PERFORMANCE

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Lithium-ion batteries are currently the dominant energy storage technology due to their high energy density, long cycle life and good efficiency. Their performance is greatly influenced by electrode manufacturing parameters, especially slurry solids content [1] and electrode calendering, which affect electrode density and microstructure [2]. However, increasing the solid content while maintaining adequate processability of the slurry, as well as optimizing calendering without compromising porosity, remains a challenge in electrode manufacturing. In this work, the use of polyvinylpyrrolidone (PVP K30) as a dispersant was investigated with the aim of increasing the solids content while maintaining favorable rheological properties required for electrode fabrication. Cathodic slurry based on NMC materials were prepared with the addition of different dispersant content, and its influence on rheological properties was systematically analyzed to determine the highest achievable solids content that maintains the processability of the system. After identifying the optimal slurry composition, the prepared electrodes were calendered at different degrees of compression. Electrochemical tests were used to investigate the effect of PVP and calendering on charge transfer and cycling stability, while scanning electron microscopy (SEM) provided insight into the microstructure of the electrodes. Additionally, contact angle and adhesion measurements provided information on the influence of the dispersant and calendering on the coating quality and resulting surface properties. The results show that the addition of 0,5% PVP K30 enables an increase in the proportion of solid content, slurry homogeneity and workability while maintaining electrochemical performance. Furthermore, a calendering degree of 25% provided the optimal balance between electrode densification and porosity, leading to improved mechanical and electrochemical properties.



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

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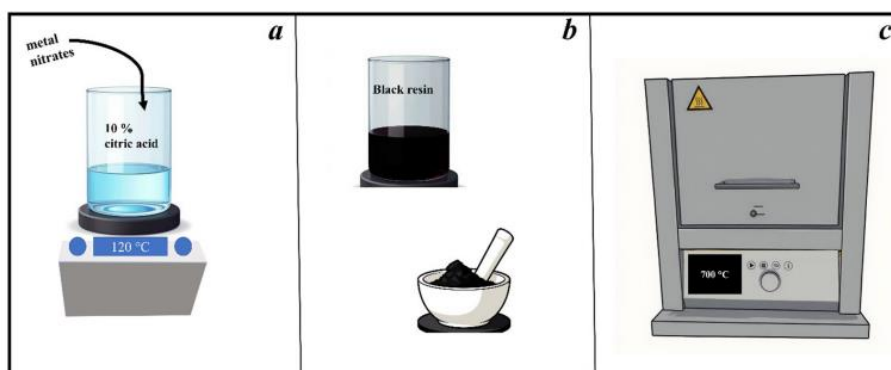


EFFECT OF Pr CONCENTRATION ON THE STRUCTURAL EVOLUTION OF CERIA-BASED HIGH-ENTROPY OXIDES

Jakov Babić, Stjepan Šarić, Dalibor Tatar, Jelena Kojčinović,
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A family of materials known as high-entropy oxides (HEOs) has attracted considerable attention due to its unique compositional complexity, structural diversity, and broad range of potential applications. These single-phase solid solutions, typically containing five or more principal metal cations, can exhibit exceptional structural stability resulting from the random distribution of cations throughout the crystal lattice [1]. In the present study, Ce–Zr–Pr–Sm–Eu-based high-entropy oxides with systematically varied Pr concentrations were synthesized using a modified sol-gel citrate method to investigate the effect of Pr incorporation on the lattice structure, defect formation, and photocatalytic performance [2]. A single-phase cubic fluorite structure was retained across all investigated compositions, while a gradual increase in lattice parameter and microstrain was observed with increasing Pr concentration, which can be attributed to the incorporation of larger Pr^{3+} ions into the crystal lattice. Morphological and surface characterization revealed the development of porous nanostructures at intermediate Pr concentrations, whereas excessive Pr incorporation resulted in increased densification and reduced surface accessibility. Spectroscopic analysis confirmed the coexistence of $\text{Pr}^{3+}/\text{Pr}^{4+}$ and $\text{Ce}^{3+}/\text{Ce}^{4+}$ redox couples, pronounced 4f–2p orbital hybridization, and an increased contribution of defect-related electronic states, resulting in a reduction of the optical bandgap. Under UV irradiation, the optimized Pr-containing composition exhibited nearly complete degradation of methylene blue within 30 minutes. This enhanced photocatalytic activity is attributed to improved charge separation and the synergistic redox cycling between Ce and Pr centers, facilitated by the reduced bandgap and increased concentration of defect-related states.



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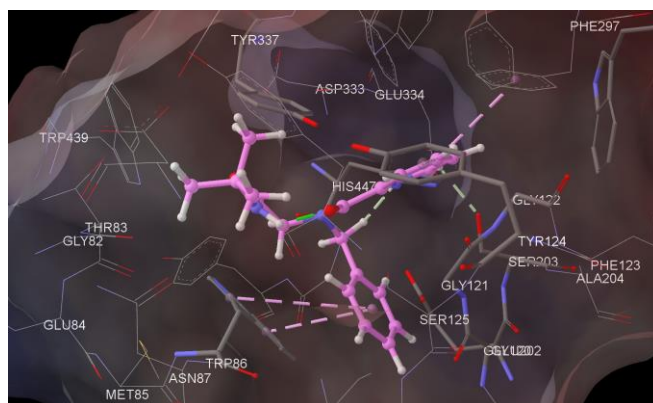


QUANTUM CHEMICAL DOCKING OF PYRIDINE UGI DERIVATIVES AS CHOLINESTERASE INHIBITORS

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Alzheimer's disease (AD) is a severe neurodegenerative disorder that causes progressive neuronal deterioration and cognitive decline. According to the *cholinergic hypothesis*, a deficiency of an important neurotransmitter, acetylcholine (ACh), caused by its inadequate biosynthesis in AD patients, drives the disease's manifestation. Two enzymes, acetylcholinesterase (AChE) and butyrylcholinesterase (BChE), catalyze the hydrolysis of ACh. Consequently, cholinesterase inhibition to maintain stable levels of ACh in the synapses and alleviate the disease's symptoms is a key strategy for AD treatment [1,2]. To identify a potent dual inhibitor of human acetylcholinesterase (hAChE) and butyrylcholinesterase (hBChE), a series of rationally designed Ugi derivatives with pyridine carboxamide motif, based on our previously investigated compounds [3,4], were evaluated *via* quantum chemical molecular docking. By systematically varying the nitrogen position within the pyridine ring, we investigated how regioisomerism affects binding affinity and orientation/interactions. To ensure accurate conformational sampling, an extensive computational protocol was employed, involving the evaluation of 5,000 single-point energy random configurations [5], from which the 1,000 lowest-energy structures underwent full geometry optimization. These were subsequently clustered and ranked by their standard enthalpies of binding. Using a combination of automated hydrogen-bond search modules and visual inspection, the key molecular interactions within both active sites were characterized. This analysis provides critical insights into the structure-activity relationship of these compounds, emphasizing the influence of the pyridine nitrogen atom position on optimizing dual inhibition. These findings will serve as a foundation for future rational design of cholinesterase inhibitors.



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

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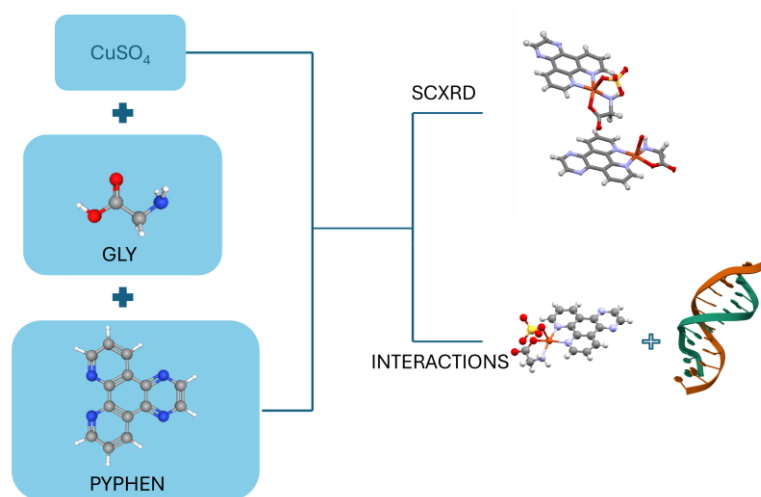


SYNTHESIS, CRYSTAL STRUCTURE AND DNA-BINDING PROPERTIES OF A TERNARY COPPER(II) COMPLEX WITH GLYCINE AND PYRAZINO[2,3-*f*][1,10]PHENANTHROLINE

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Since the introduction of cisplatin and other platinum-based compounds as antitumour therapeutics, transition-metal complexes have attracted considerable attention in cancer research [1,2]. A group of ternary copper(II) compounds containing amino acids and *N*-heterocyclic ligands has been shown to exhibit promising antiproliferative properties through interaction with double-stranded DNA [3]. This research aimed to synthesise and structurally characterise a new ternary copper(II) compound and to investigate its *in vitro* interaction with a B-DNA dodecamer (PDB code: 1BNA) [4]. A novel copper(II) compound comprising glycine (Gly) and pyrazino[2,3-*f*][1,10]phenanthroline (pyphen), $[\text{Cu}(\text{Gly})(\text{H}_2\text{O})(\text{pyphen})][\text{Cu}(\text{SO}_4)(\text{Gly})(\text{pyphen})] \cdot 6\text{H}_2\text{O}$, was synthesised, and its crystal structure was determined by single-crystal X-ray diffraction (SCXRD). The compound crystallizes in the triclinic *P*-1 space group with the unit cell parameters: $a = 7.65500(10) \text{ \AA}$, $b = 16.0940(2) \text{ \AA}$, $c = 16.7120(10) \text{ \AA}$, $\alpha = 66.1820(10)^\circ$, $\beta = 85.5420(10)^\circ$, $\gamma = 81.5850(10)^\circ$, $V_{\text{cell}} = 1862.92(4) \text{ \AA}^3$ and $Z = 2$. The asymmetric unit consists of a complex cation $[\text{Cu}(\text{Gly})(\text{H}_2\text{O})(\text{pyphen})]^+$ and a complex anion $[\text{Cu}(\text{SO}_4)(\text{Gly})(\text{pyphen})]^-$, together with six lattice water molecules. Both Cu(II) centres are five-coordinate and adopt distorted square-pyramidal geometries. Interactions with the B-DNA dodecamer were examined in solution using UV-Vis absorption spectroscopy and a *GelRed* fluorescence-quenching assay. The binding constants $K_b = 4.49 \cdot 10^4 \text{ mol}^{-1} \text{ dm}^3$ and $K_{\text{SV}} = 7.3 \cdot 10^4 \text{ mol}^{-1} \text{ dm}^3$, respectively, indicate appreciable interaction of the copper(II) compound with double-stranded DNA.



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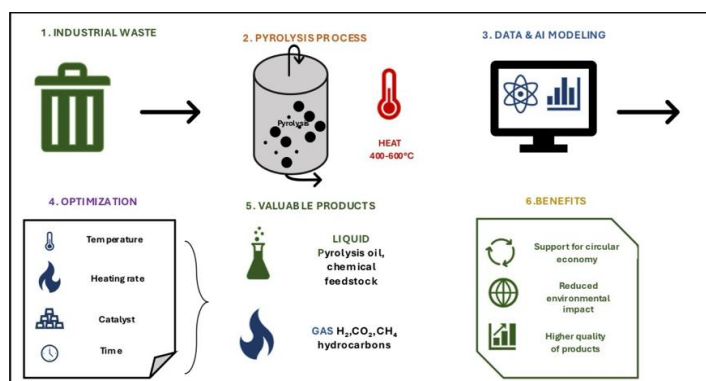


APPLICATION OF ARTIFICIAL INTELLIGENCE FOR THE OPTIMIZATION OF PYROLYSIS PROCESSES IN INDUSTRIAL WASTE VALORIZATION AND CHEMICAL FEEDSTOCK PRODUCTION

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Plastic and polymeric industrial waste was identified as a challenge for modern industry. Pyrolysis was evaluated as a process in which waste was converted into liquid, gaseous, and solid products used as fuels and chemical feedstocks. Artificial intelligence and machine learning were applied to predict product yields and optimize pyrolysis conditions using datasets. Artificial neural networks, Random Forest, and Support Vector Machines were used to analyze the effects of feedstock composition, temperature, residence time, heating rate, and catalyst properties on product distribution. Accurate predictions were obtained, while temperature and catalyst properties were identified as influential factors. Operating conditions were determined through machine learning and optimization algorithms, resulting in improved efficiency and reduced undesired product formation [1,2].



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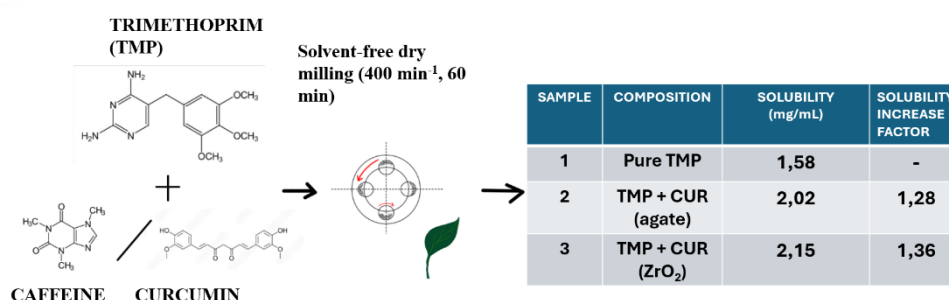


SOLID DISPERSIONS OF DRUG AND BIOACTIVE COMPOUNDS: SYNTHESIS, CHARACTERIZATION AND PHARMACEUTICAL POTENTIAL

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Trimethoprim (TMP) is a widely used antimicrobial drug belonging to Class II of the Biopharmaceutical Classification System (BCS), characterized by high membrane permeability but exceptionally low aqueous solubility, which severely limits its oral bioavailability. To overcome this biopharmaceutical hurdle without relying on synthetic co-solvents or toxic additives, solid dispersions of TMP were synthesized with natural bioactive co-formulators (curcumin and caffeine) using solvent-free dry milling in a planetary ball mill [1]. This mechanochemical approach fully complies with the principles of green chemistry, operating without organic solvents or excessive heat input [2]. Structural and thermal properties of the pure components and processed mixtures (milled in agate and ZrO₂ grinding jars at 400 min⁻¹ for 60 min) were comprehensively characterized via powder X-ray diffraction (XRPD), differential scanning calorimetry (DSC), and Fourier-transform infrared spectroscopy (FTIR). XRPD and DSC analyses demonstrated that high-energy mechanochemical activation induced structural disruption and partial amorphization of the drug within the co-formulator matrix, particularly when using ZrO₂ media. FTIR spectroscopy confirmed strong hydrogen bonding interactions in the solid state between the amino groups of TMP and the functional carbonyl/hydroxyl groups of the bioactive co-formulators. Equilibrium solubility testing in phosphate buffer (pH 6.8, 37.5 °C, 24 h) via UV-Vis spectrophotometry revealed a 1.36-fold enhancement in the apparent solubility of TMP for the ZrO₂-milled solid dispersion (reaching 2.15 mg/mL compared to 1.58 mg/mL for pure crystalline TMP). This moderate solubility boost is attributed to mechanochemically induced partial amorphization while maintaining residual crystallinity, which prevents rapid recrystallization and preserves thermodynamic stability. Overall, solvent-free mechanochemical formulation proves to be an eco-friendly and effective strategy for developing enhanced pharmaceutical dosage forms.



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

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Coordination compounds of copper(II) with amino acids and heterocyclic ligands have attracted considerable attention for their diverse structural chemistry, self-assembly capabilities, and potential applications in crystal engineering and in the development of porous materials [1]. Particular attention has been devoted to metal–organic frameworks (MOFs), which are characterized by their porosity and have been used in gas storage and separation [1,2]. One of the most important applications of MOF materials is the controlled binding and storage of water, which is particularly important given the increasing shortage of drinking water [2]. In this work, the synthesis of a novel multicomponent metal–organic framework was investigated using solvothermal and mechanochemical methods. In the crystal structure, copper(II) ions are bridged by L-asparaginate (Asn) and 4,4'-bipyridine (bpy) molecules, forming a three-dimensional framework with the formula $\{\text{Cu}_3(\mu\text{-Asn})_2(\mu\text{-bpy})_4\text{solvents}\}_n$ (**1**_{Asn}). The resulting structure contains three-dimensional channels filled with solvent molecules and nitrate ions, which together occupy approximately 61% of the unit-cell volume, with the largest pore dimensions being approximately 7.7 Å². Mechanochemical synthesis was used to investigate the possibility of preparing the same or a structurally related material with reduced solvent consumption, thereby evaluating the potential of this approach as a more sustainable alternative to conventional solution-based synthesis.

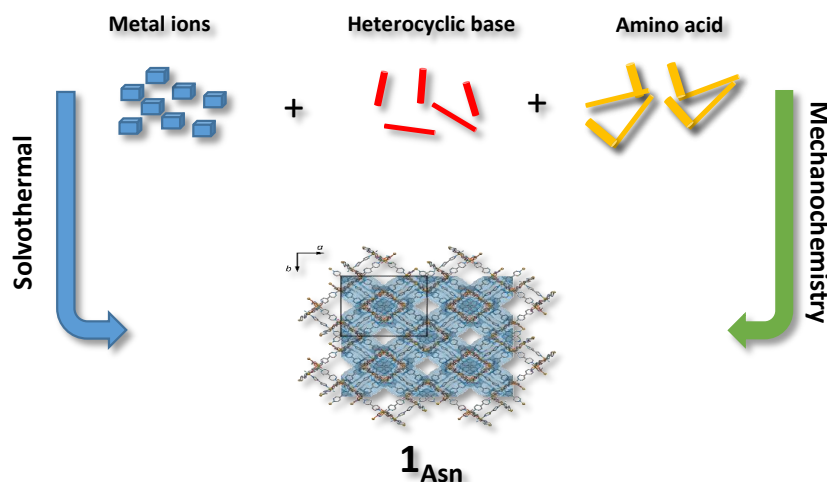


Figure 1. Schematic representation of **1**_{Asn} synthesis.

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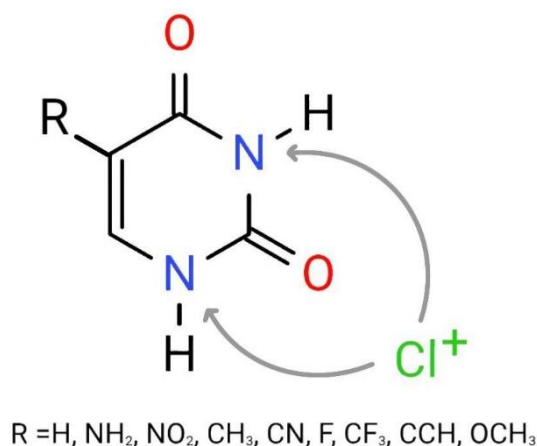


SUBSTITUENT EFFECTS IN CHLORINATION OF C5-SUBSTITUTED URACILS: A HAMMETT-TYPE DFT AND NMR STUDY

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Hypochlorous acid (HOCl) is a reactive chlorinating agent whose reactions with heterocyclic substrates are important in both synthetic and oxidative chemistry [1]. Because uracil contains multiple electronically coupled reactive sites, its chlorination provides a chemically well-defined model for examining substituent effects, competing *N*- and *C*-chlorination pathways, and the predictive value of linear free-energy relationships. In this work, the chlorination of uracil and selected C5-substituted uracils was investigated, including 5-fluorouracil and thymine, by combining experimental NMR monitoring with density functional theory calculations. Experimentally, ¹H NMR spectroscopy was used to follow substrate consumption and formation of chlorinated products. Computationally, activation barriers were calculated for competing N1- and N3-chlorination pathways, as well as pathways leading to C5-chlorinated products. The calculated activation energies were correlated with Hammett substituent constants to evaluate whether electronic substituent effects can be used to predict chlorination rates and regioselectivity. A strong linear correlation between substituent electronic properties and calculated chlorination barriers indicates that the reaction is sensitive to electron-donating or electron-withdrawing character at C5. These results support a mechanistic model in which initial nitrogen chlorination and subsequent chlorine transfer contribute to formation of the experimentally observed C5-chlorinated products. The combined NMR/DFT approach provides a molecular-level framework for predicting nucleobase chlorination under conditions relevant to food sanitation, disinfection chemistry, and HOCl-mediated biological damage.



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SYNTHESES AND CRYSTAL STRUCTURES OF MULTICOMPONENT COPPER(II) MOFS WITH L-ALANINE AND (*E*)-1,2-DI(PYRIDIN-4-YL)DIAZENE

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Metal organic frameworks (MOFs) are porous crystalline materials in which metal ions or clusters are linked by organic ligands into extended networks. Some members of the class reach BET surface areas above 6000 m² g⁻¹ [1], with applications spanning catalysis, gas adsorption and chemical sensing. Amino acids have been recognised as inexpensive, chiral and biocompatible building blocks for MOF synthesis [2]. Their combination with copper(II) and heterocyclic *N*-donor ligands was previously shown to afford architectures ranging from discrete complexes to coordination polymers [3]. In this work, two new multicomponent copper(II) MOFs were synthesised from copper(II) hydroxide, copper(II) nitrate trihydrate, L-alanine (HAla) and (*E*)-1,2-di(pyridin-4-yl)diazene (dpda) by a solution-based method using two different solvent systems: {[Cu(μ-Ala)(NO₃)(μ-dpda)]·2H₂O}_n (**1**) and {[Cu(μ-Ala)(μ-dpda)](NO₃)·solvents}_n (**2**). The products were characterised by single-crystal and powder X-ray diffraction and thermogravimetric analysis. Single-crystal XRD revealed that both MOFs crystallise as 3D coordination polymers. In **1**, water molecules of crystallisation form discrete pockets that occupy 6.6% of the unit cell volume, whereas in **2**, solvent molecules and nitrate ions form 2D channels that occupy 44% of the unit cell volume (Figure 1). The same components therefore gave two different 3D frameworks, indicating that the solvent system used for crystallisation directs which framework is obtained and how much of the unit cell is occupied by solvent molecules and nitrate ions.

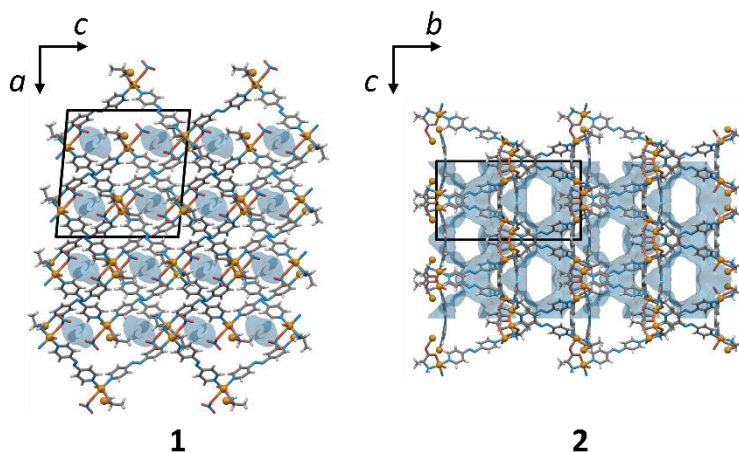


Figure 1. Crystal packing of MOFs **1** and **2**. Blue surfaces represent the surface around solvent molecules and nitrate ions (in **2**).

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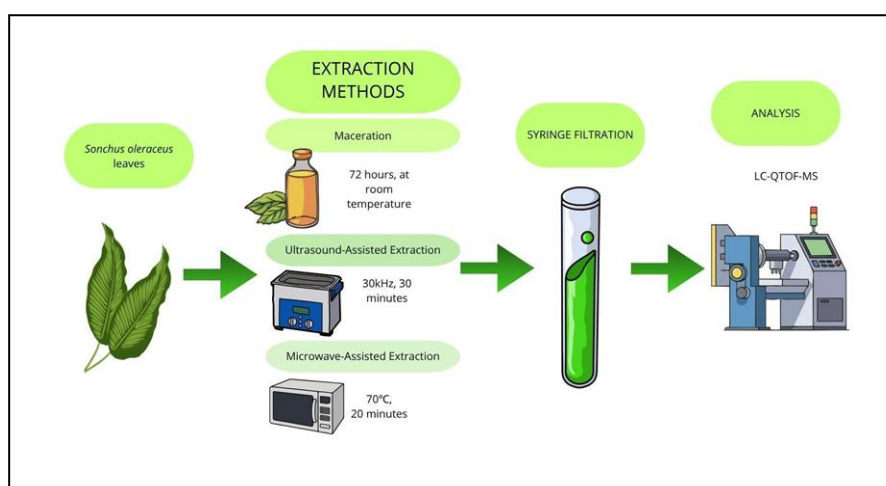


NUTRITIONAL POTENTIAL OF COMMON SOWTHISTLE (*Sonchus oleraceus* L.): INFLUENCE OF GREEN EXTRACTION METHODS

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Wild edible plants, though historically central to traditional European diets, are increasingly marginalised as weeds. This study focuses on common sowthistle (*Sonchus oleraceus* L.), a key species in “mišanca”, a traditional spring mixture of foraged wild greens from the Croatian region of Dalmatia. The aim of this research is to evaluate the nutritional potential of *S. oleraceus*, with qualitative and quantitative analysis of polyphenolic compounds. Emphasis is placed on the application of green extraction methods, such as Ultrasound-Assisted Extraction (UAE) and Microwave-Assisted Extraction (MAE), and their influence on the detection of polyphenolic compounds [1]. One of the aims of this study was to compare traditional extraction methods with “greener” ones and to obtain insight into whether traditional methods are equally successful, or whether the “greener” ones yield the same results or even better. Plant material was collected and sorted into categories according to sample preparation (fresh, freeze-dried, dried, etc.). Aliquots of the material were extracted using various solvents, followed by centrifugation and filtration to remove particulate matter. The resulting extracts were analysed using liquid chromatography coupled with quadrupole time-of-flight mass spectrometry (LC-QTOF-MS). High-resolution mass spectrometric data were acquired in negative electrospray ionisation mode to obtain accurate mass measurements and characteristic fragmentation patterns. The resulting spectral profiles were processed for peak detection, alignment and annotation of metabolites based on accurate mass, isotope distribution and MS/MS fragmentation data. Comparative analysis of the extraction methods applied provides insight into how green methods affect the result. The findings may contribute to the assessment of wild edible plants as alternative food resources and support further investigations into their potential as staple components of diets in the future.



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DIASTEREOSELECTIVE SYNTHESIS OF PHENYL-SUBSTITUTED ALDONOLACTONE DERIVATIVES VIA DOUBLE GRIGNARD ADDITION

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Monosaccharides and monosaccharide derivatives represent valuable sources of chirality in organic synthesis and are employed both as synthetic precursors for the preparation of complex molecules and as chiral auxiliaries in asymmetric synthesis [1]. Their utility arises from their rich stereochemical diversity and the ease with which they can be transformed into a variety of cyclic and acyclic structures [2]. In this study, selected aldono-lactones were investigated as substrates for the development of a new synthetic methodology based on diastereoselective double Grignard addition. The reaction conditions for the double addition were optimized, establishing a protocol in which phenylmagnesium bromide was employed as the first Grignard reagent. The scope of the developed methodology was subsequently evaluated using a range of aliphatic and aromatic Grignard reagents as the second Grignard reagent. This approach afforded several previously unreported phenyl-substituted D-ribonolactone derivatives and one phenyl-substituted D-arabinolactone derivative. The use of aliphatic Grignard reagents resulted exclusively in the formation of a single diastereomer, whereas the aromatic D-ribonolactone derivatives were isolated as mixtures of diastereomers. In the reaction with *p*-tolylmagnesium bromide, altering the order of reagent addition enabled modulation of the diastereoselectivity, highlighting the importance of the reaction sequence in determining the stereochemical outcome.

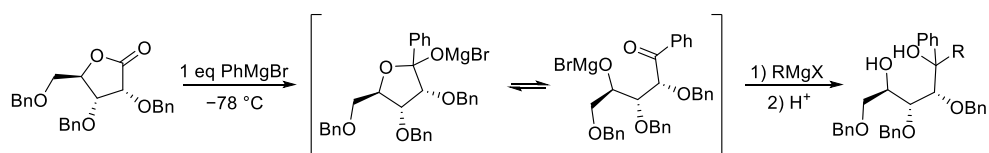


Figure 1. Phenyl-substituted D-ribonolactone derivative synthesis via established protocol.

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LOW-DIMENSIONAL HYBRID HALOCUPRATES(II) BASED ON PARA-SUBSTITUTED BENZYLAMINES

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Hybrid organic-inorganic halide perovskites constitute a versatile class of materials with the general formula A_nMX_m , comprising organic cations (A), metal cations (M), and halide anions (X = Cl⁻, Br⁻, I⁻) [1]. Appropriate selection of these building blocks enables the formation of structurally diverse architectures, ranging from three-dimensional (3D), two-dimensional (2D), one-dimensional (1D), and zero-dimensional (0D) frameworks [2,3], each exhibiting specific physicochemical properties suited for specific applications. In this study, two *para*-substituted benzylamines, namely 4-hydroxybenzylamine and 4-methoxybenzylamine, were investigated as organic components of halocuprate(II) hybrids. The presence of hydroxyl group in 4-hydroxybenzylamine, which acts as a hydrogen-bond donor, led to the formation of a 0D hybrid (Figure 1a), whereas 4-methoxybenzylamine yielded 2D structures, highlighting the role of the organic cation as a structure-directing agent (Figure 1b). Moreover, reactions with CuBr₂ yielded, in some cases, products brominated at position 3 of the benzene ring, highlighting the influence of copper(II) in this type of organic reaction. All isolated compounds were characterized by infrared spectroscopy, thermogravimetric analysis (TGA), and differential scanning calorimetry (DSC), and their molecular and crystal structures were elucidated by single-crystal X-ray diffraction.

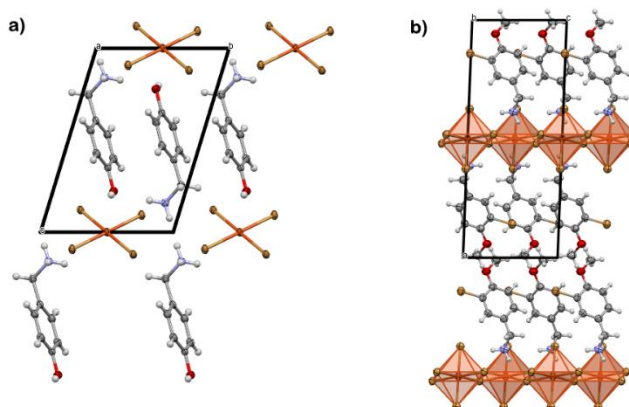


Figure 1. Crystal packing in: a) $(C_7H_{10}NO)_2[CuBr_4]$ viewed down the crystallographic *a*-axis and b) $(C_8H_{11}NOBr)_2[CuBr_4]$ viewed along the crystallographic *b*-axis.

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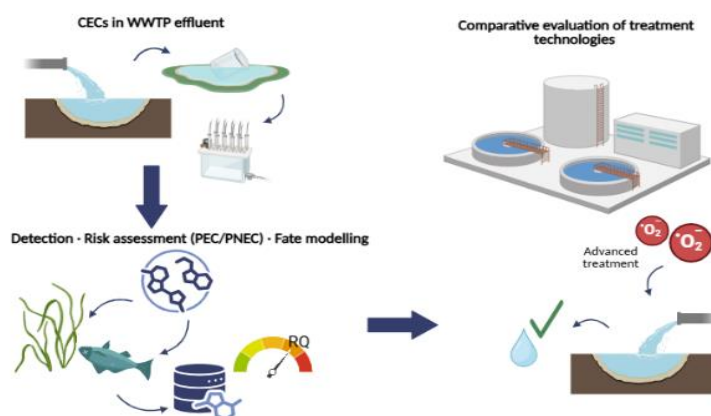
ENVIRONMENTAL FATE AND RISK ASSESSMENT OF CONTAMINANTS OF EMERGING CONCERN IN WASTEWATER: A COMPARATIVE STUDY OF SLOVENIAN AND PORTUGUESE TREATMENT SYSTEMS

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Contaminants of emerging concern (CECs) including pharmaceuticals, UV filters, and industrial chemicals are increasingly detected in aquatic environments due to their persistence and incomplete removal in conventional wastewater treatment plants (WWTPs). Previous monitoring of Slovenian coastal waters detected UV filters avobenzone and octocrylene, the pharmaceutical telmisartan, the industrial chemical TBP and the pesticide diflufenican using SPE and UHPLC-MS/MS in the south-eastern Bay of Trieste. Building on these findings, this study presents an environmental risk assessment and treatment efficiency evaluation for five priority compounds. Risk was quantified using the PEC/PNEC approach, with PNEC values derived from ecotoxicological databases (ECOTOX, ECHA). Octocrylene was the only compound exceeding the high-risk threshold ($RQ = 1.58$), while diflufenican showed moderate risk ($RQ = 0.46$). Environmental fate modelling revealed high bioaccumulation potential for UV filters ($BCF > 1000$), highlighting the limitations of conventional activated sludge for hydrophobic CECs. Treatment technologies including MBR, ozonation and AOP were evaluated based on compound physicochemical properties. A comparative analysis of CEC removal efficiency between Slovenian and Portuguese WWTPs was additionally conducted, providing a broader European perspective on current treatment challenges [1–3].



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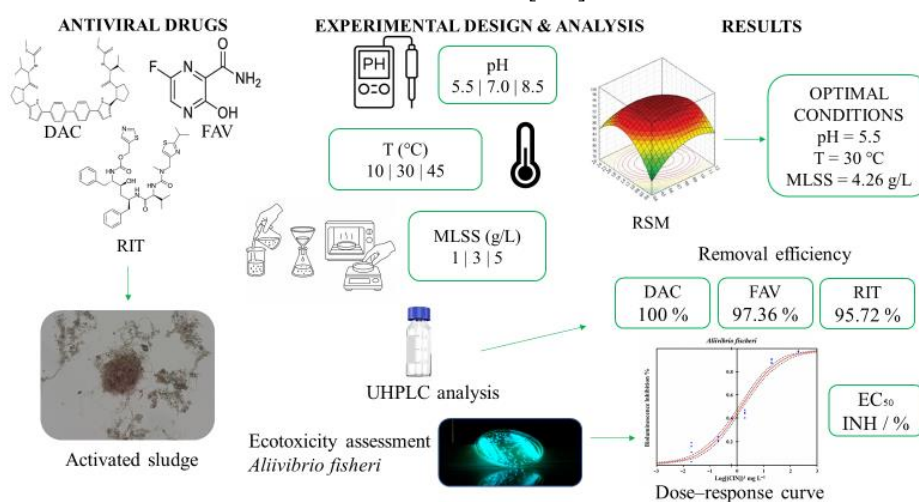


BIODEGRADATION OF THE ANTIVIRAL DRUGS RITONAVIR, FAVIPIRAVIR AND DACLATASVIR AND DETERMINATION OF OPTIMAL PROCESS CONDITIONS

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Antiviral drugs used for the treatment of COVID-19 often reach municipal wastewater and are incompletely removed during conventional wastewater treatment, resulting in their release into the environment. The aim of this study was to investigate the removal of daclatasvir (DAC), favipiravir (FAV) and ritonavir (RIT) from the aqueous phase using activated sludge and to determine the optimal process conditions. The effects of pH (5.5, 7.0 and 8.5), temperature (10 °C, 30 °C and 45 °C) and mixed liquor suspended solids concentration (MLSS; 1, 3 and 5 g/L) were investigated. Antiviral concentrations were determined by ultra-high-performance liquid chromatography (UHPLC), while physicochemical parameters, activated sludge stability and ecotoxicity using *Aliivibrio fischeri* were also evaluated. Response surface methodology was applied to determine the optimal process conditions. At 30 °C, pH of 5.5, and MLSS of 4.26 g/L, removal efficiencies of 100.00% for DAC, 97.36% for FAV, and 95.72% for RIT were achieved. Under these optimal process conditions, ecotoxicity assessment using *Aliivibrio fischeri* showed inhibition values of 16.99% for DAC, 5.08% for FAV, and 4.63% for RIT, with the highest inhibition observed for DAC. Overall, the results demonstrate the importance of combining process optimization with ecotoxicological assessment to comprehensively evaluate the effectiveness of antiviral removal from wastewater [1–3].



ACKNOWLEDGEMENTS This work was carried out as part of the project “Environmental Aspects of SARS-CoV-2 Antivirals” (EnA-SARS, IP-2022-10-2822), funded by the Croatian Science Foundation

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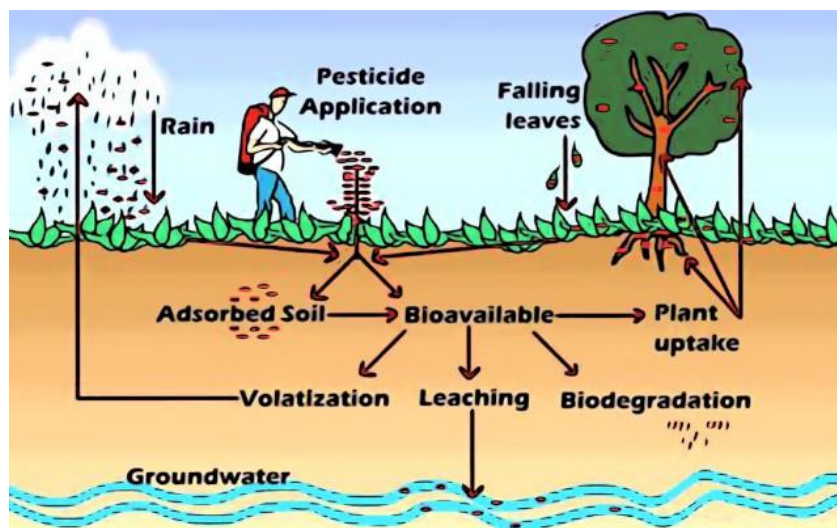


REMOVAL OF THE PESTICIDE ATRAZINE FROM GROUNDWATER AND DETERMINATION OF ITS ECOTOXICITY BY *Vibrio fischeri*

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Pesticides are widely used in agriculture to protect crops from pests and diseases; however, their extensive application can lead to contamination of water resources and pose a potential threat to aquatic ecosystems. Groundwater is particularly susceptible to pesticide contamination due to the transport and persistence of these compounds in the environment [1]. In this study, the removal efficiency of nanofiltration membrane HL and reverse osmosis membrane ESPA4 for the removal of atrazine from groundwater was investigated. The experimental study was performed using a laboratory-scale membrane system consisting of six cells operated in parallel for three hours. Atrazine concentrations in the feed and permeate were determined by UPLC-MS/MS and used to evaluate membrane retention. ESPA4 exhibited consistently high atrazine retention throughout the experiment, with values of 94,4%, 93,8% and 94,0% after 1, 2 and 3 h. In comparison, the HL membrane showed considerably lower retention, ranging from 35,2% to 39,7%. These results are consistent with previous studies reporting efficient atrazine removal using nanofiltration and reverse osmosis membranes. The results demonstrate a substantially higher efficiency of ESPA4 in atrazine removal from groundwater. In addition, the ecotoxicity of atrazine was evaluated using the bioluminescent bacterium *Vibrio fischeri*, where changes in bacterial luminescence were used as an indicator of toxic effects [2]. No relevant inhibition of bioluminescence was observed for the investigated pesticide under the applied experimental conditions, indicating no detectable acute ecotoxic effect at the tested concentrations.



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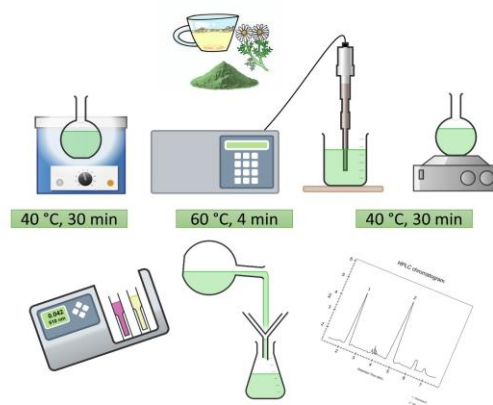


VALORIZATION OF ANTIOXIDANT COMPOUNDS FROM CHAMOMILE HERBAL DUST USING DIFFERENT EXTRACTION APPROACHES

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The production of herbal teas generates large amounts of herbal dust, very fine particles that cannot be used in filter bags and represent an underutilised by-product that is a valuable source of natural phenolic products [1]. For this reason, in this study we present a sustainable approach to extracting antioxidant components from chamomile herbal dust. Three different extraction techniques were used: ultrasound-assisted extraction (UAE) with a probe and a bath, each with two different solvent concentrations (50 and 70% (v/v)), which were compared with conventional extraction on a magnetic stirrer. The composition was examined by chromatographic and spectrophotometric methods, and the antioxidant activity was determined spectrophotometrically with different assays such as DPPH, ABTS, CUPRAC and FRAP. The results indicate the effectiveness of both solvents, as well as all three techniques. In all extracts, chlorogenic acid, neochlorogenic acid and apigenin were detected and quantified using HPLC, with very similar values. The antiradical tests yielded values in the ranges 4.85–6.15 mmol TE/g, 18.29–21.83 mmol Fe²⁺/L and 10.45–15.33 mmol Fe²⁺/L. No statistically significant differences were observed between these values. These findings indicate that chamomile plant dust is a valuable source of phenolic bioactive compounds with antioxidant potential. Comparable results obtained using all three extraction techniques and both ethanol concentrations demonstrate their effective application in the sustainable valorisation of this underutilised by-product. The results further support the potential of chamomile plant dust as an alternative source of bioactive compounds for use in the pharmaceutical, nutraceutical and cosmetic industries.



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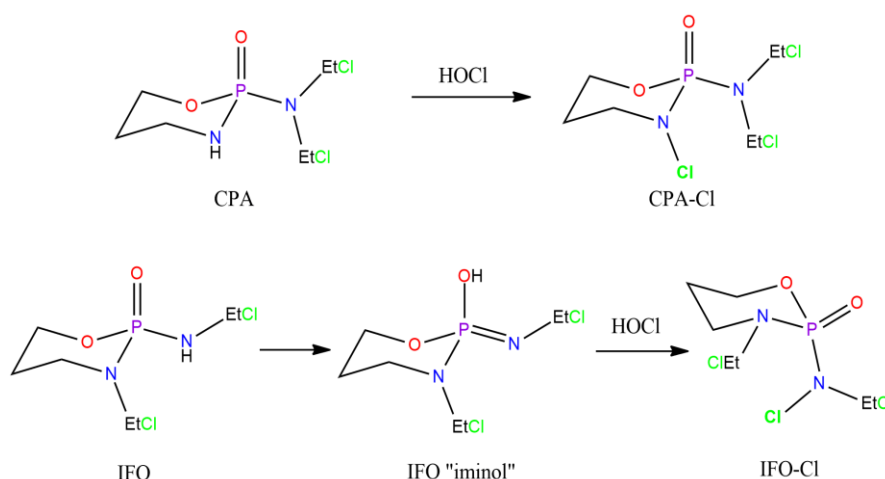
CHLORINATION OF CYCLOPHOSPHAMIDE AND IFOSFAMIDE IN AQUEOUS ENVIRONMENTS: A QUANTUM-CHEMICAL STUDY

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Hypochlorous acid (HOCl), the principal reactive chlorine species formed during wastewater chlorination, can influence the environmental fate of nitrogen-containing pharmaceuticals. In this study, the chlorination of the phosphoramidate anticancer prodrugs cyclophosphamide (CPA) and ifosfamide (IFO) was investigated using density functional theory, with particular emphasis on the effects of conformation, protonation state, and tautomerism on reaction pathways and energetics. Geometry optimizations and vibrational frequency calculations were performed at the B3LYP/6-31+G(d,p) level of theory. Stationary points were characterized by frequency analysis, and transition-state connectivity was verified by intrinsic reaction coordinate calculations. Aqueous solvation was described using the SMD continuum model, while the effect of explicit solvation on *N*-chlorination and tautomerization was examined by including up to three water molecules in the transition state structures, whose inclusion proved to be essential in earlier studies [1]. Chlorination of both CPA and IFO was found to proceed with neutral species, with the activation barriers for anions being prohibitive ($>150 \text{ kJ mol}^{-1}$), however there was a difference in the preferred tautomeric form. The “iminol” form of both compounds was substantially less stable than the “amide” form ($>90 \text{ kJ mol}^{-1}$) but combined with a very low activation barrier it was still the preferred chlorination path for IFO. In CPA, however, the tautomerisation step was prohibitive and therefore the main reaction proceeds with the “amide” form. In the calculations, the inclusion of explicit water molecules was essential in order to obtain activation barriers in the experimental range. Conformation also had to be taken into account, as chlorination changed the most stable conformation of IFO while in CPA no such effect was observed. Overall, the results show that the chlorination reactivity of CPA and IFO is governed by a combination of molecular conformation, protonation state, and tautomerism. These findings provide molecular-level insight into the transformation pathways of phosphoramidate pharmaceuticals in aqueous environments containing reactive chlorine species.



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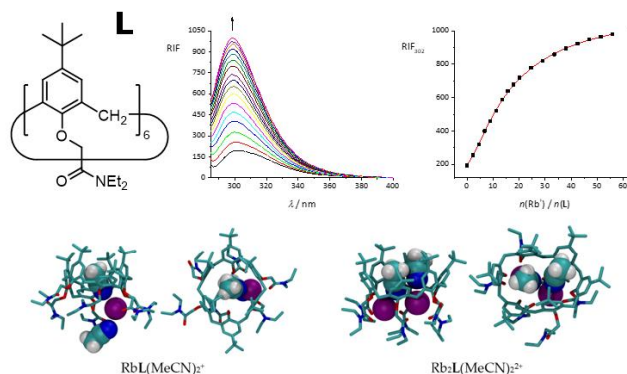
EXPLORING METAL CATION COMPLEXATION USING THE INTRINSIC FLUORESCENCE OF CALIX[6]ARENE

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The intrinsic fluorescence of a tertiary-amide calix[6]arene derivative (**L**) and its complexes with Group I and Group II metal cations was investigated by steady-state and time-resolved fluorescence spectroscopy. As previously demonstrated for the corresponding calix[4]arene analogue [1], **L** exhibits low to moderate intrinsic fluorescence despite the absence of an additionally appended fluorophore. Its emission is strongly affected by metal-ion binding, enabling complex formation to be monitored by spectrofluorimetry. Fluorimetric titrations were used to determine the stability constants of 1:1 and 2:1 (cation:ligand) complexes, which were in good agreement with those obtained by UV–Vis absorption spectroscopy and isothermal titration calorimetry. ¹H NMR spectroscopy, mass spectrometry, and molecular dynamics simulations provided complementary information on complex stoichiometries, structures, and binding processes. These results show that intrinsic calix[6]arene fluorescence provides a sensitive and low-concentration approach for monitoring and quantitatively characterizing metal-ion complexation in solution, with particular potential for systems involving poorly soluble receptors or highly stable complexes.



ACKNOWLEDGEMENTS This research was funded by the Croatian Science Foundation (projects CalixCORE, grant number IP-2024-05-3012, MacroSol (IP-2019-04-9560) POC-Sens-Bioact (IP-2022-10-9829), and MicroSyn-Total, grant number IP-2024-05-5352), European Union – NextGenerationEU through the National Recovery and Resilience Plan 2021–2026, via Institutional grants of the University of Zagreb Faculty of Science (NextGenChem and CryoLab), project ToSiAn (NPOO.C3.2.R2-I1.06.0043), and the European Regional Development Fund (infrastructural project CluK, grant number KK.01.1.1.02.0016).

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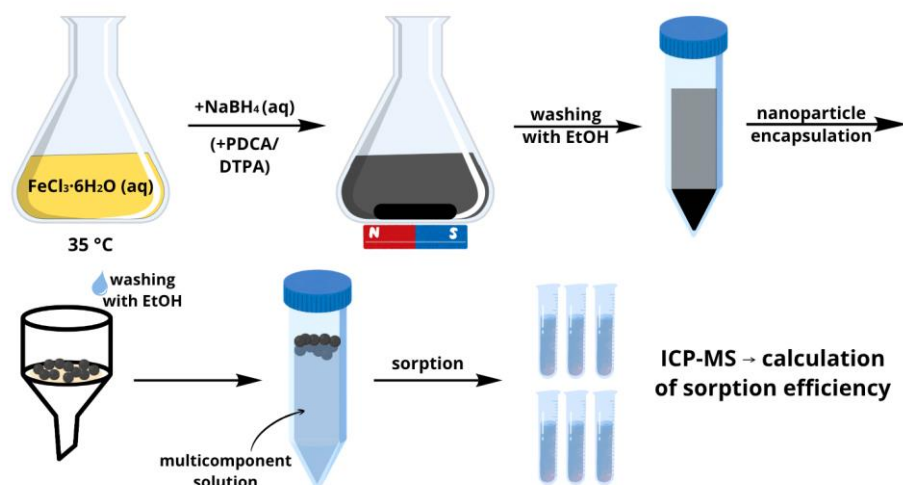
SORPTION OF LANTHANOID IONS FROM MULTICOMPONENT SOLUTIONS USING NEUTRAL AND FUNCTIONALIZED IRON NANOPARTICLES

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Lanthanoids are used as constituents of various modern technologies such as electronics and renewable energy technologies. The growing consumption, limited availability of lanthanoids in nature, and possible discharge of lanthanoids into aquatic ecosystems prompted the necessity to develop an effective method of their purification from water. Nanoparticles of iron have attracted attention as promising sorbents for water purification due to high reactivity and relatively low cost of these particles. In this work, the sorption of lanthanoid ions from multicomponent aqueous solution on neutral and modified iron nanoparticles was studied. Neutral iron nanoparticles were synthesized via reduction of ferric chloride by sodium borohydride. (PDCA)- and (DTPA)-functionalized nanoparticles were prepared introducing the corresponding ligands during nanoparticle synthesis. Sorption experiments were carried out with the use of multicomponent solutions at different initial concentrations and contact times. The residual ion concentrations were detected by inductively coupled plasma mass spectrometry, and the sorption efficiencies were calculated. It was found that the sorption efficiency depends not only on the initial concentration and the contact time but also the differences in the sorption behavior between neutral, PDCA-functionalized and DTPA-functionalized nanoparticles was observed. The results showed that sorption efficiency improved with an increase in the contact time for the studied iron nanoparticles. Sorption efficiency was determined at initial lanthanoid concentrations of 0.1, 1, 10, 20, 50, 100, and 500 ppb, and sorption efficiency was the highest within the range of 10–50 ppb. These results proved that the use of iron nanoparticles can be considered for the removal of several lanthanoid ions simultaneously from aqueous solutions [1,2].



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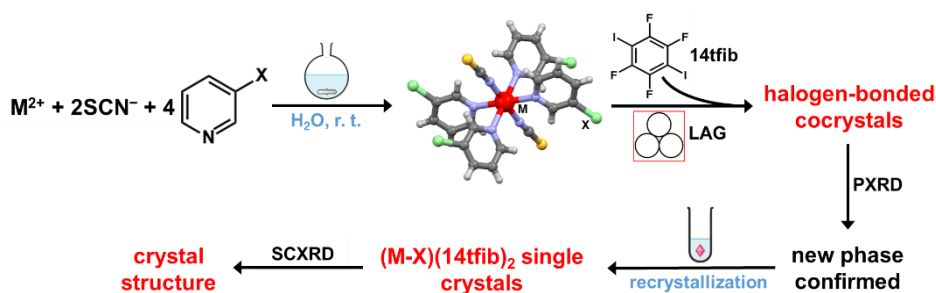
HALOGEN-BONDED COCRYSTALS OF $M(NCS)_2(3\text{-Xpyridine})_4$ COORDINATION COMPOUNDS ($M = \text{Co, Ni, Fe, Mn}$; $X = \text{Cl, Br, I}$)

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The isothiocyanate ligand has proven to be a versatile halogen bond acceptor [1], despite being less extensively studied than halide ligands in halogen-bonded metal–organic compounds [2]. In this work, we further evaluate halogen-bonding potential of this acceptor and examine how peripheral halogen atoms in coordination compounds influence halogen-bonded cocrystal structures. Building upon our previously reported findings, we have extended the scope of the present study by incorporating new coordination compounds and structural results, allowing for a more comprehensive assessment. Accordingly, we expanded our study to a series of twelve octahedral coordination compounds ($M\text{-X}$) of $M(NCS)_2(3\text{-Xpyridine})_4$ type ($M = \text{Co, Ni, Fe, Mn}$; $X = \text{Cl, Br, I}$) and cocrystallized them with the halogen bond donor 1,4-diiodotetrafluorobenzene (**14tfib**). Characterization of $(M\text{-X})(\mathbf{14tfib})_2$ cocrystals obtained by liquid-assisted grinding and crystallization from solution was performed using powder and single crystal X-ray diffraction. Structural analysis of all cocrystals revealed double chains formed by $\text{I}\cdots\text{S}$ halogen bonds between **14tfib** and isothiocyanate ligands. In $(M\text{-I})(\mathbf{14tfib})_2$, iodine atoms from 3-iodopyridine ligands emerged as halogen bond donors, forming weaker $\text{I}\cdots\text{S}$ halogen bonds between chains. In contrast, halogen-bonded chains in $(M\text{-Cl})(\mathbf{14tfib})_2$ and $(M\text{-Br})(\mathbf{14tfib})_2$ are connected via other non-covalent interactions. Beyond confirming the strong halogen-bonding propensity of isothiocyanate sulfur, this study demonstrates the halogen bonding ability of peripheral iodine atoms and reveals that the metal center in $(M\text{-X})(\mathbf{14tfib})_2$ cocrystals has no significant influence on the key features of the supramolecular architecture.



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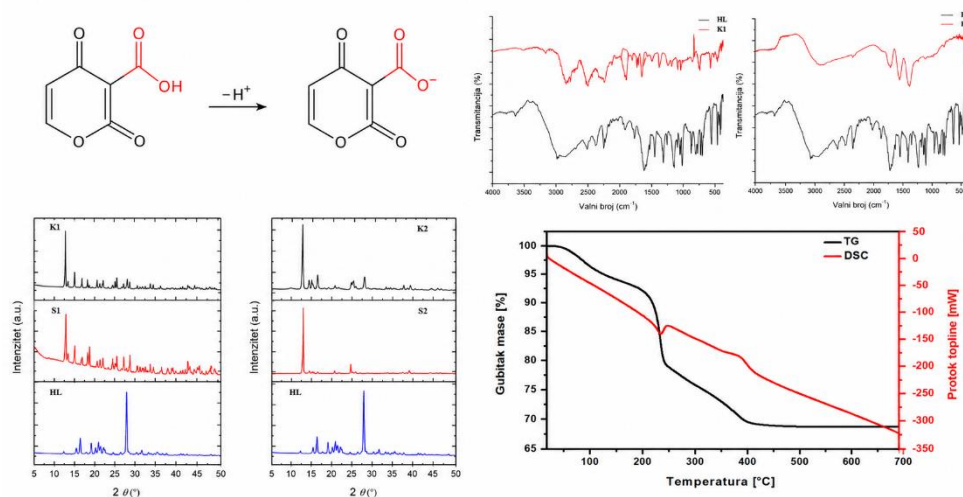


SYNTHESIS AND CHARACTERISATION OF ZINC(II) COMPLEXES WITH COUMALIC ACID

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Two zinc(II) coordination compounds with coumalic acid were synthesised to investigate the coordination behaviour of this oxygen-donor ligand towards Zn(II) ions and the influence of different zinc(II) precursor salts on the properties of the resulting products. Zinc(II) acetate dihydrate and zinc(II) nitrate hexahydrate were used as metal sources, while coumalic acid was employed as the ligand. The syntheses were performed under mild conditions in aqueous and ethanolic media, with adjustment of the reaction mixture pH to promote deprotonation of the carboxylic group and coordination to the metal centre. The isolated products were characterised by Fourier transform infrared spectroscopy (FTIR), powder X-ray diffraction (PXRD), thermogravimetric analysis coupled with differential scanning calorimetry (TGA/DSC), and UV–Vis spectroscopy. FTIR analysis indicated deprotonation of the carboxylic group and coordination of the resulting carboxylate group to Zn(II), while differences in $\Delta\nu$ values suggested different carboxylate coordination modes in the two compounds. PXRD patterns confirmed the formation of new crystalline phases distinct from those of the corresponding starting materials. TGA/DSC analysis revealed differences in the thermal behaviour of the prepared compounds and indicated the presence of water in their structures. As expected for the d^{10} electronic configuration of Zn(II), no d–d transitions were observed in the UV–Vis spectra, with the observed spectral features being predominantly associated with ligand-centred transitions. Overall, the results demonstrate that coumalic acid can coordinate Zn(II) through its deprotonated carboxylate group and indicate that the choice of zinc(II) precursor salt can influence the coordination environment, crystalline organisation, and thermal properties of the resulting compounds [1,2].



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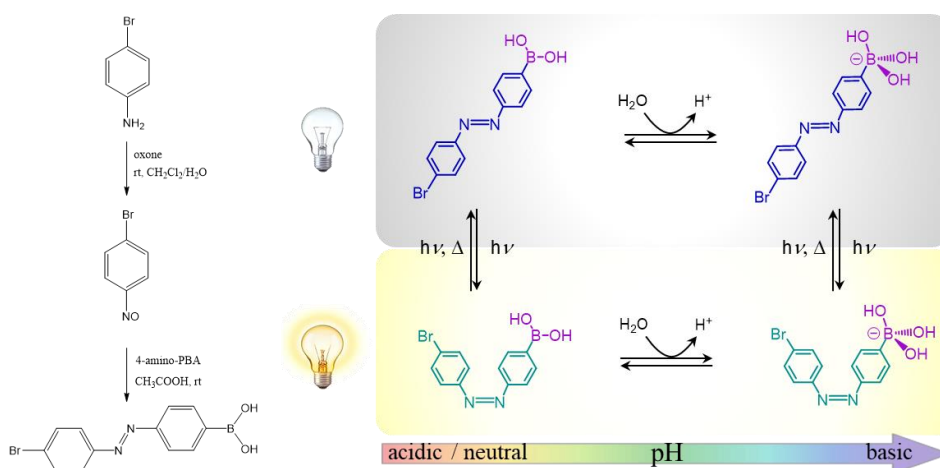


SYNTHESIS AND PHOTOPHYSICS OF AN AZOBENZENE PHENYLBORONIC ACID DERIVATIVE

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Azobenzenes are aromatic compounds characterized by an azo ($-N=N-$) group linking two phenyl rings. Their reversible *E* to *Z* photoisomerization enables light induced control over molecular structure and properties, making azobenzenes widely used components of molecular photoswitches with applications in photoactive materials and molecular devices [1]. In this work, we have synthesized an azobenzene derivative of phenylboronic acid by the Mills reaction [2], using Oxone as a mild oxidation reagent to achieve partial oxidation of aniline to a nitrosobenzene derivative. Finally, photophysical properties of the obtained compound were investigated: the photoisomerization and backphotoisomerisation quantum yields, molar absorption coefficients, the composition of the photostationary state, and rates of thermal backisomerisation were determined.



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COMPARISON OF THE ANTIOXIDANT POTENTIAL OF MULTIFLORAL AND LINDEN HONEY FROM CROATIA: PERSPECTIVES FOR HONEY VALORISATION

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Jelena Puzić⁴

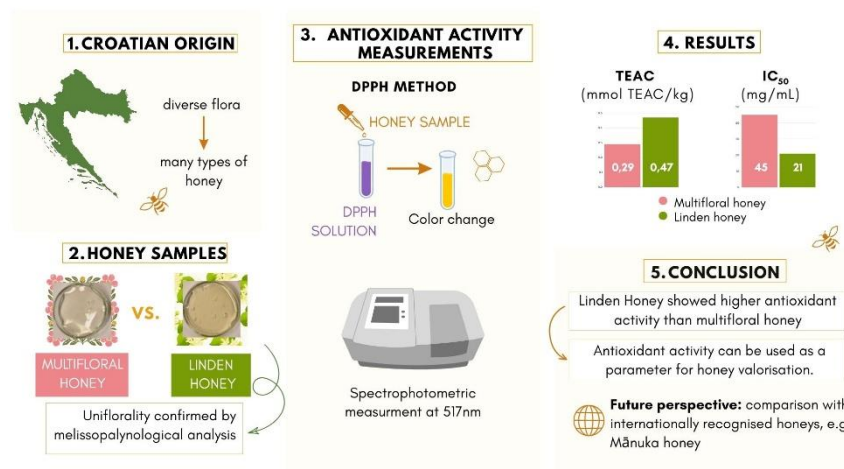
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Honey is a complex natural product whose chemical composition is influenced by its botanical and geographical origin [1]. Honey exhibits antioxidant properties largely attributed to its polyphenolic compounds. The antioxidant activity of honey depends on its botanical origin and colour, with darker honeys generally showing higher antioxidant activity [2]. Developing and applying methods for honey valorisation is important for supporting the positioning and recognition of Croatian honey in European and global markets, particularly for unifloral honey types. The Mediterranean, continental and mountain regions of Croatia offer a diverse range of melliferous plants, providing various honey types. This study compared the antioxidant activity of two honey types originating from Croatia: multifloral honey and linden honey. The uniflorality of the linden honey was confirmed by melissopalynological analysis. The antioxidant activity of the honey samples was determined using the DPPH radical-scavenging method, by spectrophotometrically measuring DPPH absorbance at 517 nm. Antioxidant activity was expressed as Trolox equivalent antioxidant capacity (TEAC) and IC₅₀ values. TEAC values were 0.29 mmol TEAC/kg for multifloral honey and 0.47 mmol TEAC/kg for unifloral linden honey, while the IC₅₀ values were 45 mg/mL and 21 mg/mL, respectively. These findings, consistent with previous studies reporting differences in antioxidant activity between honey types, support the use of antioxidant activity as a parameter for honey valorisation. In this context, further comparison of Croatian honey varieties with internationally recognised and certified honeys with well-documented bioactive potential, such as Mānuka honey, may be a valuable approach to Croatian honey valorisation.



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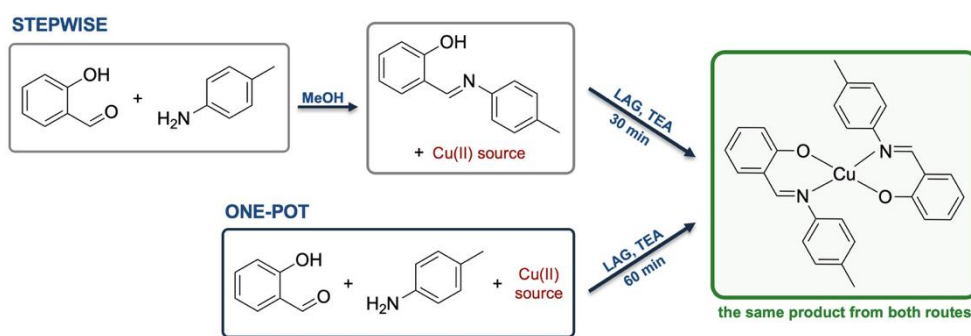
MECHANOCHEMICAL SYNTHESIS OF COPPER(II) SCHIFF BASE COMPLEXES BY STEPWISE AND ONE-POT ROUTES

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Schiff bases derived from *ortho*-hydroxy aldehydes are versatile *O,N*-ligands that are typically used to form $M(L)_2$ complexes with divalent transition metals [1]. Whereas solution-phase syntheses usually require prolonged heating under reflux, mechanochemical syntheses can be completed within minutes using little or no solvent [2], and ligand formation and metal complexation can even be combined in a single milling step [3]. Such one-pot procedures remain comparatively rare, and systematic comparisons across several ligands and metal sources are few [3,4]. In this work, six Schiff bases derived from three *ortho*-hydroxy aldehydes (salicylaldehyde, 2-hydroxy-1-naphthaldehyde and *o*-vanillin) and two aromatic amines (2-naphthylamine and *p*-toluidine) were screened with copper(II) as the metal centre. Two copper sources, $Cu(OAc)_2 \cdot H_2O$ and $Cu_2CO_3(OH)_2$ (malachite), and two routes were compared: a stepwise route, in which the pre-formed Schiff base was milled with the copper source, and a one-pot route, in which the aldehyde, the amine and the copper source were milled together in a 2:2:1 molar ratio. All reactions were carried out by liquid-assisted grinding with a small amount of triethylamine, and all products were characterized by powder X-ray diffraction. Complexes with all six ligands were obtained from copper(II) acetate, and the same complexes were obtained from malachite despite its low solubility, with residual reactants in some systems. For most systems the same crystalline phase was obtained by the one-pot route as by the stepwise route, showing that ligand formation and complexation can be coupled in a single milling step. In two cases the one-pot product was amorphous. Where the complex was already known, the powder patterns matched those simulated from structures in the Cambridge Structural Database; in two systems a phase absent from the database was obtained, identically from both copper sources and by both routes. Isolation of the ligand was therefore avoided in most systems, and the screening is being extended to further Schiff bases and metal centres.



Shown for one of six Schiff bases. $Cu(II)$ source: $Cu(OAc)_2 \cdot H_2O$ or $Cu_2CO_3(OH)_2$

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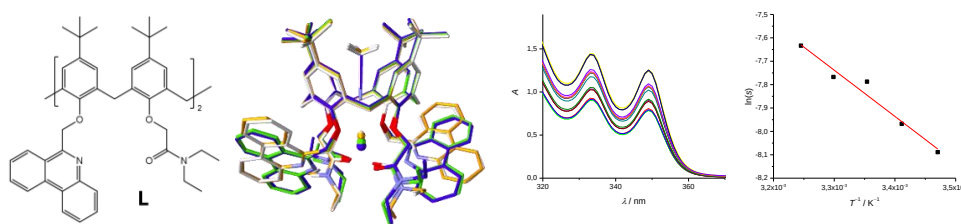
SOLVENT INCLUSION IN CALIX[4]ARENE: A COMPREHENSIVE EXPERIMENTAL, THERMODYNAMIC, AND COMPUTATIONAL STUDY

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 groups, particularly those containing carbonyl moieties, have attracted considerable attention due to their ability to form highly stable complexes with a variety of cations in different solvents [1]. The inclusion of solvent molecules within the hydrophobic cavity of calixarenes plays an important role in determining the extent and thermodynamics of cation-complexation reactions [2]. In our previous studies [3], the thermodynamics of the complexation of first- and second-group metal cations by the calix[4]arene derivative **L** in acetonitrile, methanol, and ethanol was studied in detail. In the present work, particular emphasis was placed on elucidating the influence of solvent molecule inclusion within the *basket* of the free ligand and its metal complexes on the corresponding complexation equilibria. The structures of ligand-solvent and complex-solvent adducts were investigated using a combination of experimental and computational approaches, including NMR spectroscopy, classical molecular dynamics simulations, and DFT calculations. The principal difference between the adducts of alkali and alkaline earth metal cation complexes was found to arise from the orientation of the included solvent molecule within the calixarene cavity. In the alkali metal complexes, the solvent methyl group was directed towards the metal center, whereas in the alkaline earth metal complexes, the –CN or –OH group was oriented towards the cation, resulting in its additional coordination. The orientation and position of the included solvent molecule were shown to significantly influence the thermodynamic stability of the complexes. The solvent inclusion process was quantitatively investigated by isothermal titration calorimetry and UV absorption spectrophotometry, enabling determination of the corresponding thermodynamic parameters. Furthermore, the thermodynamic cycles describing the complexation of alkali and alkaline earth metal cations by **L** in methanol and ethanol were prepared using the measured solubilities and solution enthalpies of the ligand in both solvents. These findings provided a comprehensive thermodynamic description of solvent inclusion phenomenon and its influence on the cation-binding ability of **L**.



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

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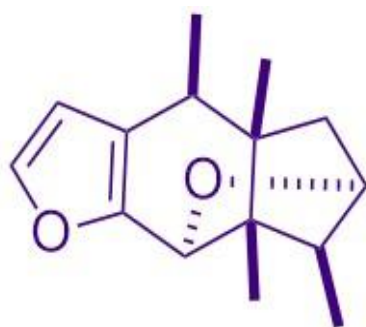


COMPLETE NMR ASSIGNMENT OF PINGUISANIN AND DEOXYPINGUISONE

Katarina Nejić, Miljana Đorđević Zlatković, Dragan Zlatković, Niko Radulović

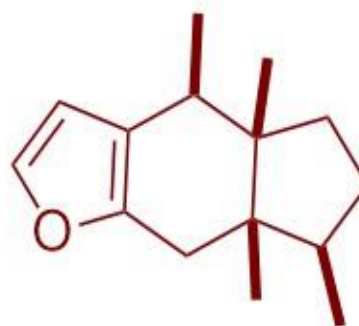
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Although the structures of the pinguisane-type sesquiterpenoids pinguisanin [1,2] and deoxypinguisone [3] were established in early literature, their published NMR data rely largely on low-field 1D and early 2D experiments. Consequently, full proton coupling networks and complete heteronuclear long-range correlations for quaternary carbons remain incomplete. Here, we report the complete ^1H and ^{13}C NMR spectral assignment of both natural products using modern high-field gradient-enhanced 2D techniques (gCOSY, gHSQC, gHMBC, and NOESY). Analysis of long-range ^1H – ^{13}C correlations resolved historical ambiguities in the crowded aliphatic and quaternary carbon regions of the pinguisane core, providing a definitive, high-resolution reference dataset for future natural product identification.



pinguisanin

isolated by Asakawa *et al.* [1]
structure revised by Asakawa *et al.* [2]



deoxypinguisone

isolated by Krutov *et al.* [3]

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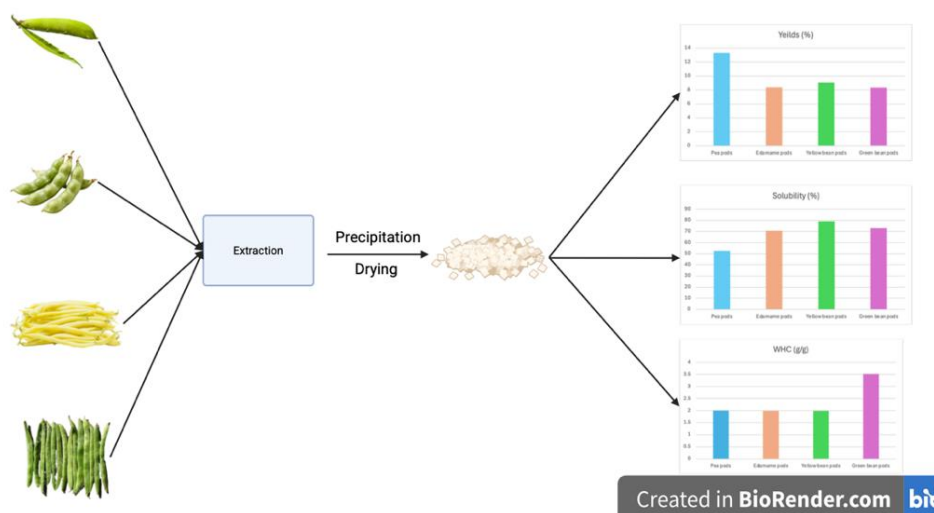


TOWARDS ZERO WASTE CONCEPT – PLANT SECONDARY WASTE AS PROMISING SOURCE OF HEMICELLULOSE

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The Zero Waste concept has gained increasing importance in the context of modern mass production, where the focus is not only on minimizing waste but also on identifying valuable uses for industrial by-products. One of the many useful products that can be obtained from biowaste is hemicellulose, owing to the near unlimited supply of this sustainable polysaccharide and its excellent physical and chemical properties, hemicellulose was used in the production of various materials (emulsifiers, films, and hydrogels, etc.) and fine chemicals (xylitol, ethanol, furfural, etc.) for food, medical, and energy storage applications [1]. In this research, hemicellulose was isolated from pea pods, edamame pods, yellow bean pods, and green bean pods. The extraction was performed by alkaline hydrothermal extraction after phenols and proteins were removed. The extraction yields obtained were 13%, 8%, 9%, and 8% for pea pods, edamame pods, yellow bean pods, and green bean pods, respectively. Isolated hemicelluloses were characterized in terms of functional and antioxidant properties, and the best results for WHC, OHC, and solubility were exhibited by hemicellulose from green beans (3.52 g/g), yellow beans (1.32 g/g), and green bean pods (73%), respectively. The highest potential for scavenging ABTS-radicals was shown by pea pods. Considering the obtained results, the waste material was shown to be a good and promising source of hemicellulose, in addition to previously extracted polyphenols and proteins.



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TERNARY COPPER(II) COORDINATION COMPOUND WITH L-PHENYLALANINE: SYNTHESIS, CHARACTERIZATION AND INTERACTIONS WITH DNA

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Ternary copper(II) coordination compounds with amino acids and heterocyclic ligands are rising in prominence due to their applications as anticancer drugs. The antiproliferative activity is a result of interactions between these compounds and DNA of tumorous cells [1]. The key objective of this research is to prepare coordination compounds with various amino acids and heterocyclic bases and analyse their interactions with DNA. A coordination compound of copper(II) with L-phenylalanine (L-HPhe) and 2,2'-bipyridine (bipy)— $[\text{Cu}(\text{L-Phe})(\text{H}_2\text{O})(\text{bipy})][\text{Cu}(\text{L-Phe})(\text{SO}_4)(\text{bipy})]\cdot 8\text{H}_2\text{O}$ (**1·8H₂O**) was synthesised by a solution-based method and also mechanochemically by liquid-assisted grinding (LAG), as described in the literature [2]. Compound **1·8H₂O** was analysed by single-crystal X-ray diffraction (SCXRD), powder X-ray diffraction (PXRD), FTIR spectroscopy and thermogravimetric analysis (TGA). The crystal structure revealed that the copper(II) atom is pentacoordinated by 2,2'-bipyridine and L-phenylalaninate in the equatorial plane, while the apical position is occupied by either a water molecule or a sulphate ion (Figure 1). The interactions and binding affinity of **1·8H₂O** with a double-stranded DNA dodecamer were investigated using spectroscopic methods.

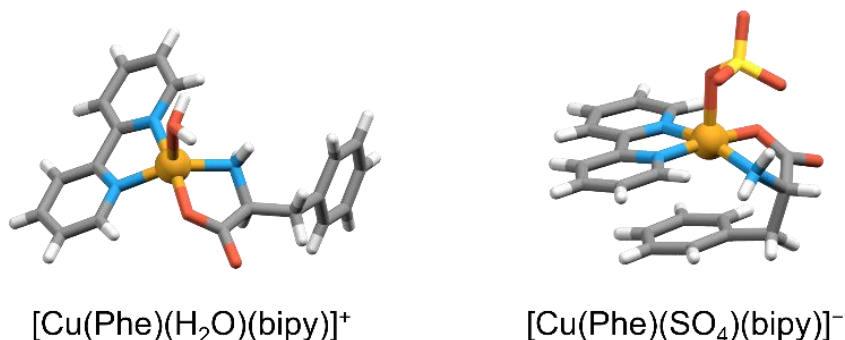


Figure 1. Coordination species in the crystal structure of **1·8H₂O**.

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THE USE OF TEMPLATED ZINC IMIDAZOLATE (ZnIm₂) FRAMEWORKS IN THE SEPARATION OF SOLID MIXTURES

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Zeolitic imidazolate frameworks (ZIFs) are a subclass of metal-organic frameworks. They are highly porous, crystalline materials made of tetrahedral metal nodes and imidazolate organic linkers and are characterized by chemical and thermal stability, as well as large surface areas. Unsubstituted zinc imidazolate (ZnIm₂) is the simplest ZIF material and it is known for its great topological diversity—19 topologies and 24 crystallographically distinct forms have been published so far [1,2]. ZnIm₂ is usually synthesized using the solvothermal method, where the solvent serves as a putative template and structure directing agent, but it has recently been shown that mechanochemical synthesis is faster, more efficient, and allows the use of templates not compatible with solvothermal synthesis. For example, it was shown that nonpolar liquids such as cyclohexane can easily be used in conjunction with protic and ionic reagents such as imidazole and zinc oxide [3]. This approach can be expanded to many different templates, including combining templates with additional auxiliaries such as simple liquids, where the preparation of different ZIF products can be led to by the synergistic effect of the template/liquid pairing [4]. Here it is proposed that this methodology can not only be used for templating new ZIFs, but also for separation of solid template mixtures. It is shown, by us, that judicious choice of liquid additive can switch on or switch off the absorption of target templates, allowing for their separation.

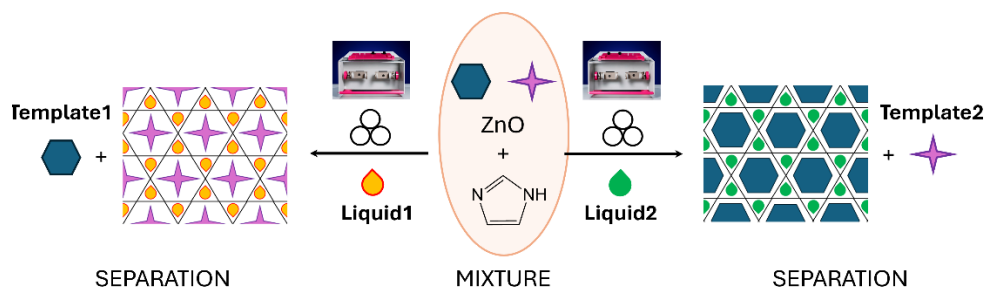


Figure 1. Schematic representation of mechanochemical mixture separation.

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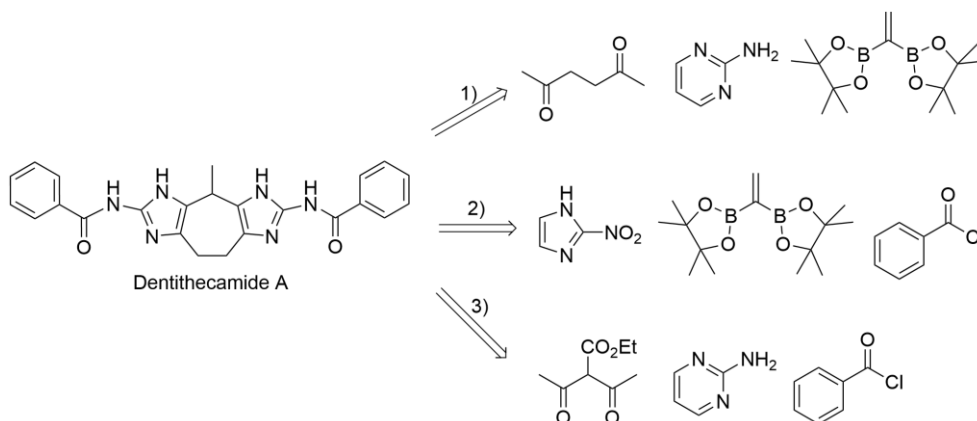
TOWARD THE TOTAL SYNTHESIS OF DENTITHECAMIDE A

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Dentitheca habereri is a marine hydroid commonly found on coral reefs throughout the Indo-Pacific and remains relatively understudied from a chemical perspective. An extract of *D. habereri* collected in Palau was found to inhibit the transcriptional activity of the PAX3–FOXO1 oncoprotein, which plays an important role in fusion-positive rhabdomyosarcoma. Chemical investigation of the active extract led to the isolation of eight new zoanthoxanthin alkaloids, dentithecamides A–H, together with three known analogues. Dentithecamide A was identified as a diacylated zoanthoxanthin alkaloid. Its intriguing polycyclic structure and PAX3–FOXO1 inhibitory activity makes it an attractive target for total synthesis. The first approach towards total synthesis consisted of functionalization of a linear γ -diketone, followed by formation of imidazo[1,2-*a*]pyrimidine structure and Suzuki cross-coupling after further functionalization. This approach was abandoned due to poor results of Suzuki cross-coupling. The second approach consisted of functionalization of a 2-nitroimidazole derivative and subsequent Suzuki cross-coupling, but the desired coupling was unsuccessful. The third approach involved the construction and further functionalization of a linear β -diketone followed by the introduction of a 2-aminopyrimidine moiety intended to establish the fused heterocyclic system. However, the subsequent opening of the pyrimidine ring required for further functionalization could not be achieved [1–3].



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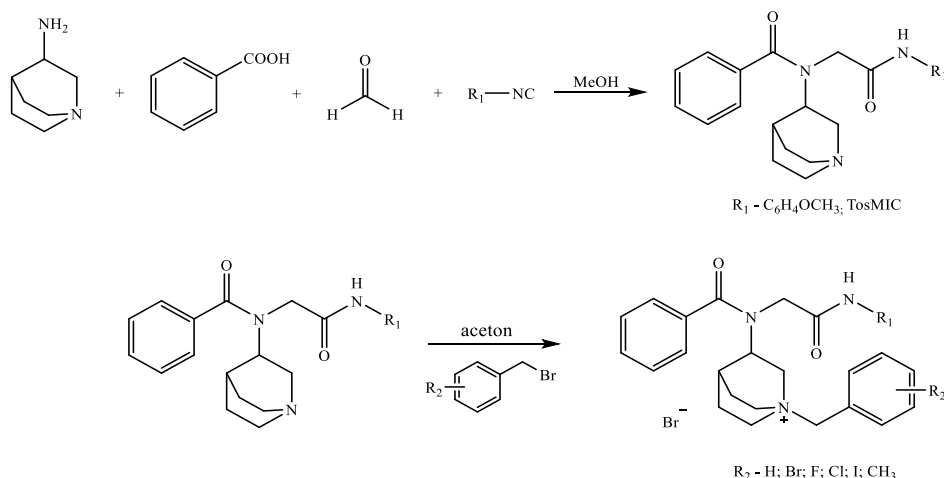
SYNTHESIS AND CHARACTERIZATION OF NOVEL UGI PRODUCTS

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The Ugi reaction, named after the German scientist Ivar Karl Ugi, is a multicomponent exothermic reaction that allows for the high-yield production of a condensation product [1]. The classic Ugi reaction is a four-component process that includes reaction of carbocyclic acid, aldehyde or ketone, amine and an isocyanide and usually proceeds in two steps. The first step involves the condensation of an amine and an aldehyde or ketone to form an imine. In the second step, the resulting imine reacts with a carboxylic acid and an isocyanide to yield the final product [2]. Variations of the Ugi reaction using three components are also possible, provided one of the components possesses two functional groups, such as an amino acid. Due to the possibility of using a wide range of starting compounds to synthesize peptidomimetics, the reaction is also applied in the discovery of potential drugs [3]. In this work, we have synthesized a small library of structurally related peptidomimetics using benzoic acid, paraformaldehyde, quinuclidine-3-amine and different isocyanides. Next, prepared peptidomimetics were used in a Menshutkin reaction in which the quinuclidine nitrogen atom was quaternized with differently substituted benzyl bromides. In total, novel nine compounds were synthesized and characterized with standard analytical methods (FTIR, 1D and 2D ¹H and ¹³C nuclear magnetic resonance spectroscopy).



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

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SYNTHESIS OF HYBRID HALIDE PEROVSKITES WITH *p*-HALOGENATED BEZYLAMINES

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Perovskite refers to a mineral with an ABX_3 crystal structure, which may adopt either a two-dimensional (2D) or three-dimensional (3D) framework. In organic-inorganic hybrid perovskites, typically, the A site is occupied by an organic cation, site B by a metal cation and site X by a halide anion (Cl^- , Br^- , I^-) [1]. For the synthesis of 2D perovskites bulky organic cations are used. These cations form a physical barrier that minimises water absorption and enhances material's stability [2]. Two-dimensional perovskites have found numerous applications in light emitting diodes (LED), solar cells, photovoltaic devices, while many of their potential applications remain to be explored. Also, their magnetic properties are of considerable interest [3]. In this work, the synthesis of 2D perovskites was investigated. *p*-Chlorobenzylammonium, *p*-bromobenzylammonium and *p*-iodobenzylammonium cations were used in combination with $MnCl_2$, $MnBr_2$, $CuCl_2$ and $CuBr_2$. The synthesized compounds were characterized by IR spectroscopy, thermal analysis (TGA, DSC) and their crystal structures were determined by single crystal X-ray diffraction.

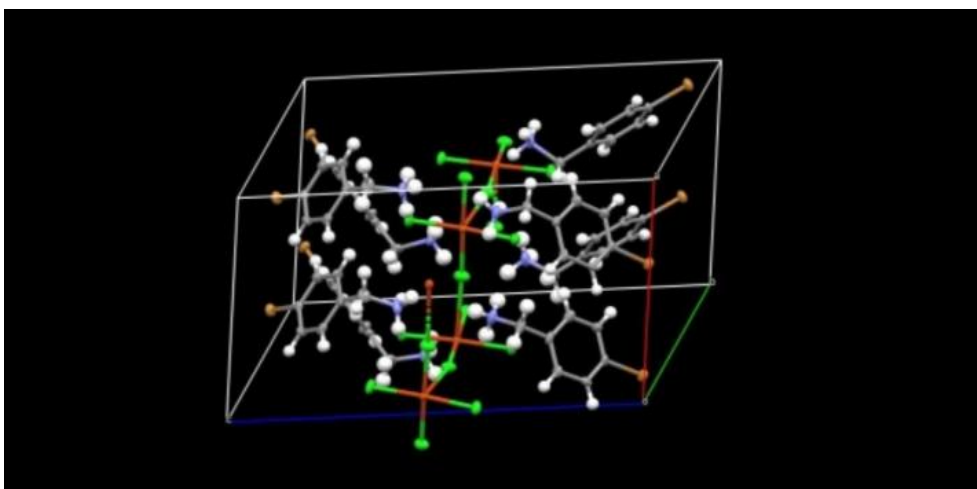


Figure 1. Structure of the *p*-bromobenzylamine and $CuCl_2$ synthesis product (Mercury).

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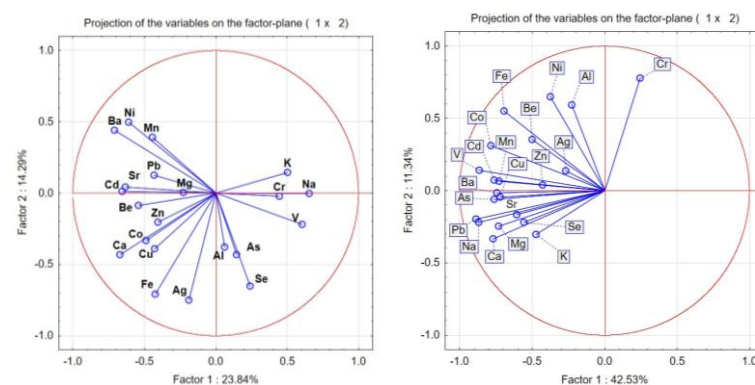
DIFFERENTIATION OF “GRAŠEVINA” AND “PLAVAC MALI” WINES USING ICP-MS AND NMR METHODS

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The elemental composition of wine can serve as a distinctive chemical fingerprint, providing valuable information for assessing its authenticity and geographical origin [1]. This study focuses on two of the most important grape varieties in the Republic of Croatia: “Graševina”, predominantly cultivated in Slavonia and the Croatian Danube region, and “Plavac mali”, mainly cultivated in central and southern Dalmatia. Inductively coupled plasma mass spectrometry (ICP-MS) is a highly sensitive analytical technique capable of providing reliable multi-elemental analysis. The obtained elemental profiles, combined with Deep Reinforcement Learning (DRL) analysis, can contribute to the development of advanced tools for the characterization and classification of wines [2]. In this study, ICP-MS was used to determine the elemental composition of “Graševina” and “Plavac mali” wine samples. Variations in elemental profiles were observed among the analyzed samples, allowing differentiation and classification of the “Graševina” and “Plavac mali” wines. The results demonstrate the applicability of ICP-MS for elemental characterization of Croatian wines and emphasize the importance of combining elemental analysis with appropriate statistical and computational approaches for reliable wine classification and geographical traceability. The analyzed wine samples were additionally subjected to ¹H and DOSY NMR analyses to qualitatively and quantitatively characterize the main metabolites present in the wines. The obtained experimental results coupled with DRL can further be used to develop a predictive model for vine quality assessment.



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THERMODYNAMIC AND STRUCTURAL INSIGHTS INTO CATION COMPLEXATION BY A THIOAMIDE CALIX[4]ARENE DERIVATIVE

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Calix[*n*]arenes are macrocyclic oligomers composed of *n* phenolic residues linked by methylene bridges in the *ortho*-position [1]. Modification of their upper and/or lower rim enables tuning of their chemical properties, yielding highly efficient and selective receptors for diverse ionic and neutral guests [1–7]. The introduction of sulfur-based functional groups promotes the formation of stable complexes with soft, polarizable metal cations [8–10]. In the scope of this work, binding affinity of thioamide calix[4]arene derivative **L** (Figure 1) towards alkali, alkaline earth, and soft metal cations in acetonitrile was investigated by means of spectrophotometry, NMR spectroscopy, isothermal titration calorimetry, and X-ray crystallography. Ligand **L** forms stable complexes with alkali and alkaline earth metal ions, while exhibiting exceptionally high affinity towards soft metal ions. Consequently, receptor **L** represents a promising model compound for designing calixarene-based hosts tailored for soft metal cations.

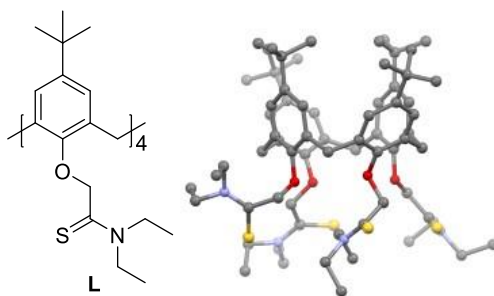


Figure 1. Molecular structure of thioamide calix[4]arene derivative **L**.

ACKNOWLEDGEMENTS This work has been supported by Croatian Science Foundation (projects CalixCORE (IP-2024-05-3012) and MicroSynTotal (IP-2024-05-5352)), and the European Union – NextGenerationEU through the National Recovery and Resilience Plan 2021-2026. via Institutional grants of the University of Zagreb Faculty of Science (NextGenChem and CryoLab).

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TOTAL PHENOLIC CONTENT AND BIOACTIVITY OF SLOVENIAN HONEY SAMPLES OF DIFFERENT ORIGIN

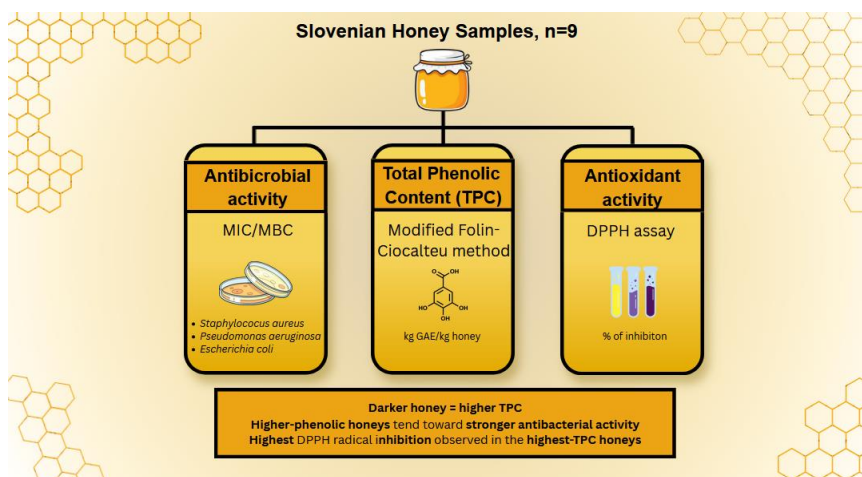
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Honey has been widely studied for its antimicrobial and antioxidant properties, which are commonly attributed to its phenolic content [1,2]. In the framework of a CEEPUS student mobility program at the Biotechnical Faculty, University of Ljubljana, Slovenian honey samples of different botanical and geographical origin were investigated. Antimicrobial activity was evaluated against *Escherichia coli*, *Staphylococcus aureus* and *Pseudomonas aeruginosa* by the microtiter broth microdilution method, and minimum inhibitory and minimum bactericidal concentrations were determined. Total phenolic content was determined by a modified Folin-Ciocalteu assay, adapted to acidic conditions to reduce interference from the high sugar content of honey [3], while antioxidant activity was assessed by the DPPH radical scavenging assay. Darker honey varieties, such as chestnut and forest honey, were found to contain higher phenolic content than lighter varieties, such as acacia and linden, consistent with previously reported trends. A Gram-dependent pattern of antimicrobial susceptibility was observed, with *S. aureus* generally inhibited at lower concentrations than the Gram-negative species, and *P. aeruginosa* was found to be the most resistant. Bioactivity of samples broadly correlated with phenolic content ranking. However, antioxidant and antimicrobial activity did not consistently follow the same trend, indicating that further work is needed to clarify the relationship between phenolic content and different types of bioactivity in different honey samples.



ACKNOWLEDGEMENTS This work was supported by the CEEPUS networks HR-0306: For Safe and Healthy Food in Middle-Europe, and RS-1512: Improving quality with Novel Food Processing Technologies. Mellifera s. p. kindly provided the honey samples.

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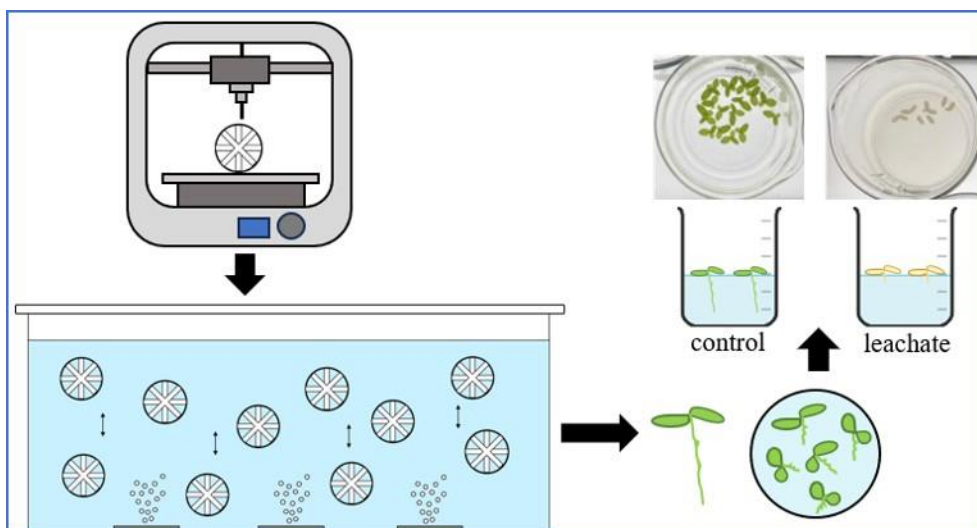


STABILITY ASSESSMENT OF 3D-PRINTED MBBR BIOMASS CARRIERS IN MUNICIPAL WASTEWATER

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Among advanced biological wastewater treatment technologies, the Moving Bed Biofilm Reactor (MBBR) has gained considerable attention due to its operational stability, resistance to hydraulic and organic load fluctuations, and compact design. Biomass carriers are the key components of MBBR systems, providing a large surface area for biofilm development and microbial growth. Recent advances in additive manufacturing have enabled the production of customized three-dimensional (3D)-printed carriers; however, their environmental safety and material stability remain insufficiently investigated. The aim of this study was to evaluate the stability of 3D-printed biomass carriers produced from a photopolymer resin and assessed the ecotoxicological effects of their leachates on the aquatic plant *Lemna minor*. Carriers occupying 70% of the reactor volume were exposed to municipal wastewater in a 10-day leaching experiment under continuous mixing. Samples were analysed for pH, chemical oxygen demand (COD), and total organic carbon (TOC), while toxicity was determined using the *Lemna minor* growth inhibition test according to OECD Guideline 221. The results showed increased TOC and COD concentrations in wastewater exposed to the carriers, indicating the release of organic compounds from the photopolymer material. Moreover, the leachates caused significant growth inhibition of *Lemna minor*, demonstrating a pronounced toxic effect. These findings suggest that the tested 3D-printed carriers may release harmful organic substances into aquatic environments, highlighting the need for further material optimization before their application in biological wastewater treatment systems [1,2].



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MECHANOCHEMICAL SYNTHESIS OF EXPANDED MOF-74

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Metal-organic frameworks (MOFs) are a class of crystalline porous materials composed of metal cations and polydentate organic linkers. They have proven to be promising materials for various applications, including gas storage, purification, separation, catalysis, and sensing [1]. Among various MOFs reported, MOF-74 represents one of the most thoroughly investigated families composed of divalent metal ions (such as zinc, magnesium, nickel or cobalt) and 2,5-dihydroxyterephthalic acid in a 2:1 ratio. They are characterized by a high density of coordinatively unsaturated metal sites and exhibit exceptional properties including high surface area, tunable porosity, thermal stability, and magnetic behavior [2,3]. Currently, common synthesis methods for MOF-74 still require solvothermal conditions and primarily use dimethylformamide as the solvent, resulting in high costs and toxic waste. For more efficient synthesis, it is meaningful to identify other, more economical and environmentally friendly processes for synthesis. As an alternative approach, mechanochemical synthesis has emerged as a promising strategy [4]. In addition to offering improved reaction efficiency, shorter reaction times, and high product purity, mechanochemical methods enable the use of extended organic linkers, facilitating the synthesis of MOFs with significantly enlarged pore dimensions [4]. Herein, we present a thermomechanical approach [5] for the controllable, rapid, green, and efficient synthesis of an expanded MOF-74 using 3,3'-dihydroxy[1,1'-biphenyl]-4,4'-dicarboxylic acid as an organic linker. Furthermore, we obtained an intermediate phase, a coordination polymer in a 1:1 metal-to-ligand ratio, which provides valuable insight into the reaction mechanism and possibly opens a pathway towards a new class of bimetallic MOF-74 materials based on extended isophthalic linkers [6].

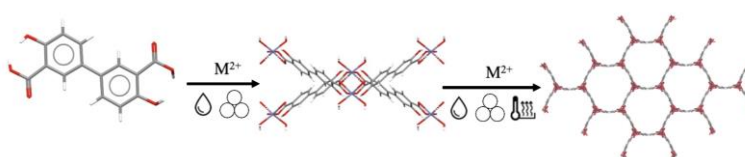


Figure 1. Templated preparation of expanded MOF-74 derivatives.

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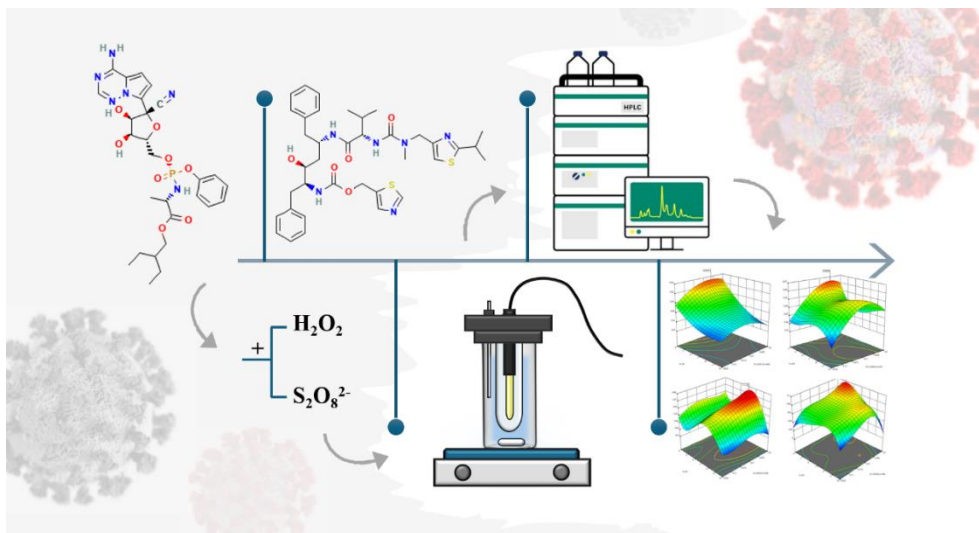


UV-C INDUCED OXIDATION OF REMDESIVIR AND RITONAVIR

Leonarda Zovko, Luka Večenaj, Dora Lastovčić, Kristina Bule Možar, Lidija Furač, Marinko Markić, Dajana Kučić Grgić, Matija Cvetnić, Tomislav Bolanča

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Pharmaceuticals, which stand out among micropollutants due to their high biological activity and persistence, can appear in the aquatic environment, where their presence represents a potential ecological risk. Antivirals attract special attention, as their use during the COVID-19 pandemic has increased their input into wastewater systems and the aquatic environment [1]. Since conventional treatment processes are not suitable for the complete removal of pharmaceuticals, advanced oxidation processes (AOPs) represent one option for their degradation. Among these, photolytic and photooxidative processes stand out, in which degradation is induced by UV radiation alone or in combination with oxidants [2]. The aim of this work was to examine the effectiveness of UV-C-induced AOPs in the degradation of the COVID-19 antivirals remdesivir and ritonavir. Antiviral degradation was examined using UV photolysis and the combined processes UV/H₂O₂ and UV/S₂O₈²⁻ at different pH values and oxidant concentrations. The experimental data were statistically processed in the *Design Expert 12* program, where analysis of variance (ANOVA) was performed and optimal process conditions were determined. Degradation of the antivirals in the tested processes followed pseudo-first-order kinetics. The highest degradation efficiency for both antivirals was achieved with the UV/S₂O₈²⁻ process, followed by the UV/H₂O₂ process, while the lowest efficiency was observed with UV photolysis.



ACKNOWLEDGEMENTS This work was produced as part of the research project „Environmental Aspects of SARS-CoV-2 Antiviral Substances“ (IP-2022-10-2822), funded by the Croatian Science Foundation.

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