

29th CROATIAN MEETING of
CHEMISTS & CHEMICAL ENGINEERS
7th symposium Vladimir Prelog

HSKIKI^{XXIX}

Split **2.-5.9.25.**
Campus of the University of Split

— Book of **Abstracts**



HDKi
HRVATSKO DRUŠTVO
KEMIJSKIH INŽENJERA I
TEHNOLOGA



29th Croatian Meeting of Chemists and Chemical Engineers

with international participation

7th Symposium Vladimir Prelog

University of Split

Faculty of Chemistry and Technology (KTF), and Faculty of Science (PMF)

Ruđera Boškovića 33, 21000 Split, Croatia

BOOK OF ABSTRACTS





IMPRESSUM

ORGANIZERS

Croatian Chemical Society
Croatian Society of Chemical Engineers

PUBLISHED BY

Croatian Chemical Society

EDITORS

COVER DESIGN

Vesna Uglješić

ISSN: 2757-0754 (Online)

VENUE

University of Split
Faculty of Chemistry and Technology (KTF), and Faculty of Science (PMF)
Ruđera Boškovića 33, 21000 Split, Croatia

Zagreb, 2025





Dear Colleagues, Partners and Friends,

On behalf of the Scientific and Organizing Committee, it gives me a great privilege and pleasure to welcome you all to the 29th Croatian Meeting of Chemists and Chemical Engineers, which will be held from September 2 to 5, 2025 in Split, Croatia.

Approximately 400 to 500 chemists and chemical engineers from universities, research institutes and industry are expected to participate and to contribute to the Meeting with posters and oral presentations.

The Meeting will provide an interdisciplinary platform for leading academic scientists, researchers, and research scholars to present and share their experiences and research results on all aspects of chemistry and related fields in a friendly, interactive and collaborative atmosphere, while discussing the latest achievements and novel approaches, the most recent innovations, trends as well as challenges and adopted solutions.

An exhibition of chemical industrial and laboratory equipment and instrumentation, computer software and hardware, literature, and other relevant material, will be organized as an accompanying manifestation.

We will be glad to host you at this Meeting as we believe, other participants and coming delegates would love to hear and learn from your experience.

We look forward to welcoming you at the 29HSKIKI in Split!



Prof. Mirta Rubčić, chair



ORGANIZERS



Croatian Chemical Society
Croatian Society of Chemical Engineers

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Spužević, Marina Tranfić Bakić, Nives Vladislavić

CONFERENCE VENUE

University of Split
Faculty of Chemistry and Technology (KTF), and Faculty of Science (PMF)
Ruđera Boškovića 33, 21000 Split, Croatia

<https://29hskiki.hkd.hr/>

AUSPICES



Under the high auspices of Zoran Milanović,
President of the Republic of Croatia



Under the special auspices of the
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SAXS group, Elettra – Sincrotrone Trieste, Trieste, Italy

Professor Pablo Domínguez de María

Sustainable Momentum, S.L. (SusMom), Las Palmas de Gran Canaria, Spain

Professor Jiří Kaleta

Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Prague, Czech Republic

Professor Spas D. Kolev

School of Chemistry, University of Melbourne, Australia

Professor Boelo Schuur

Faculty of Science and Technology (TNW), Department of Chemical Engineering (DCE), Universiteit Twente, Netherlands

Professor Martin D. Smith

Chemistry Research Laboratory, University of Oxford, UK

Professor Vladislav Tomišić

Faculty of Science, Department of Chemistry, University of Zagreb, Croatia



INVITED LECTURERS

Professor Ana Vrsalović Presečki

Associate Professor Boštjan Genorio

Associate Professor Torsten Mayr, Dipl.-Chem., Dr. rer. nat.

Associate Professor Vilko Mandić

Professor Lidija Ćurković

Associate Professor Ivana Grčić

Gordana Pehnek, PhD, Senior Research Associate

Ivana Brekalo, PhD, Research Associate

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Nikola Basarić, PhD, Senior scientist with tenure

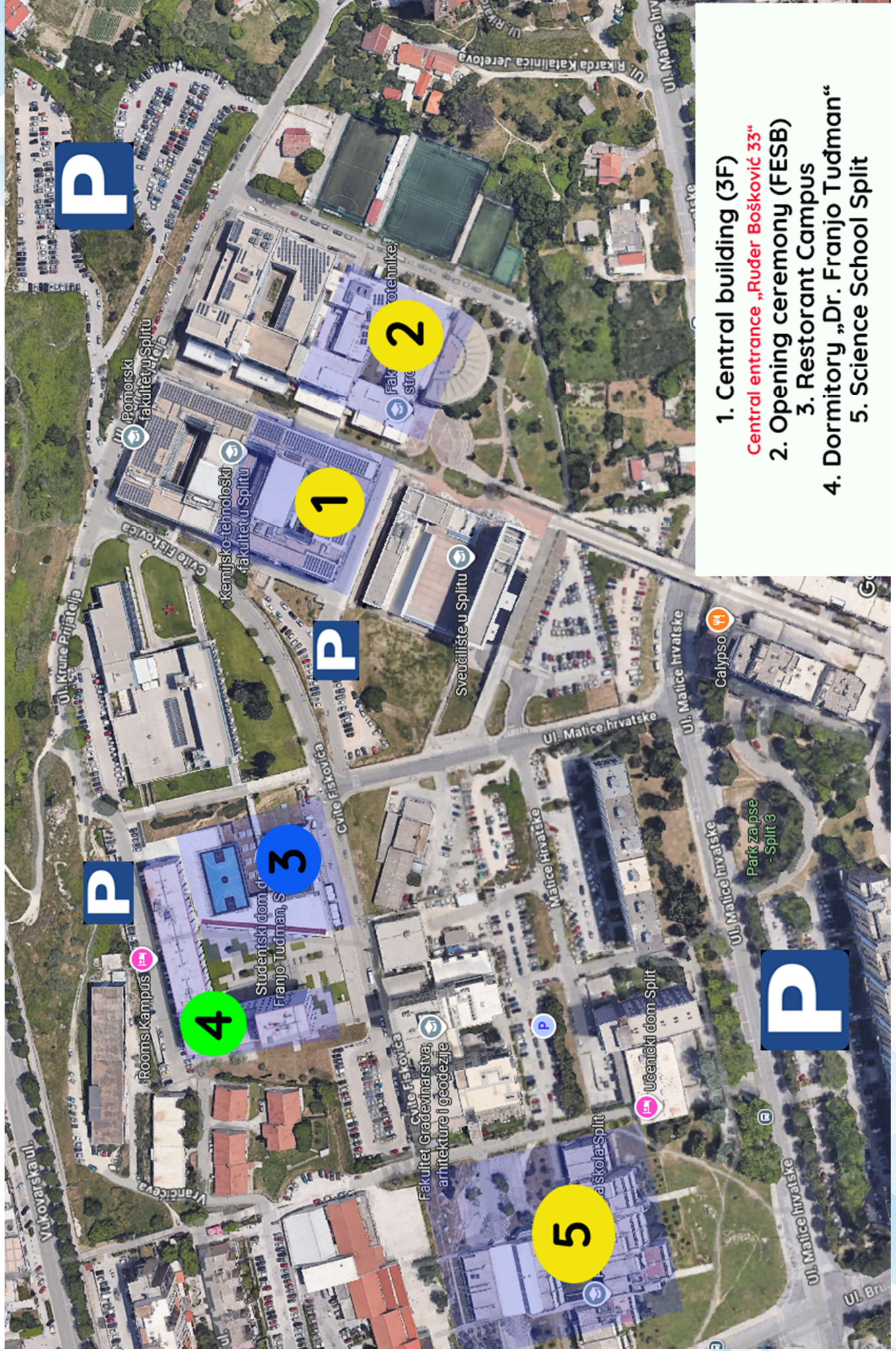
Nađa Došlić, PhD, Senior scientist with tenure

Professor Ante Kolak

Associate Professor Vladimir Stilinović

Associate Professor Milan Nikolić

Ana Ratković, PhD



1. Central building (3F)
2. Opening ceremony (FESB)
3. Restorant Campus
4. Dormitory „Dr. Franjo Tuđman“
5. Science School Split

Central entrance „Ruđer Bošković 33“



Tuesday, September 2, 2025

14.00 – 16.00 **Registration**

Atrium of 3F ①

16.00 – 16.30 **Opening ceremony**

Lecture Hall **A100 of FESB ②**

16.30 – 17.30 ***PLENARY LECTURE***

Spas D. Kolev

ECO-FRIENDLY CHEMICAL SEPARATION BASED ON POLYMER
INCLUSION MEMBRANES AND BEAD

Chair: Lea Kukoč-Modun

Lecture Hall **A100 of FESB ②**

17.30 – 18.30 **Sponsors**

Lecture Hall **A100 of FESB ②**

19.00 – 21.00 **Welcome reception**

Lecture Hall **A100 of FESB ②**

Wednesday, September 3, 2025

8.00 – 9.00	Registration	Atrium of 3F ①
9.00 – 10.00	PLENARY LECTURE Sigrid Bernstorff SMALL ANGLE SCATTERING AND ITS APPLICATION IN CHEMISTRY, LIFE AND MATERIAL SCIENCE <i>Chair: Dražan Jozić</i>	A-02 (3F)
10.00 – 10.30	Coffee Break	
10.30 – 12.30	A – CHEMISTRY <i>Chair: Vladislav Tomišić</i>	A-01 (3F)
10.30 – 11.00	INVITED LECTURE Nađa Došlić Modeling excited-state molecular dynamics with classical trajectories	
11.00 – 11.30	INVITED LECTURE Aleksandra Maršavelski Harnessing ancestral sequence reconstruction to engineer thermostable enzymes for plastic degradation	
11.30 – 12.30	ORAL PRESENTATIONS (A – CHEMISTRY) <i>Chair: Rosana Ribić</i>	A-01 (3F)
11.30 – 11.50	Antonija Tomić Influence of dpp3 inactivation on its interaction with the Kelch domain of KEAP1	
11.50 – 12.10	Donna Danijela Dragan Exploring pantoprazole–cyclodextrin interactions <i>via</i> coffee ring imaging and thermodynamic profiling/electrospinning technology in the development of medical applications	
12.10 – 12.30	Ivana Kekez Stabilization and structural characterization of metagenomic esterases for enhanced bioplastic degradation	

10.30 – 12.30	B – CHEMICAL ENGINEERING AND BIOTECHNOLOGY <i>Chair: Marko Rogošić</i>	A-03 (3F)
10.30 – 11.00	INVITED LECTURE Ana Jurinjak Tušek Artificial intelligence in biochemical engineering: application and future perspective	
11.00 – 11.30	INVITED LECTURE Ana Vrsalović Presečki Multienzyme systems in the production of nutraceuticals from renewable sources	
11.30 – 12.30	ORAL PRESENTATIONS (B – CHEMICAL ENGINEERING AND BIOTECHNOLOGY) <i>Chair: Krunoslav Žižek</i>	A-03 (3F)
11.30 – 11.50	Želimir Kurtanjek Causal AI modelling of chemical process plant	
11.50 – 12.10	Antonija Čelan Ultrasound vs. mechanical mixing in batch crystallization, comparison of key hydrodynamic parameters and effect on final product	
12.10 – 12.30	Filip Car Application of 3D-printing for production of ceramic monolithic catalysts for oxidation of aromatic volatile organic compounds	
10.30 – 12.30	7th SYMPOSIUM VLADIMIR PRELOG <i>Chair: Matija Gredičak</i>	A-02 (3F)
10.30 – 11.00	INVITED LECTURE Ana Ratković Photochemical strategies for the design of cholinesterase-targeting small-molecules	
11.00 – 11.30	INVITED LECTURE Xavier Guinchard Bifunctional chiral ligands for enantioselective catalysis <i>via</i> tethered counterion-directed catalysis	
11.30 – 12.30	ORAL PRESENTATIONS (7th SYMPOSIUM VLADIMIR PRELOG) <i>Chair: Matija Gredičak</i>	A-02 (3F)

11.30 – 11.50	Marina Tranfić Bakić Photoactive phenylboronic acid derivative: Synthesis and interactions with sialic acids	
11.50 – 12.10	Gabriel Glotz Phototruncation of cyanines	
12.10 – 12.30	Marko Purić Chiral multisubstituted binol–cyclopentadienyl ligands and their complexes with transition metals	
12.30 – 14.00	Lunch	
14.00 – 15.00	PLENARY LECTURE Martin D. Smith <i>CONTROLLING AXIAL CHIRALITY</i> Chair: Matija Gredičak	A-02 (3F)
15.00 – 15.30	Coffee Break Place	
15.00 – 16.30	Poster presentations Place	
17.00 – 18.30	A – CHEMISTRY Chair: Marina Tranfić Bakić	A-02 (3F)
17.00 – 17.30	INVITED LECTURE Gordan Horvat Ion-binding properties of linear and cyclic oligopeptides	
17.30 – 18.30	ORAL PRESENTATIONS (A – CHEMISTRY) Chair: Marina Tranfić Bakić	A-02 (3F)
17.30 – 17.50	Laura Nuić Azodioxy thin films <i>via</i> on-surface polymerization of aromatic dinitroso compounds	
17.50 – 18.10	Mario Pajić Uncovering the role of ABCs in the solid-state Suzuki-Miyaura reaction <i>via in situ</i> Raman monitoring	
18.10 – 18.30	Matija Modrušan Anion binding by phenylalanine and leucine cyclopeptides: thermodynamic and structural study	

17.00 – 18.30	B – CHEMICAL ENGINEERING AND BIOTECHNOLOGY <i>Chair: Krunoslav Žižek</i>	A-01 (3F)
17.00 – 17.30	INVITED LECTURE Boštjan Genorio “Green” graphene in electrocatalysis	
17.30 – 18.30	ORAL PRESENTATIONS (B – CHEMICAL ENGINEERING AND BIOTECHNOLOGY) <i>Chair: Zoran Mandić</i>	A-01 (3F)
17.30 – 17.50	Hongwei Yu Electrolyte engineering enables long-life in high-energy-density lithium metal batteries	
17.50 – 18.10	Yunyun Luo Interface-tailored separators via iCVD for lithium metal batteries with extended lifespan	
18.10 – 18.30	Maris Minna Mathew Nickel electrocatalysts for HER: Bridging material performance and data integrity	
17.00 – 18.30	ORAL PRESENTATIONS (C – MATERIALS AND NANOTECHNOLOGY) <i>Chair: Fabio Faraguna</i>	A-03 (3F)
17.00– 17.20	Ivana Panžić Environmentally friendly lead-free thin films for high-performance dielectric capacitors	
17.20 – 17.40	Mia Mesić The influence of preparation parameters on the morphology and ferroelectric properties of metal-organic thin films based on bicyclic amines	
17.40 – 18.00	Sanja Burazer Understanding battery failure mechanisms through structure changes during operando XRD measurements	
18.00 – 18.20	Andrea Szpecht Unlocking the potential of ionic liquids in epoxy resin design and composite performance	

Thursday, September 4, 2025

8.00 – 9.00 Registration

Atrium of 3F ①

9.00 – 10.00 **PLENARY LECTURE**

Boelo Schuur

CHALLENGES & DIRECTIONS TO CONVERT LINEAR PRODUCTION INTO CIRCULAR & BIOBASED

Chair: Vesna Tomašić

A-02 (3F)

10.00 – 10.30 **Coffee Break**

10.30 – 12.30 **A – CHEMISTRY**

Chair: Karl Gademann

A-02 (3F)

10.30 – 11.00 **INVITED LECTURE**

Nikola Basarić

Bodipy compounds: fluorescent labels, photocages and potential drugs

11.00 – 11.30 **INVITED LECTURE**

Ines Primožič

New class of therapeutics for Alzheimer's disease symptom control

11.30 – 12.10 **ORAL PRESENTATIONS (A – CHEMISTRY)**

Chair: Danijela Musija

A-02 (3F)


11.30 – 11.50 **Antea Hrepić**

Modern approaches to laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) analysis

11.50 – 12.10 **Sara Krivačić**

Carbonized metal-organic frameworks as ultra-hydrophobic solid transducer in potentiometric potassium probes

10.30 – 12.10	C – MATERIALS AND NANOTECHNOLOGY <i>Chair: Matko Erceg</i>	A-01 (3F)
10.30 – 11.00	INVITED LECTURE Vilko Mandić Optimising the device architecture for small molecule bulk-heterojunction photovoltaics	
11.00 – 11.30	INVITED LECTURE Lidija Ćurković Microwave-assisted synthesis and application of a molecularly imprinted core-shell photocatalyst	
11.30 – 12.10	ORAL PRESENTATIONS (C – MATERIALS AND NANOTECHNOLOGY) <i>Chair: Nataša Stipanelov Vrandečić</i>	A-01 (3F)
11.30 – 11.50	Marijana Đaković From mechanical properties to atomic-level mechanism of elastically flexible crystals	
11.50 – 12.10	Martina Perić Bakulić Harnessing optical properties of quantum noble metal bio-nano hybrids	
10.30 – 12.10	D – ENVIRONMENTAL PROTECTION AND SUSTAINABLE DEVELOPMENT <i>Chair: Ivona Nuić</i>	A-03 (3F)
10.30 – 11.00	INVITED LECTURE Ivana Grčić Photocatalytic decomposition of methane as a technology for reducing emissions from low-methane municipal waste landfills	
11.00 – 11.30	INVITED LECTURE Gordana Pehnec Polycyclic aromatic hydrocarbons in particulate matter and total deposited matter in Croatia	
11.30 – 12.10	ORAL PRESENTATIONS (D – ENVIRONMENTAL PROTECTION AND SUSTAINABLE DEVELOPMENT) <i>Chair: Marina Trgo</i>	A-03 (3F)
11.30 – 11.50	Andrea Špoljarić Development and evaluation of nZVI-based materials for arsenate removal from water: Adsorption performance	



11.50 – 12.10	Patrik Bubalo Effect of process parameters on removal of acetamiprid with nanofiltration membranes
12.10 – 13.30	Lunch
13.30 – 14.30	<i>PLENARY LECTURE</i> <i>Pablo Dominguez de Maria</i> <i>CHALLENGING SUSTAINABILITY: ESTIMATING THE CO₂ PRODUCTION IN (BIO)CATALYTIC REACTIONS</i> <i>Chair: Zvezdana Findrik Blažević</i> A-02 (3F)
14.30 – 15.00	Coffee Break
14.30 – 16.00	<i>POSTER PRESENTATIONS</i>
17.00 – 20.00	Excursion
21.00 – 24.00	Gala Dinner

Friday, September 5, 2025

9.00 – 10.00	PLENARY LECTURE Jiří Kaleta <i>SURFACE-MOUNTED MOLECULAR DEVICES</i> <i>Chair: Katarina Varga</i>	A-02 (3F)
10.00 – 10.30	Coffee Break	
10.30 – 11.40	A – CHEMISTRY <i>Chair: Zoran Kokan</i>	A-02 (3F)
10.30 – 11.00	INVITED LECTURE Ivana Brekalo The use of templates in the mechanochemical synthesis of Zeolitic Imidazolate Frameworks	
11.00 – 11.40	ORAL PRESENTATIONS (A – CHEMISTRY) <i>Chair: Zoran Kokan</i>	A-02 (3F)
11.00 – 11.20	Nela Malatesti Tripyridyl porphyrins in photodynamic therapy on melanoma cells under the CoCl ₂ -induced hypoxia	
11.20 – 11.40	Nataša Šijaković Vujičić Self-sorting versus co-assembly: Structural insights into supramolecular oil gels	
10.30 – 11.20	ORAL PRESENTATIONS (B – CHEMICAL ENGINEERING AND BIOTECHNOLOGY) <i>Chair: Bruno Zelić</i>	A-01 (3F)
10.30 – 11.00	INVITED LECTURE Torsten Mayr Shining light on microbioreactors: Exploring the power of optical sensing	
11.00 – 11.20	ORAL PRESENTATIONS (B – CHEMICAL ENGINEERING AND BIOTECHNOLOGY) <i>Chair: Anita Šalić</i>	A-01 (3F)
11.00 – 11.20	Desislava Yordanova Apostolova Electrocatalytic approaches to high-efficiency hydrogen peroxide generation in microfluidic systems	

11.20 – 12.20	ORAL PRESENTATIONS (C – MATERIALS AND NANOTECHNOLOGY) <i>Chair: Ladislav Vrsalović</i>	A-03 (3F)
11.20 – 11.40	Mateja Filković Challenges of glass as a primary packaging material in pharmaceutical industry	
11.40 – 12.00	Jakov Tenžera Improvements of tin halide perovskite thin films by crystallization mediators and plasma-assisted crystallization	
12.00 – 12.20	Grgur Mihalinec Perovskite-based anodes: a new hope for next-gen lithium-ion batteries	
12.40 – 13.00	Closing ceremony and poster awards	A-02 (3F)

8.45 – 13.45	E – EDUCATION <i>Chairs: Olgica Martinis and Željka Soldin</i>	Science School Split
8.45 – 9.00	OPENING CEREMONY	
9.00 – 9.45	PLENARY LECTURE Vladislav Tomišić CONDUCTIVITY OF ELECTROLYTE SOLUTIONS: MACROSCOPIC AND MICROSCOPIC VIEWS ON THE MOTION OF IONS UNDER THE INFLUENCE OF AN ELECTRIC FIELD	
9.45 – 10.45	INVITED LECTURE Ante Kolak Strengthening basic teaching competencies in chemistry teaching	
10.45 – 12.15	INVITED LECTURE Vladimir Stilinović New recommendations for Croatian nomenclature of inorganic chemistry	
12.15 – 13.45	WORKSHOPS	
	Innovative Pedagogy – Chemistry Board Games <i>Milan Nikolić</i>	
	Pub Quiz – Chemical Elements <i>Vladimir Stilinović</i>	

13.45 – 14.45 Poster session and lunch break

14.45 – 16.00 **ORAL PRESENTATIONS (E – EDUCATION)**

Chair: Olgica Martinis and Željka Soldin

Science School Split

14.45 – 15.00 **Ana Magovac**

Integrated approach to teaching radioactivity: Connecting chemistry and physics for better understanding

15.00 – 15.15 **Đani Škalamera**

Lego photometer as a tool for studying chemical reaction kinetics

15.15 – 15.30 **Marijana Žgela Putniković**

Green chemistry in high school experiments

15.30 – 15.45 **Tajana Kovačević**

Differentiated teaching of chemistry

15.45 – 16.00 **Final remarks and closing**

POSTER SCHEDULE

Wednesday, September 3, 2025

Section: CHEMISTRY

Thursday, September 4, 2025

Section: CHEMICAL ENGINEERING AND BIOTECHNOLOGY

Section: MATERIALS AND NANOTECHNOLOGY

Section: ENVIRONMENTAL PROTECTION AND SUSTAINABLE DEVELOPMENT

Friday, September 5, 2025

Section: EDUCATION

POSTER PRESENTATIONS

CHEMISTRY	
P-A01	<u>Marija Alešković</u>, Jasna Alić, Wolfgang E. Ernst, and Marina Šekutor Emergence of diamondoid clusters in helium nanodroplets
P-A02	<u>Petra Bajt</u>, Ivančica Vicković, Jelena Kovačić, Petra Turčić, Daniela Amidžić Klarić, and Ana Mornar Turk Deucravacitinib Tablet Dosage Forms: Achieving Analytical Excellence Through a Novel HPLC-DAD Method
P-A03	<u>Konrad Barnowski</u>, Łukasz Skalniak, Katarzyna Nakielska, Anna Stasiłowicz-Krzemień, Judyta Cielecka-Piontek, and Jacek Plewka Natural Compounds as LAG-3 Inhibitors in Cancer Immunotherapy
P-A04	<u>Maja Biočić Šormaz</u>, Dora Županović, and Lea Kukoč-Modun Development and Validation of a Flow Injection Method for the Determination of Ascorbic Acid in Pharmaceutical Preparations
P-A05	<u>Narendra Bisht</u> and Nikola Topolovčan Shortening the Linker-Distance in Binol-derived Cyclopentadiene Ligands
P-A06	<u>Barbara Bogović</u>, Ivanka Jerić, and Vilko Smrečki Fmoc Solid-Phase Synthesis and Structural Characterization of C-Glycopeptides
P-A07	<u>Jakov Borovec</u>, Toni Divjak, Alma Ramić, Nika Jakobović, Bruna Bakota, Ines Primožič, and Tomica Hrenar Machine Learning Prediction of Cholinesterase Inhibition by α -Benzoylamino Acetamides
P-A08	<u>Lidija Brkljačić</u> and Matija Gredičak Development of LC-MS/MS Method for Simultaneous Determination of Thiamine, Folic Acid, and Niacin in Fermented Milk Supplements Containing Probiotic Bacteria
P-A09	<u>Franko Burčul</u>, Ana Vučak, Kristina Jurlina, Azra Đulović, Ivica Blažević, Petra Brzović, and Ivana Generalić Mekinić Quantitative Determination of the Chiral Compounds in the Sea Fennel Essential Oil Using GC-MS/MS
P-A10	<u>Mia Bušljeta</u>, Bernard Denegri, and Mirela Matić Nucleofugality of Phenylsulfinate Leaving Group in Aqueous Acetone and Aqueous Ethanol
P-A11	<u>Mia Bušljeta</u>, Mirela Matić, and Bernard Denegri Duality in S_N1 and S_N2 Mechanisms in Reactions of Benzyl Chlorides with Amines Under Solvolytic Conditions
P-A12	<u>Mario Cetina</u>, Silvija Maračić, and Silvana Raić Malić Conformation and Supramolecular Structures of <i>n</i> -Heterocyclic Hybrids Based on 1,2,3-Triazole and Quinoline
P-A13	<u>Lara Čižmek</u>, Filip Stipić, Iva Erak, and Dunja Božić Development of a Dye Ingress Test Comparable to Microbial Ingress for Assessing Container Closure Integrity
P-A14	<u>Karla Čižmešija</u> and Nataša Šijaković Vujičić Innovative Gelled Emulsions for General Use

P-A15	Marija Cvetnić, Dajana Barišić, Nikola Bregović, Vladislav Tomišić Binding of Carboxylate Anions by (Thio)urea-calix[4]arenes
P-A16	Vladimir Damjanović, Dino Kuzman, Marina Cindrić, and Višnja Vrdoljak The Mechanochemical Synthesis of Co(III)-ammine Heteropolyoxomolybdates $[X_xMO_mO_y]^{n-}$ (X = Al, Si, Ge or Te)
P-A17	Andrea Dandić, Aleksandar Széchenyi, Mateja Budetić, Mirela Samardžić, Ines Drenjančević, and Nikolina Kolobarić Development and Characterization of a 1,8-Naphthalimide-based Fluorescent Probe for Hydrogen Sulfide Detection in Human Blood Serum
P-A18	Barbara Debanić Monitoring and Characterization of Subvisible Particles in Pharmaceutical Products Using Micro-flow Imaging (MFI)
P-A19	Toni Divjak and Ines Primožič Synthesis of α -Nicotinoylamino Acetamide Derivatives as Butyrylcholinesterase Inhibitors
P-A20	Senka Djaković, Jasmina Lapić, Matea Bakota, Ema Živković, and Valerije Vrčec Substituent Effects on the Regioselectivity of the Ferrocenylation of Purines
P-A21	Nikolina Filipović, Tomislav Balić, Martina Medvidović-Kosanović, Dominik Goman, Anamarija Stanković, Marija Jozanović, Martina Šrajer Gajdošik, Stjepan Šarić, Sunčica Roca, and Elvira Kovač-Andrić Coordination-driven Selectivity: Ternary Copper(II) Bipyridine Complexes with Antitumor Potential
P-A22	Tea Frey, Matija Popović, Ivana Biljan, and Ivan Kodrin Strategic Design of Porphyrin-based Porous Organic Polymers for CO ₂ Capture: A Computational Study
P-A23	Marcela Šišić, Leo Frkanec, and Ruža Frkanec Biomimetic Nanomaterials Functionalized with Peptidoglycan Monomer: Studying Carbohydrate-Mediated Interactions for Biomedical Use
P-A24	Dominik Goman, Tatjana Gajić, Iva Kurtović, Ivica Đilović, Krištof Kranjc, Ivana Balić, Tomislav Balić, Martina Medvidović-Kosanović Electrochemical Study of Novel Hydrazone Macrocylic Compounds
P-A25	Filip Grdović, Zoran Kokan, and Srećko I. Kirin Enantioselective Transition Metal Catalysis with Self-Assembled Host-guest Systems
P-A26	Ita Hajdin and Ante Prkić 3D Printed Ion Selective Electrodes for Potassium Ion Determination
P-A27	Ivan Ilakovac, Ivan Marić, Anđela Pustak, Ivana Landripet, and Tanja Jurkin Comparison of Microstructural and Magnetic Properties of Radiolytically Synthesized Feroxyhyte and Magnetite Nanoparticles for Magnetic Hyperthermia Treatment
P-A28	Ana Ivančić, Zhenxue Zhang, Krunoslav Bojanić, Iana Fomicheva, Hyoungwon Park, Katarina Marušić, Silke Christiansen, Maja Dutour Sikirić, and Darija Domazet Jurašin Dimeric Metallosurfactant with Zinc: Physicochemical Properties in Solution and Application as Antibacterial Coating
P-A29	Nika Jakobović, Tomica Hrenar, and Ines Primožič Multiligand Docking of Three-membered Heterocycles in the Active Site of Butyrylcholinesterase
P-A30	Jasmina Jukić, David Kučera Čavara, and Tajana Begović Adsorption of Poly(<i>N</i> -ethyl-2-vinylpyridinium bromide) on Silica Nanoparticles and Flat surfaces

P-A31	Tea Juračić, Tajana Begović, and Adriana Kendel Effect of Chloride Ions Adsorption on the SERS Activity of Silver Nanoparticles
P-A32	Filip Lešić, Dijana Jureša, and Leo Štefan Nitrosamine Impurity Risk Assessment in Ophthalmic Pharmaceutical Product
P-A33	Sandra Jurić and Emanuela Erceg Solvolytic Reactivity of Triphenylphosphonium Salts
P-A34	Sandra Jurić and Emanuela Erceg Comparison of the Nucleofugalities of the Neutral Leaving Groups
P-A35	Lucija Jurko, Alja Štern, Karlo Wittine, Olivija Plohl, Matej Bračić, Damjan Makuc, Janez Plavec, Bojana Žegura, and Rupert Kargl Design and Antimicrobial Activity of Polyallylamine- <i>N</i> -hydroxysuccinamide Conjugates
P-A36	Antonija Karakaš and Davor Margetić Mechanochemistry as a Green Route to Trisubstituted Guanidines
P-A37	Maja Karnaš Babić, Vesna Rastija, Milan Vraneš, Dejan Agić, and Domagoj Šubarić Ecotoxicity Estimation of Imidazole-Based Ionic Liquids: The Effect of Alkyl Side Chain Length
P-A38	Ivana Kavain, Vlatka Paštar, Marijana Franičević, Krunoslav Aladić, and Ivana Carev Variability, Composition, and Chemical Profiling of Lavender Extract from Croatia Obtained with Supercritical Extraction
P-A39	Luka Klemen, Andrea Usenik, Karla Kukina Gradečak, Ivana Nikšić-Franjić, Mateja Belovari, Marta Jurković, Nikola Cindro, Nađa Došlić, Ivo Piantanida, and Vladislav Tomišić Fluorescence "Without Fluorophores": Investigating Cation Complexation by Calixarenes
P-A40	Ivan Kodrin and Tea Frey Polymorphism and Mechanical Behavior in Molecular Crystals: a Computational Study
P-A41	Robert Junior Kolman and Matija Gredičak Dearomative [3+3] Annulation for The Construction of Polycyclic Skeletons
P-A42	Mario Komar, Maja Molnar, Katarina Jukić, Martina Jakovljević Kovač, and Tihomir Kovač Mechanochemical Synthesis of 1,2,3-Triazoles via Copper(I)-catalysed 1,3-Dipolar cycloaddition: a Green Approach to Antifungal Agents
P-A43	Dino Koranić, Lucija Brtan, Ivana Kekez, and Aleksandra Maršavelski Identification and Functional Characterization of Metagenomic Esterases for Biodegradation of Bioplastics
P-A44	Veronika Kovač, Ivana Kmetič, Teuta Murati, and Marina Miletić Biological Activity of New Ferrocenylpyrimidine Derivatives of Curcumin
P-A45	Marija Hefer, Nikolina Filipović, Stjepan Šarić, Ana Petrović, Martina Smolić, Martina Šrajer Gajdošik, and Elvira Kovač-Andrić Spectroscopic Characterization of (–)-Epicatechin-lipid Interactions in a MASLD Model
P-A46	Petra Kovačec, Leentje Persoons, Dirk Daelemans, and Tatjana Gazivoda Kraljević Synthesis and Biological Activity of New Benzoxazolinone–coumarin Hybrids
P-A47	Luka Krstulović, Marijana Leventić, Ivan Ćorić, and Ljubica Glavaš-Obrovac Antiproliferative Activity of Novel Benzimidazole- Coumarin Hybrids

P-A48	Filip Kučas, Robert Pendelić, Morana Dulić, Marko Močibob, Ita Gruić-Sovulj, and Vesna Petrović Peroković Synthesis of Arginine Hydroxamate – a Potential Inhibitor of Aminoacyl-tRNA Synthetase
P-A49	Lea Kukoc-Modun, Matea Vukorepa, Maja Biocic-Sormaz, Sanja Perinovic-Jozic, and Spas D. Kolev A New Generation of Polymer Inclusion Membranes with Superior Performance
P-A50	Bojan Kuridža, Julien Boixel, and Ivo Piantanida Diarylethene-based Photoswitches: Photochemical Behavior and Biomolecular Interactions
P-A51	Matea Laučan, Alma Ramić, and Ines Primožič Novel Bioactive Quaternary Quinuclidine Peptidomimetics
P-A52	Katarina Leko, Nikola Cindro, Andrea Usenik, Gregor Talajić, and Vladislav Tomišić Complexation Reactions of Soft Metal Cations with Calix[4]arene Derivatives Containing Sulphur and Glucose Functionalities
P-A53	Vilma Lovrinčević, Dragana Vuk, Irena Škorić, and Nikola Basarić Mechanistic Study of Aminobiphenyl Photocages
P-A54	K. Majerová Varga, D. Lončarić, E. Kaletová, C. Santos Hurtado, M. Mašat, and J. Kaleta Photoswitchable Cucurbit[7]urils
P-A55	Martina Mušković, Martin Lončarić, Nikola Basarić, Ivana Ratkaj, and Nela Malatesti Synthesis and Evaluation of (Oxidopyridyl)porphyrins in Photodynamic Therapy
P-A56	Iva Džeba, Anđela Goluža, Đani Škalamera, and Ivan Ljubić Design and Development of Quinazoline White Light Emitters for Lightning Application
P-A57	Maja Friščić, Ivanka Maleš, Sanja Radman, Željko Maleš, and Igor Jerković Essential Oil and Hydrosol Composition of <i>Globularia alypum</i> L. from Croatia
P-A58	Antonija Mamić, Kristina Butković, Kristina Starčević, Leentje Persoons, Dirk Daelemans, Robert Vianello, and Marijana Hranjec Synthesis and Biological Activity of Novel Methoxy and Hydroxy Substituted Pyridine Benzamides
P-A59	Sven Marinac, Andrea Usenik, Matija Modrušan, Jakov Borovec, Katarina Pičuljan, Katarina Leko, Gordan Horvat, Josip Požar, Nikola Cindro, Tomica Hrenar, and Vladislav Tomišić Calorimetric, Spectroscopic, and Computational Studies of Calixarene-solvent Adducts Formation
P-A60	Jan Meixner, Vilma Lovrinčević, Dragana Vuk, and Ines Despotović Quantum-chemical Study of Thermal Transformations of <i>o</i> -Divinylbenzene Derivatives
P-A61	Tihana Mlinarić, Donna Danijela Dragun, Iva Rezić Meštrović, and Ernest Meštrović Crystals on the Edge: Coffee-ring Symmetry, Diffusion, and Unpredictability in a Single Drop of Pantoprazole
P-A62	Krešimir Molčanov, Petra Stanić, and Lidija Androš Dubraja Phase Transformation and Self-healing of a Charge-transfer Crystal
P-A63	Lidija Molčanov, Krešimir Molčanov, Filip Torić, Mirta Herak, Sanja Burazer, and Marijana Jurić Structural and Magnetic Properties of the Oxalate-based [Cu ^{II} Cr ^{III}] Complexes: the Influence of Solution on Dimensionality
P-A64	Maja Molnar, Mario Komar, Martina Jakovljević, Nika Rak, Nora Slivar, and Dragica Suknović Mechanochemical Synthesis of Coumarin Based Thiosemicarbazides

P-A65	Danijela Musija, Dino Kuzman, Tomica Hrenar, and Višnja Vrdoljak Vanadium(V) Aroylhydrazone Complexes: Synthesis, Characterization, Cytotoxic and Antibacterial Activity
P-A66	Kristian Nakić, Zhejian Cao, Ita Hajdin, Ante Prkić, Ivan Mijaković, and Ivana Mitar Green Microwave-hydrothermal Synthesis of Mixed-phase Copper/copper oxides: Chamomile Extract's Effect on Relative Phase Abundance and Antibacterial Potential
P-A67	Renata Odžak, Antonio Sabljic, and Matilda Šprung Quinuclidine BisQACs: Structure–Activity Relationship Analysis with Focus on Antimicrobial Resistance
P-A68	Mario Oraić, Želimira Filić, Lucija Brtan, Ivana Kekez, and Aleksandra Maršavelski Identification and Characterization of Novel PLA-Degrading Esterases from Metagenomic Databases
P-A69	F. Pahović, J. S. Sajko, and I. Jerić Preparation of a Potential Urea-based Organocatalyst from D-(–)-Quinic acid
P-A70	Barbara Panić, Mladen Borovina, Matija Popović, and Ivana Biljan Azo-bridged Porous Organic Polymers for CO ₂ Capture and Conversion
P-A71	Dijana Pavlović Saftić, Natalie Mutter, Filippo Savini, Željka Ban, Andrea Hloušek-Kasun, Branimir Bertoša, Ivo Piantanida, and Ivan Barišić Smart Biosensor Design: Harnessing G-Quadruplex and Antimicrobial Peptides for Selective Pathogen Detection
P-A72	Vesna Pehar, Ivana Cetina, Valentina Ključarić, and Donna Vadlja Toxicity of Carbamate Herbicides – Impact on Human
P-A73	Petra Petrović and Snežana Miljanić Shape Matters: the Role of Gold Nanoparticle Morphology in SERS Detection of G-Quadruplex
P-A74	Danijela Beneš, Vesna Petrović Peroković, Željka Car, and Rosana Ribić Synthesis of Cholesterol Derivatives of Mannosylated Desmuramyl Peptide
P-A75	I. Picek, D. Musija, V. Damjanović, B. Foretić, and Z. Štefanić Supramolecular Self-assembled Hexacyano-ferrate(II)-based Charge-transfer Complexes
P-A76	Matija Popović, Mladen Borovina, Barbara Panić, and Ivana Biljan Porphyrin-based Azo-bridged Porous Organic Polymers: CO ₂ Capture and Conversion Towards Sustainable Solutions
P-A77	J. Požar, M. Modrušan, N. Cindro, M. Cvetnić, A. Usenik, K. Leko, S. Petrović, J. Borovec, G. Horvat, V. Stilinović, T. Hrenar, and V. Tomišić Thermodynamic Insights into the Chelate Effect; the Calix[4]arene Conformation Influence on Cation Complexation
P-A78	Mila Radan, Vedrana Čikeš Čulić, Ivana Carev, and Marina Tranfić Bakić Photoactive Phenylboronic Acid Derivatives: Light-Modulated Antiproliferative Action of Azobenzene Boronic Acid on Breast Cancer Cells
P-A79	Lucija Klobučar, Alma Ramić, and Nikola Cindro Total Synthesis of Dispyrrolopyridine A
P-A80	Josip Rešetar, Karla Remar, Ana Mikleušević, Josipa Suć Sajko, Ines Bašić, and Matija Gredičak One-Pot Synthesis of Functionalized Pyrrolo[3,4-b]indoles via a Tandem Barton–Zard and Friedel–Crafts Approach

P-A81	Petra Glagolić, Tihana Mlinarić, Donna Danijela Dragun, Ernest Meštrović, and Iva Rezić Meštrović Green Synthesis of Metal Nanoparticles for Investigation of the Coffee – Ring Effect
P-A82	Mirta Rubčić, Nikola Miše, Edi Topić, Dario Barišić, and Damir Pajić Tuning the Magnetism in Copper(II) systems: From Discrete Complexes to Low-dimensional Hybrid Organic-inorganic Materials
P-A83	Antonio Sabljic, Matilda Šprung, and Renata Odžak Design and Synthesis of <i>Soft</i> Quaternary Ammonium Salts Based on 3-Aminoquinuclidine with Amide-Linked Alkyl Chains
P-A84	Leon Sačer, Marina Ter, Doris Babić, Martin C. Taylor, John M. Kelly, and Silvana Raić-Malić Synthesis and Structural Characterization of New Nitro(triazole/imidazole)-appended quinolines with Potential Antitrypanosomal Activity
P-A85	Hanna Zhukouskaya, Marija Jozanović, Robert Vianello, Lucija Vrbanić, Martin Hruby, Jiri Panek, Marija Kraševac Sakač, Sunčica Roca, Dražen Vikić-Topić, Dean Marković, and Nikola Sakač New Potentiometric Sensor for Anionic Surfactants
P-A86	Marija Jozanović, Marija Miloš, Rozelindra Čož-Rakovac, Petra Ivančan, Bojan Šarkanj, Nada Glumac, Domagoj Drenjančević, Nikolina Filipović, Nikola Sakač, and Dean Marković Influence of Alkyl Chain Length on Antibacterial and Antifungal Activities of Vinylimidazolium Quaternary Ammonium Compounds
P-A87	Mirela Samardžić, Ema Vlahović, Mateja Budetić, and Andrea Dandić Development of the New MIP-based Thiabendazole-selective Sensor
P-A88	Tijana Stanić, Marina Zekić, and Anđela Zečić Volatile Aroma Compounds of Traditional Croatian Cheese “Prigica”
P-A89	Leo Štefan, Ivan Sušan, Marin Roje, Mladenka Jurin, Anđela Buljan, Marijana Pocrnić, Nives Galić, and Ana Čikoš Degradation Profiling and <i>In Silico</i> Toxicity Assessment of Lifitegrast
P-A90	Elza Štefanović and Nataša Šijaković Vujičić Self-healing Oil Organogelators as Fat Substitutes in Food Spreads
P-A91	Josipa Suć Sajko and Ivanka Jerić Conformational Control and Functional Modulation of Peptides Using Aminoshikimic Acid
P-A92	Dario Šušnić, Berislav Perić, and Zoran Kokan Benzene-1,3,5-Tricarboxamide Systems: Host-guest Interactions, Photoswitching, and Ion Coordination
P-A93	Dhanesh Tiwary, Rajat Singh, and Yogendra Pal Singh Synergistic UV Photocatalysis Using ZnO and Biomass Carbon in a Hydrogel Matrix
P-A94	Edi Topić, Juraj Toplak, Dino Kuzman, Damir Pajić, Filip Torić, and Višnja Vrdoljak Structural Features and Magnetic Properties of Copper(II) Hydrazonato Complexes
P-A95	Nikolina Vidović, Karla Selar, Rafaela Šilje, Nikola Cindro, Matija Modrušan, Gordan Horvat, and Vladislav Tomišić Efficient Cyclization of Functionalized Peptides <i>via</i> Chloride Templating
P-A96	Nives Vladislavić, Ivana Škugor Rončević, Marijo Buzuk, Josipa Dugeč, and Martina Maričević Antioxidant Characterization of Spices and Autochthonous Dalmatian Species by Electrochemical and Spectrophotometric Methods

P-A97	Nina Vukadinović, Lidija-Marija Tumir, and Marijana Radić Stojković Noble Metal Nanostructures and Cannabinoids: A Synergistic Approach to Bioactivity
P-A98	Alma Vuran and Nataša Šijaković Vujičić Effect of Additives on the Structural Properties of Oleogels
P-A99	Ivana Zdravec, Ernest Meštović, Edi Topić, and Donna Danijela Dragun Azithromycin Solvates: Correlating Crystal Structure and Surface Properties with Taste Prediction

CHEMICAL ENGINEERING AND BIOTECHNOLOGY	
P-B01	Iva Zokić, Bianca Lerotić, Marija Jurak, Marko Sejdić, and Jasna Prlić Kardum Evaluation of Various Scale-up Criteria for Ceritinib Spherical Crystallization
P-B02	Anita Šalić, Renata Vičević, Ana Jurinjak Tušek, and Bruno Zelić Development of Deep Eutectic Solvents with ADJUSTABLE Properties for Sustainable Enzymatic Processes
P-B03	Renata Vičević, Anita Šalić, Marina Cvjetko Bubalo, Ana Jurinjak Tušek, Davor Valinger, and Bruno Zelić Integration of Computational Modelling and Experimental Validation to Improve the Stability of GDH and Hydrogenase in DES-based Systems
P-B04	Jelena Jakić, Lea Goreta, Miće Jakić, and Ivana Smoljko Salinity-dependent Corrosion Properties of Copper in Seawater
P-B05	Dino Skendrović and Ana Vrsalović Presečki Optimization of the Activating Agents in the Immobilization of Laccase on Mesoporous Silica and Magnetic Nanoparticles
P-B06	Iva Blažević, Aleksandra Sander, Dajana Kučić Grgić, and Maja Bival Štefan Characterization of Ginger and Turmeric Extracts
P-B07	Vesna Tomašić, Marina Duplančić, and Zoran Gomzi The Influence of Intraphase Diffusion on the Oxidation of Toluene Over Manganese-based Oxide – a Comprehensive Theoretical and Experimental Study
P-B08	Mirjana Čurlin, Marina Fusco, and Virgijina Lipoveci AI-driven Modeling for Quality Optimisation of the Wastewater Treatment Plant's Output stream
P-B09	Ana-Marija Gotal Skoko, Ivana Flanjak, Martina Skendrović Babojelić, and Ante Lončarić The Mold Battle: Traditional and Conventional Apple Cultivars vs <i>Penicillium expansum</i>
P-B10	Mia Božiković, Matea Raić, and Zoran Mandić Impact of C-rate on Battery Formation and Solid Electrolyte Interphase Layer Development
P-B11	Vanja Kosar, Veronika Gorup, Maja Klasić, and Nikol Jović Optimisation of the Imidacloprid Photodegradation in a Rotating Photoreactor Using the Response Surface Methodology
P-B12	Matija Cepanec, Anja Damjanović, Marijan Logarušić, Marina Cvjetko Bubalo, and Marko Rogošić Prediction and Correlation of Water Activity Using the COSMO-RS, Wilson and Redlich-Kister Models in Deep Eutectic Systems (DES)

P-B13	Lan Julij Zadavec, Simon Schröder, Sandy Schmidt, Angelina Osipyan, and Zvezdana Findrik Blažević Investigation of Reaction Kinetics of Two Piperazate Syntheses
P-B14	Leo Mandić, Klara Maruševac, Jana Gašperov Kašuba, Ivana Šoljić Jerbić, Fabio Faraguna, and Ante Jukić Polymer-solvent Molecular Interactions in PDLLA/PLGA-DMSO Systems
P-B15	Petra Pongrac, Jana Gašperov Kašuba, Ivana Šoljić Jerbić, and Fabio Faraguna Insights into Copolymer Solution Viscosity Behaviour – Potential Systems for Drug Delivery
P-B16	Karlo Blažević, Rafael Anelić, Ivana Šoljić Jerbić, Dorina Kružić, and Fabio Faraguna Thermal Degradation Kinetics of the PLGA Copolymers of Different Molar Mass and Composition (Lactide to Glycolide Molar Ratio)
P-B17	Hrvoje Tašner, Grgur Mihalinec, Sanja Burazer, and Zoran Mandić Impact of Mass Loading and Active Material Microstructure on Capacity of Lithium Iron Phosphate Electrodes
P-B18	Lara Štorga, Donna Danijela Dragun, Ernest Meštrović, and Iva Rezić Meštrović Simulation of Lung Tissue in a “Lung-on-a-chip” Model
P-B19	Ana-Katarina Marić, Holly Stolterfoht-Stock, Margit Winkler, Martina Sudar, and Zvezdana Findrik Blažević Carboxylic Acid Reductase: a Key for Enzymatic Aldehyde Synthesis
P-B20	Nevena Milčić, Ivana Čevd, Maja Majerić Elenkov, and Zvezdana Findrik Blažević Biocatalytic Synthesis of (<i>R</i>)-3-Hydroxy- γ -butyrolactone
P-B21	Marta Pleše, Donna Danijela Dragun, Ernest Meštrović, Petra Pongrac, and Fabio Faraguna Simulation of Pulmonary Soft Tissue Using a Lung-on-a-Chip Platform with Integrated Respiratory Monitoring Sensors
P-B22	Anđela Marković, Donna Danijela Dragun, Karlo Blažević, Ernest Meštrović, and Fabio Faraguna Development and Characterization of Sustained-Release Indomethacin Delivery Systems <i>via</i> Electrospinning
P-B23	Vladić Jelena, Dina Balaić, Anja Golemac Lipovac, Stela Jokić, Krunoslav Aladić, Ivana Flanjak, and Igor Jerković Phytochemical Characterization and Skin Cell Modulatory Potential of Supercritical CO ₂ Extracts from <i>Foeniculum Vulgare</i> and <i>Juniperus Communis</i>
P-B24	Monika Znika, Zvezdana Findrik Blažević, Etienne Séverac, Magali Remaud Siméon, and Martina Sudar Enzymatic Synthesis of Glucolipids for Sustainable Consumer Products
P-B25	Marija Kovačević Babić, Daniela Horvat, Krešimir Dvojković, Gordana Šimić, Jurislav Babić, Vinko Krstanović, Krešimir Mastanjević, and Kristina Habschied Croatian Wheat Varieties and Beta Glucan Content
P-B26	Tonči Rezić, Ivan Perković, Roland Ludwig, Florian Csarman, Ana Jurinjak Tušek, and Marina Cvjetko Bubalo Activation of LPMO in Low-temperature Deep Eutectic Solvent

MATERIALS AND NANOTECHNOLOGY

P-C01	Mateja Filković and Domagoj Vrsaljko Challenges of Glass as a Primary Packaging Material in Pharmaceutical Industry
P-C02	Elizabeta Forjan, Marijan-Pere Marković, Dajana Kučić Grgić, Katarina Šulek, and Domagoj Vrsaljko Fabrication and Properties of COC/Cu Composite Filaments
P-C03	Marijan-Pere Marković, Elizabeta Forjan, Matea Milovac, and Domagoj Vrsaljko Influence of 3D Printing Parameters on the Mechanical Properties of 17-4 PH Stainless Steel Parts
P-C04	Antonija Mravak, Vlasta Bonačić-Koutecký, and Stefan Vajda The Role of Size-selected Metal Nanoclusters in Catalytic CO ₂ Mitigation
P-C05	Suresh Kumar Pandey, Sandra Romic, Josipa Papac Zjačić, Hrvoje Kušić, Marin Kovačić, Marijana Kraljić Roković, Ana Lončarić Božić, Boštjan Žener, Boštjan Genorio, and Urška Lavrenčič Štanger Fe-substituted SrTiO ₃ : A Route Toward Tailored Electronic and Optical Properties
P-C06	Nikola Zdolšek, Mia Božiković, Marijana Kraljić Roković, and Zoran Mandić Exploring 1-Ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide Ionic Liquid as Advanced Electrolyte for Calcium-oxygen Batteries
P-C07	Ena Miletić and Katarina Mužina Synthesis and Characterization of Mesoporous Zinc Oxide Doped with Copper and Nickel
P-C08	Tara Balen, Margarita Bužančić Milosavljević, Antonija Mravak, Ita Hajdin, Marina Tranfić Bakić, and Martina Perić Bakulić Enhancing DSSC Performance with Natural Dyes and Noble Metal Nanoclusters
P-C09	Gabrijela Ljubek, Kaltrina Stajku, Marijana Kraljić Roković, Leonarda Vugrin, Pierluigi Bilotto, and Markus Ostermann Mechanochemistry for Unique Fluoride-free MXene
P-C10	Andrej Molnar, Grgur Mihalinec, and Zoran Mandić Utilization of Ionic Liquids in Next-generation Carbon Based Supercapacitors
P-C11	Rafael Anelić, Karlo Blažević, Monika Mihaljević, Ivana Perković, Martin Keleminić, Patrik Grahovac, Fabio Faraguna, and Ivana Šoljić Jerbić Influence of Blending Parameters on the Structural and Thermal Properties of PLA/PGA Systems for Drug Delivery Applications
P-C12	Ivana Biljan, Laura Nuić, Ana Senkić, Nataša Vujičić, Matej Bubaš, Marko Kralj, and Igor Rončević Polymer Semiconductor Thin Films Based on Dinitrosobiphenyl Moiety
P-C13	Dawid Zielinski, Andrea Szpecht, and Marcin Smiglak Tailoring Mechanical Performance of Epoxy Composites Using Dicyanamide-based Ionic Liquid Mixtures
P-C14	Adrian Zajac, Małgorzata Nyga, Małgorzata Kopytko, and Katarzyna Komorowska New Surface Passivating Ionogel Technology for Mesa-Type Detector Structures (PASION project)
P-C15	Ivana Landripet, Ivan Marić, Ivan Ilakovac, Anđela Pustak, Marijan Gotić, and Tanja Jurkin Tailoring Properties of Sr-ferrite and Doped Iron Oxide Nanoparticles for Hyperthermia Effect
P-C16	Željka Boček, Elizabeta Forjan, Andrej Molnar, Marko Zubak, Domagoj Vrsaljko, and Petar Kassal Fully Printed Modularized Microfluidic Setup for <i>In Situ</i> Analytical Monitoring Based on Electrochemical Detection of Methylene Blue

P-C17	Jozefina Katić, Sara Krivačić, Elizabeta Horvat, Željka Petrović, and Dajana Mikić Surface Modification of Titanium Implants with Electrodeposited Multifunctional Calcium Phosphate Coatings
P-C18	Lucija Fiket, Yuhka Uda, Xin Sun, Bicheng Zhu, Zoran Žujović, Jadranka Travaš-Sejdić, and Zvonimir Katančić Conductive PEDOT-Thermoplastic Elastomer Films for Stretchable Electronics Applications
P-C19	Katarina Sokač Pogrmilović, Vittorio Coen, and Krunoslav Žižek Formulation of Dasatinib-loaded Cyclodextrin Nanosponges for TARGETED Drug Delivery
P-C20	Lina Šepić, Filip Dlačić, Lea Raos, Sanja Burazer, Grgur Mihalinec, and Zoran Mandić Enhancing Lithium-ion Battery Performance with Silicon-graphite Composite Negative Electrodes
P-C21	Tamara Holjevac Grgurić, Karla Knežević, Lucija Lasić, Primož Mrvar, Stevica Hodić, Vilko Mandić, Sanja Martinez, and Emi Govorčin Bajsic Surface Modification of Ti-6Al-4V Alloy
P-C22	Floren Radovanović-Perić, Michael Burtscher, and Vilko Mandić Spark Ablation Coupled with Aerosol Direct Writing in Thin Film Fabrication
P-C23	Irena Krešić, Branka Andričić, Matko Erceg, and Petra Joskić Influence of LiBOB Concentration on the Structure and Thermal Properties of Poly(ethylene-oxide)/lithium Montmorillonite Nanocomposite
P-C24	Teodora Prebeg, Maja Stanković, Ardita Lazami, and Gordana Matijašić Enhancement of Antimicrobial Properties of DECM-based Hydrogels for Application in Skin Tissue Engineering

ENVIRONMENTAL ENGINEERING AND SUSTAINABLE TECHNOLOGIES

P-D01	Martina Miloloža, Dora Lastovčić, Želimira Cvetković, Marin Ganjto, Matija Cvetnić, Marinko Markić, Tomislav Bolanča, Dajana Kučić Grgić, Šime Ukić Isolation and Identification of Microorganisms from Activated Sludge Polluted with Antivirals
P-D02	Anita Ivanković, Luka Barić, Danijela Petrović, Anita Martinović Bevanda, and Stanislava Talić IT Devices as Detectors in Surface Water Quality Monitoring
P-D03	Sandra Romac, Suresh Kumar Pandey, Martina Kujavić, Josipa Papac Zjačić, Marin Kovačić, Ana Lončarić Božić, Urška Lavrenčić Štanger, and Hrvoje Kušić Light-driven Degradation of PFAS Using Fe-modified SrTiO ₃ Photocatalysts
P-D04	Ivana Škugor Rončević, Nives Vladislavić, Marijo Buzuk, and Josipa Dugeč Investigation of the Corrosion-inhibiting Properties of Rosemary Extract for Aluminum
P-D05	Jelena Milić, Dušan Karan, Aleksandar Dimitrijević, Bojan Radak, Ivana Petronijević, and Branko Dunjić Bridging the Gaps: Green Startup Accelerators and Sustainability Innovation in Serbia
P-D06	Jelena Milić, Jelena Avdalović, Tatjana Šolević Knudsen, and Mila Ilić Harnessing Microbial Power for Sustainable Remediation in Circular Economy
P-D07	Silva Žužul, Jasmina Rinkovec, Ivan Bešlić, and Magdalena Vincetić Winter Levels of Metals in Zagreb Air During 2014 and 2024
P-D08	Ivona Nuić and Sunčica Mileta Sweet and Sour Cherry Pits as Sustainable Green Sorbents for the Treatment of Heavy Metal-Contaminated Water

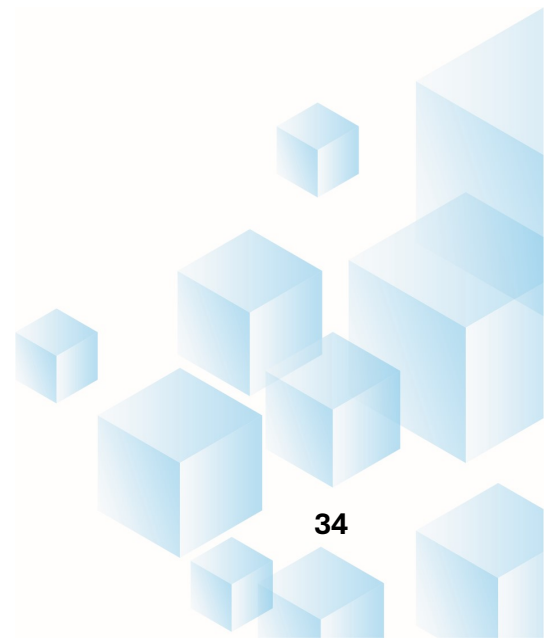
P-D09	Karlo Grgurević, Vesna Ocelić Bulatović, Dora Bramberger, Martina Miloloža, Matija Cvetnić, Marinko Markić, Šime Ukić, Tomislav Bolanča, Mirela Leskovac, Elvira Vidović, Jasmina Ranilović, Kristina Kanižaj, and Dajana Kučić Grgić Tuning Properties of PLA/PHBV Blends with Bioplasticizers for Food Packaging
P-D10	Tajana Horvat, Ivana Jakovljević, and Gordana Pehnec Comparison of Selected Volatile Organic Compounds in Zagreb City Households Across Two Seasons
P-D11	Tatjana Šolević Knudsen, Gordana Dević, Jelena Avdalović, Mila Ilić, Jelena Milić, Sandra Bulatović, and Nenad Marić Biomarker Fingerprint as a Forensic tool for Oil Spill Source Identification in Alluvial Sediments
P-D12	Tatjana Šolević Knudsen, Aleksandra Tasić, and Ivan Kojić Pesticides Burden in Surface Waters Adjacent to Small Agricultural Holdings in Eastern Serbia
P-D13	Silvia Morović, Paula Šimun, Marija Katarina Drmić, Matija Cvetnić, Sandra Babić, and Krešimir Košutić Enhancing RO Membrane Selectivity for <i>N</i> -Nitrosamine and Boric Acid Rejection via 1,10-Diaminodecane Plugging
P-D14	Petra Štefanec Vesić, Ivan Gabrijel, and Kristina Dropučić Comparative Characterization of Fluidized Bed Fly Ash and Conventional Fly Ash for Use in Self-compacting Concrete
P-D15	Nikolina Račić, Mario Lovrić, Gordana Pehnec, Ivana Jakovljević, Zdravka Sever Štrukil, Iva Smoljo, Silva Žužul, and Jasmina Rinkovec From Airborne Particles to Soil Deposits: Understanding the Distribution of PAHs and Heavy Metals
P-D16	Antonija Avdalović, Milica Mandić, Mirko Đurović, Nataša Stipanelov Vrandečić, and Ladislav Vrsalović Application of ATR-FTIR Spectroscopy for the Identification of Microplastics

EDUCATION

P-E01	Dražen Crnčec Adoption of Educational Outcomes in Chemistry Through the Extra-curricular Activity "Orchardists Group" Using the Example of Determining the Streif Index
P-E02	Marija Pustak, Ljilja Mišević, and Nives Vladislavić From Theory to Practise: Scientia Projects as a Model for Modern STEM Teaching
P-E03	Monika Pavić and Maja Jurić-Babaja AI and Chemistry – Smart Science of the Future
P-E04	Martina Šeler Namjesnik and Martin Buljubašić Introducing Advanced Analytical Methods to High School Students: Can Different Candle Waxes be Distinguished by ¹ H NMR Spectroscopy?
P-E05	Mirta Malčić and Suzana Lovrić A Journey Through Time – A Chemistry Lesson with the Help of Artificial Intelligence



PLENARY LECTURES



SMALL ANGLE SCATTERING AND ITS APPLICATION IN CHEMISTRY, LIFE, AND MATERIAL SCIENCE

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Small Angle X-ray Scattering (SAXS) is a versatile technique used on synchrotrons and many laboratories all over the world. It provides information on nanostructures regarding dimensions, shapes and aggregation states from roughly 1 nm to > 100 nm. All states of matter, i.e. solid, liquid, aerosol and thin surfaces can be probed. The opportunity to investigate samples in their “natural” environment and with high time resolution is one of the strong points of this technique.

The experimental possibilities at the Austrian SAXS beamline operated at the synchrotron radiation source Elettra – Sincrotrone in Trieste will be presented. Here the focus will be on in-situ and in-operando experiments, as well as on results obtained for self-assembled thin films.

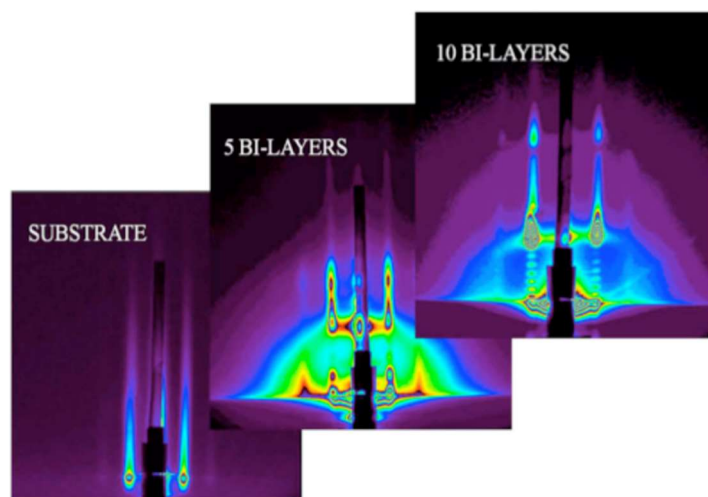


Figure 1. Grazing Incidence SAXS images from thin multilayer films on a rippled substrate.



CHALLENGING SUSTAINABILITY: ESTIMATING THE CO₂ PRODUCTION IN (BIO)CATALYTIC REACTIONS

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Enzymes may offer eco-friendly options to traditional organic synthesis. Yet, like any other chemical process, biocatalysis require water, solvents and energy, what inevitably generates waste. Developing reliable metrics to evaluate the environmental impact of enzymatic reactions, particularly at early stages, results crucial.^[1] The traditional E-Factor ($\text{kg waste} \cdot \text{kg product}^{-1}$)^[2] is intuitive, albeit it is often used to assess wastes that are fully treated in the chemical plant (wastewater, solvents, etc), and do not remain in the planet.^[3] When such wastes are treated, CO₂ is the ultimate residue, formed upon wastewater treatment, from solvent incineration, and from the energy used in the (bio)catalytic reaction.^[3,4] That CO₂ remains in the planet and should be therefore the key aspect to be environmentally considered, to put forth processes that may balance sustainability with commercial viability. This talk discusses a rapid tool to estimate the “Global Warming Potential (GWP)” – expressed as $\text{kg CO}_2 \cdot \text{kg product}^{-1}$ – of (bio)catalytic reactions, deducing equations based on reaction parameters such as “conversion”, “substrate loading”, “reaction time”, and “temperature”.^[5] The method compares reaction conditions and identifies key CO₂-producing hotspots, pinpointing greener biomanufacturing options while preserving the efficiency of biocatalytic systems.

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SURFACE-MOUNTED MOLECULAR DEVICES

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Surface-mounted molecular devices represent a distinctive class of stimuli-responsive smart materials that continue to garner significant scientific interest due to their broad range of potential applications - from modulating physical properties to enabling photopharmacological functions. These systems generally comprise two essential components: a stimuli-responsive head group, which serves as the functional core, and a molecular platform that performs several critical roles. Specifically, the platform: (i) ensures reliable surface attachment through appropriately designed anchoring groups; (ii) provides sufficient spacing between adjacent molecules; (iii) facilitates electronic decoupling of photoactive units from metallic substrates to reduce quenching of excited states; and (iv) ideally positions functional units in a well-defined and predictable geometry above the surface.^[1] In this presentation, three conceptually distinct strategies for constructing such responsive two-dimensional molecular arrays will be discussed: Langmuir-Blodgett films,^[2] self-assembled monolayers, and surface inclusions within porous nanocrystals.^[3,4] These approaches offer complementary advantages and will be compared in terms of structural control, functional performance, and suitability for specific applications.

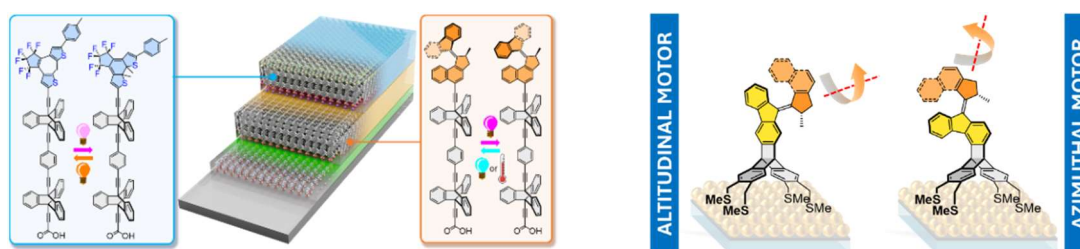


Figure 1. Photoswitchable Langmuir-Blodgett films (left) and self-assembled arrays of tetrapodal light-driven molecular motors (right).

Acknowledgements. This work has been supported by the Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences (RVO: 61388963), the Czech Science Foundation (grant number: 20-13745S), and the Ministry of Education, Youth and Sports of the Czech Republic (grant number: LUAUS23144).

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ECO-FRIENDLY CHEMICAL SEPARATION BASED ON POLYMER INCLUSION MEMBRANES AND BEADS

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Separation based on Polymer Inclusion Membranes (PIMs), a relatively recently introduced type of liquid membranes, offers an attractive alternative to conventional solvent extraction by mimicking this important separation process, utilised extensively in industry and chemical analysis, but without the use of a large inventory of volatile, flammable and often toxic diluents.^[1–3] In addition to minimizing the amounts of extractants used, thus reducing the cost of separation, PIMs provide possibilities for substantial improvements to the overall speed of the separation process and to the reduction of its complexity based on allowing both extraction and back-extraction to proceed simultaneously at opposite sides of the membrane. In most cases a PIM is composed of a base polymer (e.g., PVC, cellulose triacetate) and an extractant (e.g., Aliquat 336), acting as plasticiser. However, in some cases, the inclusion in the PIM composition of a plasticiser or a modifier may be required for improving the membrane homogeneity, flexibility and extraction properties. PIMs allow the complete transfer of a target chemical species from a feed solution to a receiving solution, separated by the membrane, by a facilitated transport mechanism.

Micro Polymer Inclusion Beads (μ PIBs) with compositions similar to those of PIMs have been fabricated recently using a microfluidic technique and applied to the separation of Au(III) [3], rare earth metal ions^[4] and Zn(II).

PIMs and μ PIBs have been used successfully for the selective separation of metallic and non-metallic ionic species of industrial and environmental importance. This presentation will outline some of them to illustrate the potential of these advanced polymeric extracting materials in industrial separation (e.g., clean-up of mine tailings water, recovery of noble and strategic metals from electronic waste) and online separation in chemical analysis.

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CHALLENGES & DIRECTIONS TO CONVERT LINEAR PRODUCTION INTO CIRCULAR & BIOBASED

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The current society is heavily dependent on fossil fuel that is used for both energy applications such as heating and cooling dwellings, and as transportation fuel, but also as feedstock for the chemical industries. For many transport applications, firing fossil fuels can already be replaced by driving electric, but to construct consumer goods, electrons only are not sufficient and the carbon atoms are needed.

With 10 % of the fossil fuel being used in production processes, the amount of oil equivalents needed worldwide are so much, that if transported by train, it would require on every single day a train of 600 km. Replacing this amount of oil equivalents by biobased chemicals seems a humongous challenge. Would we be able to maintain enough biodiversity? It would be better to reduce the demand for freshly sourced carbons by recycling strategies. If we can recycle up to 80 % of all the carbon in our consumer goods, that train with oil equivalents would already reduce to 120 km per day.

So, we need both effective and efficient recycling approaches, and accepting we can never recycle 100 %, we also need biorefineries in which we source the make-up carbon that is lost in the life cycle. In both recycling and biorefineries, the carbon sources are typically much more complex than in crude oil, and that means that the standard processes in the petrochemical industry cannot be applied without any modification. Being a separation technologist, in this conference contribution, next to outlining the challenges and possible directions on a generic level, I will also show that developing new separation processes is key to realizing effective production routes based on complex feedstocks. This includes a new approach towards regeneration of solvents that we are currently developing in my group.

CONTROLLING AXIAL CHIRALITY

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Axially chiral compounds are of growing importance within the fields of catalysis, medicine and agrochemistry and hence new approaches for their stereocontrolled synthesis remain valuable.^[1] Here we describe a series of strategic approaches for the enantioselective synthesis of axially chiral compounds including oxidative cross coupling^[2] and dynamic stereochemical methods^[3] employing chiral counterions.^[4]

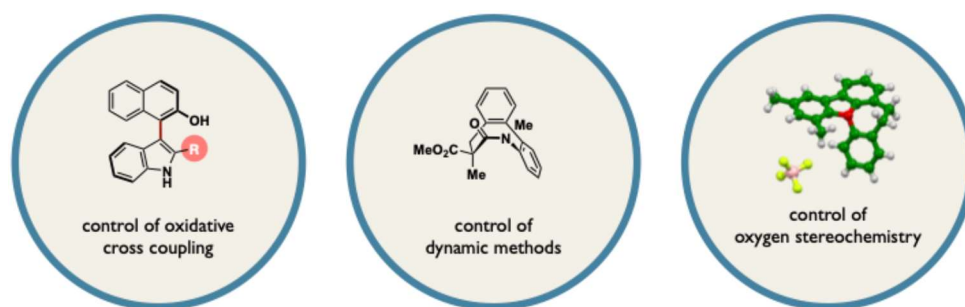


Figure 1. Strategic approaches to selectivity within this work.

We also extend this approach to an examination of stereochemistry at trivalent oxygen,⁵ and outline the unexplored chemistry of triaryloxonium ions.⁶

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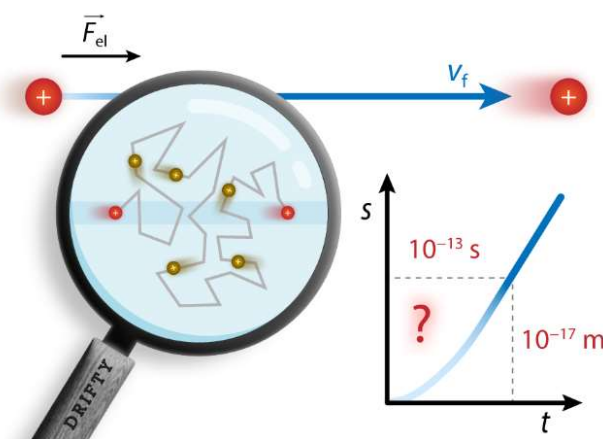
CONDUCTIVITY OF ELECTROLYTE SOLUTIONS: MACROSCOPIC AND MICROSCOPIC VIEWS ON THE MOTION OF IONS UNDER THE INFLUENCE OF AN ELECTRIC FIELD

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Comprehending the phenomena lying behind the conductivity of electrolyte solutions is essential at all levels of electrochemistry learning. However, the traditional macroscopic approach to teaching the motion of ions under the influence of an electric field can lead to misconceptions about what actually happens at the submicroscopic scale.^[1,2] In this talk, the macroscopic and microscopic views on the motion of ions in solution, with and without the applied electric field, will be compared and discussed. By setting the appropriate equations, solving them, and analyzing the obtained results, it will be shown that the macroscopic model cannot be simply mirrored to account for the properties of particles at the submicroscopic level.^[2] An interactive simulation ([available for download](#))^[2] is proposed for use in teaching the migration of ions in solution. It provides the opportunity to simulate the purely Brownian motion of ions in the absence of an electric field and that when the field is “switched on”, i.e. when a directional component resulting from the action of the electric force is superimposed to the completely random motion. The implementation of this tool can help a wide range of students, from secondary school to university ones, to visualize the fact that the averaging of movements of many ions in solution results in the macroscopically observed properties corresponding to (unrealistic) uniform motion of the species comprising ion and its solvation sphere through solution. The described approach to teaching the ionic conductivity facilitates students’ insight into the distinction and relation between the macro- and microscopic properties of the moving charged particles, and can be readily extended to other transport phenomena.

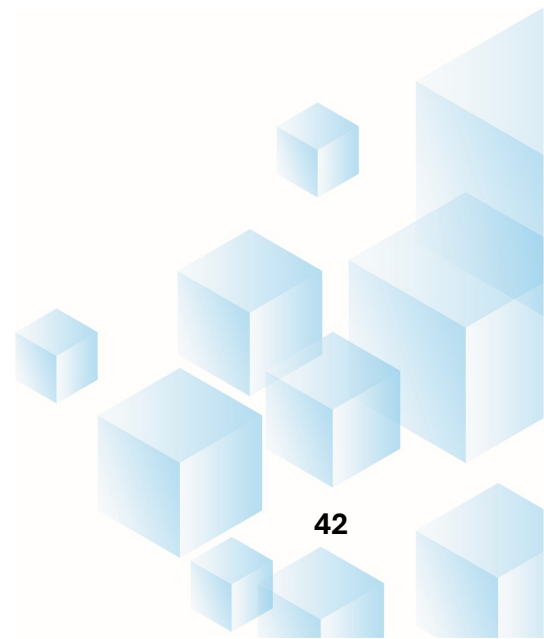


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INVITED LECTURES



BODIPY COMPOUNDS: FLUORESCENT LABELS, PHOTOCAGES AND POTENTIAL DRUGS

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BODIPY is a trade name for heterocyclic compounds with the IUPAC name 4,4-difluoro-4-bora-3a,4a-diaza-s-indacene. Owing to their excellent spectral and photophysical properties and easy structural modifications, they have gained a significant scientific interest with applications in fluorescence sensing,^[1a] molecular biology as fluorescent markers^[1b] and phototherapeutics.^[1c]

In the past decade at the Ruđer Bošković Institute we developed a series of BODIPY compounds (such as **1**, Figure 1) which show unusual photochemical reactivity from higher excited states (also known as anti-Kasha photoreactivity) and have applicability in fluorescent labeling of proteins.^[2] Moreover, we extended the study of photoreactive BODIPY compounds to photocleavable protective groups, also known as photocages. Contrary to the ubiquitous BODIPY photocages that undergo cleavage at the *meso*-methylene position,^[3] we develop dyes that are cleavable at boron (such as **2**),^[4] which have potential for the development of new phototherapeutics that do not base their action on singlet oxygen formation.^[5] Furthermore, the photocages have potential for the use in organic synthesis as protective groups, as well as in biology or medicine for the targeted temporally and spatially controlled delivery of biologically active substances. In addition to photoreactive BODIPY compounds, we were also interested in fluorescent dyes that selectively accumulate in intracellular organelles and can be used in cell biology (such as **3** for labeling mitochondria).^[6] The lecture will feature different BODIPY dyes, their synthesis, photophysical properties and photoreactivity as well as applications in different fields of research.

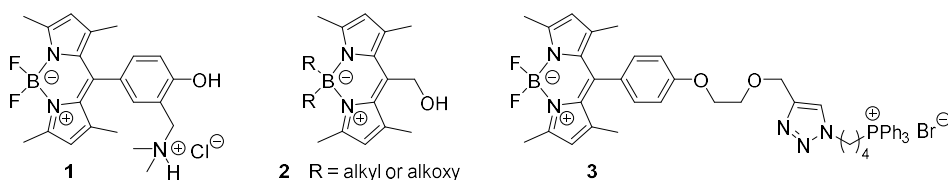


Figure 1. Different BODIPY derivatives investigated at the Ruđer Bošković Institute.

Acknowledgements. This work has been supported by the Croatian Science Foundation by research grants HrZZ-IP-2024-05-8565 and HrZZ-IP-2019-04-8008.

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THE USE OF TEMPLATES IN THE MECHANOCHEMICAL SYNTHESIS OF ZEOLITIC IMIDAZOLATE FRAMEWORKS

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Zeolitic imidazolate frameworks (ZIFs) are an extensively studied class of porous materials built from tetrahedral metal centers and imidazolate ligands, with potential uses in separations, catalysis and guest capture.^[1] They exist in many different solid forms which often appear concomitantly, so the control of their polymorphism is crucial. Mechanochemistry has been shown to offer not only high yields, fast reaction times and little to no waste, but also good control over solid form selection in ZIFs.^[2]

We here show that combining templation effects with mechanochemistry can not only allow for the controlled synthesis of many solid forms of the simplest ZIF, zinc imidazolate, but the judicious use of templates can also provide new forms of ZIFs that can't be made solvothermally.^[3] Periodic DFT calculations are performed to rationalize the results of mechanochemical screening, and to predict future reaction outcomes.

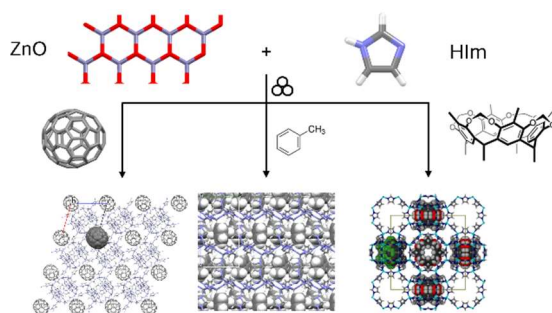


Figure 1. Graphical representation of the templation effect in mechanochemical ZIF synthesis.

Acknowledgements. This work has been supported by the European Union from the NextGenerationEU programme through grant NPOO.C3.2.R2-I1.06.0049

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MICROWAVE-ASSISTED SYNTHESIS AND APPLICATION OF A MOLECULARLY IMPRINTED CORE-SHELL PHOTOCATALYST

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In this study, magnetic molecularly imprinted $\text{Fe}_3\text{O}_4/\text{SiO}_2/\text{TiO}_2/\text{MIP}$ photocatalyst with selected pharmaceutical as the template was prepared by microwave-assisted synthesis method (Figure 1). For reference, non-imprinted magnetic nanoparticles ($\text{Fe}_3\text{O}_4/\text{SiO}_2/\text{TiO}_2$) were prepared using the same procedure. The synthesis of the non-imprinted magnetic core-shell $\text{Fe}_3\text{O}_4/\text{SiO}_2/\text{TiO}_2$ nanocomposite involved coating magnetite (Fe_3O_4) nanoparticles with a protective silica (SiO_2) layer, followed by a titania (TiO_2) outer shell. For preparation of molecularly imprinted core-shell photocatalyst, acetonitrile was used as porogen and solvent, methacrylic acid as monomer, 2,2'-azobis(metil-propionitril) as initiator, ethylene glycol dimethacrylate as crosslinker, and diclofenac as pharmaceutic template. The molecularly imprinted TiO_2 layer has specific cavities designed for the diclofenac target molecule (imprint), resulting in a synergistic effect of extraction by adsorption and photocatalysis^[1]. Microwave radiation enables fast and uniform heating rate, rapid nucleation and growth of particles, shortens reaction time, and enables energy savings. The structure and properties of the synthesized materials ($\text{Fe}_3\text{O}_4/\text{SiO}_2/\text{TiO}_2$ and $\text{Fe}_3\text{O}_4/\text{SiO}_2/\text{TiO}_2/\text{MIP}$) were characterized using XRD, FTIR, SEM, VSM, BET, and DRS techniques.

The synergistic effect of adsorption and photocatalysis as well as the kinetics and mechanism of diclofenac degradation using $\text{Fe}_3\text{O}_4/\text{SiO}_2/\text{TiO}_2$ and $\text{Fe}_3\text{O}_4/\text{SiO}_2/\text{TiO}_2/\text{MIP}$ were determined and analysed. The results demonstrated that the developed photocatalyst enables efficient degradation of diclofenac under simulated solar irradiation, combined with easy magnetic separation, underscoring its potential for practical application in wastewater treatment.

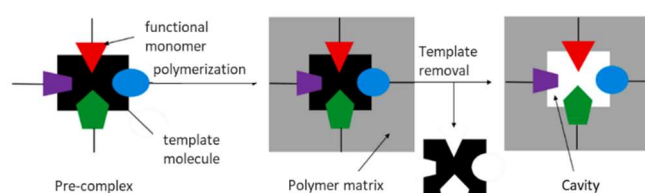


Figure 1. Synthesis procedure of molecularly imprinted polymers.

Acknowledgements. This work was funded by the Croatian Science Foundation under the project [IP-2022-10-4400]: Development of molecularly imprinted polymers for use in analysis of pharmaceuticals and during advanced water treatment processes (MIPdePharma).

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MODELING EXCITED-STATE MOLECULAR DYNAMICS WITH CLASSICAL TRAJECTORIES

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Understanding how molecules behave after absorbing light is essential for explaining a wide range of photochemical and photophysical phenomena—from fluorescence and photostability to charge transfer and energy conversion. Theoretical investigation of these light-induced processes often relies on nonadiabatic molecular dynamics methods, which account for the coupling between nuclear and electronic motion.

Among these methods, Trajectory Surface Hopping (TSH) is widely used. It combines classical nuclear trajectories with stochastic transitions between electronic states, providing an efficient and intuitive way to simulate excited-state dynamics.

In this contribution, we present an overview of how TSH can be effectively applied to simulate photoinduced processes in molecular systems. We discuss key methodological aspects, including the sampling of initial conditions, the choice of hopping algorithms and electronic structure methods, and strategies for analyzing simulation outcomes.

Through selected case studies, we demonstrate how TSH can reproduce time-resolved spectroscopic observables and reveal key mechanistic features such as internal conversion, bond rearrangement, and nonradiative decay. Our goal is to make TSH more accessible to chemists interested in excited-state reactivity by providing both theoretical context and practical guidance for its successful application.

PHOTOCATALYTIC DECOMPOSITION OF METHANE AS A TECHNOLOGY FOR REDUCING EMISSIONS FROM LOW-METHANE MUNICIPAL WASTE LANDFILLS

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Landfills present environmental, economic, and social challenges, primarily due to pollution caused by the decomposition of organic waste within the landfill itself. The breakdown of organic waste generates methane (CH_4), a greenhouse gas that contributes significantly to climate change. CH_4 is typically managed through flaring, which converts it into carbon dioxide (CO_2) and water vapor (H_2O). However, when methane concentrations fall below 20 %, flaring becomes economically unfeasible, resulting in its direct release into the atmosphere. This study investigated the potential of photocatalytic oxidation with the aim of developing a suitable air protection technology for landfill sites. This process utilizes solar radiation and a photocatalyst and has proven to be both effective and cost-efficient in degrading pollutants such as CH_4 in landfill gas. Additionally, a mathematical model was developed for multiphysics simulation and for designing future systems to reduce landfill gas emissions at the source.

Laboratory tests of photocatalytic degradation on a gas sample containing CH_4 from the Totovec non-hazardous waste landfill showed an average CH_4 concentration reduction of 19.91 % across three measurements: 21.59 % in the first, 18.15 % in the second, and 20.00 % in the third, at slightly lower initial methane concentrations in gas samples (<10%). The tests confirmed the effectiveness of photocatalytic oxidation, as CH_4 was oxidized to carbon monoxide (CO) and CO_2 , which was evidenced by a 30 % increase in CO levels. The mathematical model identified key factors influencing CH_4 degradation in the annular reactor, particularly the importance of pipe length. Although the model proved effective, the proper design of a photocatalytic system for application at landfill sites remains a challenge due to the need for extensive customization and specialized expertise for this specific use.

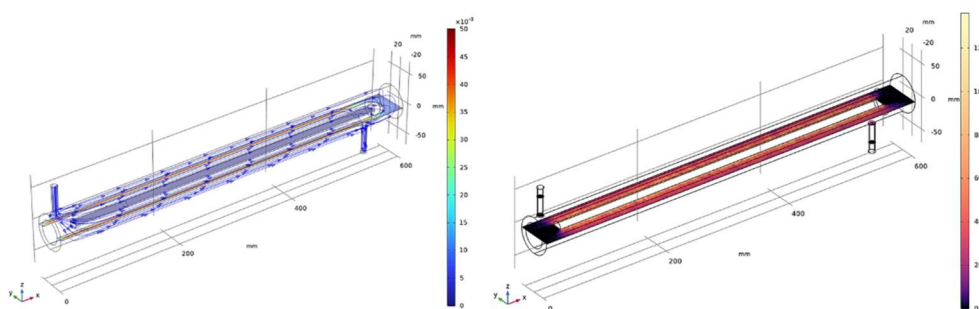


Figure 1. CFD and Ray trace modelling results in the annular reactor

Acknowledgements. This work has been supported by the project “Recycling rubber & solar photocatalysis: ecological innovation for passive air and health protection” supported by the European Regional Development Fund, KK.01.1.1.07.0058.

“GREEN” GRAPHENE IN ELECTROCATALYSIS

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Carbon, a fundamental element of life and a cornerstone of the life sciences has attracted much attention in materials science since the revolutionary isolation of graphene — a two-dimensional carbon allotrope — in 2004. The extraordinary mechanical, thermal, electrical, and optical properties of graphene have brought it to the forefront of research and innovation. Since its discovery, graphene-based materials have shown enormous potential for a wide range of applications, including composites, sensors, transistors, spin valves, radio frequency identification tags, flexible displays, ultrafast lasers, and nano-healthcare applications (e.g. drug delivery systems, cancer therapy, and biological imaging), as well as various energy-related devices such as fuel cells, supercapacitors and ultra-light batteries. However, to fully exploit the potential of graphene-based materials in energy storage and conversion, a thorough understanding of their role in electrocatalysis is crucial.

Graphene-based derivatives can serve “actively” as electrocatalysts or “passively” as catalyst supports. In this area, our research focuses on uncovering the complex interplay between morphology and chemical structure in electrocatalytic reactions, particularly in the oxygen reduction reaction (ORR). ORR is crucial for fuel cells^[1], metal-air batteries^[2], and H₂O₂ electrosynthesis^[3] and is therefore a key area of research. By elucidating the intricate relationships between morphology, chemical composition, and catalytic activity, we aim to advance the development of efficient and durable electrocatalysts for various energy conversion applications.

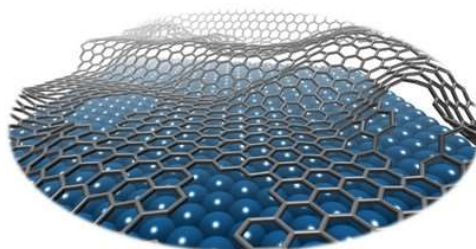


Figure 1. Schematic of graphene electrochemical interface.

Acknowledgements. This work has been supported by Slovenian Research Agency: ARIS through program P2-0423 and projects J7-50227, J2-50086, and J7-4636.

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BIFUNCTIONAL CHIRAL LIGANDS FOR ENANTIOSELECTIVE CATALYSIS VIA TETHERED COUNTERION-DIRECTED CATALYSIS

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The access to enantioenriched molecules via selective catalytic methods is of utmost importance. The **ligand-based approach** (Figure 1a) to enantioselective catalysis often relies on the use of either functionalized or very bulky ligands to trigger geometrical constraints and steric repulsions. The alternative **Asymmetric Counteranion-Directed Catalysis (ACDC) approach**^[1a] relies on the use of chiral counteranions as the source of stereochemical information during the key bond-forming step (Figure 1b). The strong pairing between the cationic metal-substrate complex and the chiral anion is hence central to the transfer of the chiral information. This concept,^[1a] pioneered in Au(I)^[1c] and Pd(0)^[1a] catalysis, was rapidly applied to other transition metals. However, 15 years later, the field did not bloom as much as expected and examples remain sporadic. Why ACDC has met little success probably results from the flexible and poorly defined spatial arrangements of the chiral phosphate-cation pairs (Figure 1b). In this context, we have established (Figure 1c) that tethering the chiral anion to the metal center could be a suitable strategy to increase geometrical constraints and molecular organization in the intermediates involved in catalytic processes and therefore generate higher enantioselectivities. This strategy, named **Tethered Counterion-Directed Catalysis (TCDC)** relies on the use of CPA-Phos chiral bifunctional ligands that are phosphine/phosphoric acid new chiral bifunctional ligands.^[2a] The corresponding Au(I) complexes have been prepared and used successfully as catalysts in a number of enantioselective reactions. The synthesis, coordination and catalytic applications of these chiral ligands will be discussed.^[2]

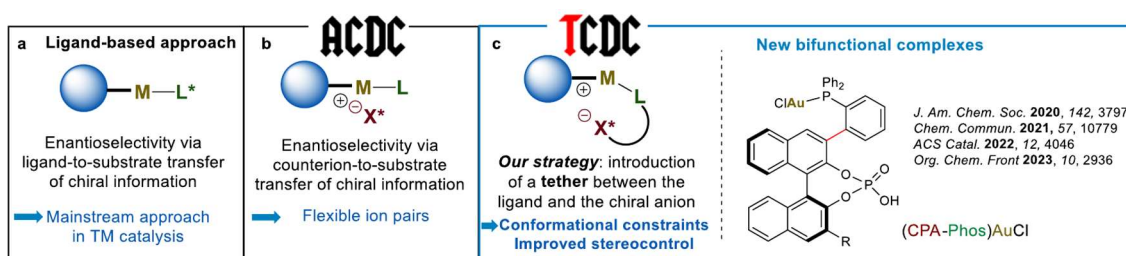


Figure 1. Context of the work.

Acknowledgements. This work has been supported by ANR grant TCDCat.

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ION-BINDING PROPERTIES OF LINEAR AND CYCLIC OLIGOPEPTIDES

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The complexation of anions by both natural and synthetic receptors has become a central theme in the rapidly evolving field of supramolecular chemistry. Among these, cyclopeptides have emerged as a promising and versatile class of macrocyclic anion receptors. Their ability to bind anions arises from the hydrogen-bond donating capacity of the amide groups in the peptide backbone, the structural flexibility of the macrocyclic ring, and the tunability of their subunits. In addition, they can also bind metal cations with their backbone carbonyl groups. Compared to their linear counterparts, cyclopeptides demonstrate enhanced metabolic stability and stronger affinity for charged species.

In this talk, we will present our recent contributions to the field, focusing on the effects of ring size and solvent on the anion-binding properties of cyclopeptides.^[1] The binding of cations by cyclohexapeptides will also be discussed. Additionally, the ion-binding affinities of cyclic peptides will be compared with those of their linear counterparts.^[2] Finally, newly developed macrocyclization strategies for cyclopeptide ring closure will be introduced.^[3]

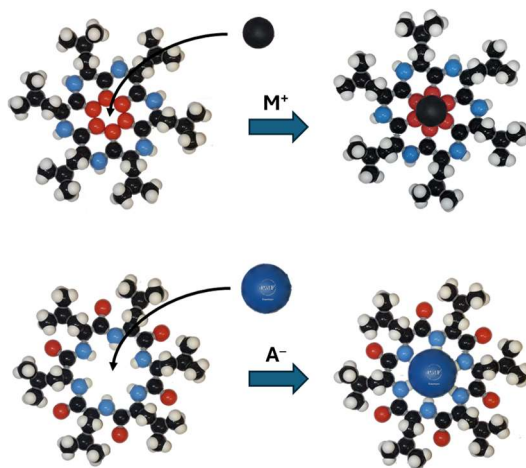


Figure 1. Cyclohexaleucine as ion receptor.

Acknowledgements. This work is supported by Croatian Science Foundation (IP-2024-05-3012).

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ARTIFICIAL INTELLIGENCE IN BIOCHEMICAL ENGINEERING: APPLICATION AND FUTURE PERSPECTIVE

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Artificial intelligence (AI) is revolutionizing the field of biochemical engineering by introducing powerful tools for modelling, optimization, and automation of complex biological systems. AI techniques, particularly machine learning and artificial neural networks (ANN), have significantly improved the ability to make accurate predictions and informed decisions in processes characterized by high variability, non-linearity, and biological complexity. These data-driven approaches are especially valuable in cases where traditional mechanistic models fall short due to incomplete system understanding or dynamic behaviour, as is often the case in fermentation, metabolic engineering, enzyme extraction, and biowaste processing. As the demand for more efficient, sustainable, and cost-effective biotechnological processes continues to grow, the integration of AI and big data analytics becomes increasingly vital. This lecture highlights practical and effective applications of AI-driven modelling in biochemical engineering, emphasizing real-world case studies where intelligent algorithms have provided meaningful advancements. These include the prediction of physicochemical properties of medicinal herb extracts, the use of near-infrared spectroscopy (NIR) coupled with artificial neural networks for real-time monitoring and control of grape skin composting, and the optimization and modelling of lipase extraction using low-toxicity deep eutectic solvent (DES)-based aqueous two-phase systems (ATPS). Together, these examples illustrate how AI enhances data analysis, optimizes process parameters, and supports the development of sustainable solutions across a wide range of biotechnological applications.



OPTIMISING THE DEVICE ARCHITECTURE FOR SMALL MOLECULE BULK-HETEROJUNCTION PHOTOVOLTAICS

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The last generation of solar cells, which are one of the most prominent types of renewable energy sources, includes various technologies and materials. Among the last generation solar cells, organic bulk-heterojunction (BHJ) stand out with advantageous high absorption coefficients, tuneable bandgaps, economically efficient synthesis and low-cost production of high area and flexible panels, as well as modularity e.g. for indoor light harvesting. They however suffer from multiple energy losses, which can be surpassed by synthesizing new systems, such as squaraine derivatives reported hereafter.

Specifically, this work wraps around challenges faced during characterizing, assembling and examining viability of competitive BHJ photovoltaics solar cells from small molecule squaraine derivatives. Squaraines are electron donors and needed blending with a model acceptor such as PC₇₁BM. Firstly, physical and optoelectronic properties of the system were determined. The solubility of squaraines turned out to be the major concern, whereas it was found that prolonged alkyl chains at the ends of the molecule facilitated solubility in non-polar solvents, such as chloroform.

Thereafter it made sense to preliminary address architecture and processing conditions suitability. In-depth analysis was conducted on 2,4-bis(4-(benzyl(isopropyl)amino)-2,6-di-hydroxyphenyl)cyclobuta-1,3-diene-1,3-bis(olate) and 2,4-bis(4-(diisobutylamino)-2,6-dihydroxyphenyl)cyclobut-1-ene-1,3-bis(olate) systems, comprising (micro)structural properties of the BHJ layer, i.e. domain size, crystallinity, preferred orientation, obtained through atomic force microscopy and grazing incidence wide angle X-ray scattering. By improving the squaraine crystallinity in BHJ, short-circuit current of the solar cell increases, likely due to improved equilibrium between charge carrier mobilities.

Altogether, it was confirmed that a low hole mobility of the squaraine derivatives limits device performance by inducing a high charge carrier imbalance, which hinders the transport. Majority of the prepared squaraines proved viable for a full solar cell assembly.

Acknowledgements. This work has been supported by MINGO under the grants NPOO.C3.2.R3-I1.05.0091 and NPOO.C3.2.R3-I1.04.0324. Financial sustenance of University of Zagreb is acknowledged.

HARNESSING ANCESTRAL SEQUENCE RECONSTRUCTION TO ENGINEER THERMOSTABLE ENZYMES FOR PLASTIC DEGRADATION

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Plastic pollution presents an escalating threat to environmental and public health, underscoring the urgent need for innovative strategies to degrade synthetic polymers such as polylactic acid (PLA).^[1] In this study, we report the engineering of a novel PLA-degrading enzyme, MGY, originally identified from a metagenomic dataset. Although MGY exhibited promising catalytic activity, its low solubility, poor expression yield, and limited thermostability restricted its practical application. To address these limitations, we employed ancestral sequence reconstruction^[2] to generate ancestral MGY variants. All variants maintained significant PLA-degrading activity, with one also demonstrating activity against polycaprolactone (PCL). These ancestral enzymes showed enhanced solubility, improved expression levels, and markedly increased thermal stability. Differential scanning calorimetry revealed a melting temperature (T_m) of 84 °C for the most stable variant—the highest reported for any PLA-degrading enzyme to date. In addition, characterization of both PLA and PCL polymers^[3] identified the optimal temperature ranges for their efficient enzymatic degradation. Together, these findings provide insights into the structural determinants of enzyme stability and activity, highlighting ancestral sequence reconstruction as a powerful strategy for engineering robust biocatalysts.

Acknowledgements. This research was funded through National Recovery and Resilience Programme, The Development Research Support (NextGenerationEU), project Enzyme engineering for sustainable recycling of bioplastics (NPOO.C3.2.R2-I1.06.0041).

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SHINING LIGHT ON MICROBIOREACTORS: EXPLORING THE POWER OF OPTICAL SENSING

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Optical chemical sensors are established in process monitoring tools in industry and research laboratories. They basically comprise of a luminescent indicator dye based in a host polymer. They are easy to integrate, non-invasive, do not need any reference element and can be read-out contactless from outside. However, to fully exploit the potential in microfluidic systems or microreactors, the sensors have to fulfil several demands including high brightness, capability to be applied as thin film, excellent photo stability, cheap and accurate read-out systems, ease in use (simple calibration and drift free), simple mass production compatible preparation steps, compatibility with the chip materials, resistance towards sterilization and no toxicity.

We present sensors for important chemical parameters such as oxygen, pH, glucose, lactate, ammonia and hydrogen peroxide fulfilling these demands. Our sensors can be excited with red-light and emit light in the near infra-red range (<700 nm). This suppresses background fluorescence and scattering from biological material. Sensor can be prepared in different formats including coated fibers, ink-jet printed sensor spots or knife-coated spots. Compact measurement instruments enable the read-out of integrated sensor elements in microreactors in sizes from 300 to 800 micrometers or miniaturized probes.

Oxygen and pH sensor are applied in microbio reactors and microfluidic cell culture systems. The integrated sensors are used to monitor cell culture conditions and the cell metabolism. We demonstrate the influence of model drugs and nanomaterials on the cell respiration and acidification.^[1,2] Integrated oxygen sensors are also presented in organ-on-chip to measure the oxygen consumption of cardiac cells during beating motion with electrical stimulation.^[3] We also present glucose and lactate sensors in microfluidic format to measure additional important metabolic parameters. We also developed sensors for ammonia and hydrogen peroxide – analytes that were not able to be monitored continuously, so far. These sensors can be applied to monitor ammonia in trace levels for environmental monitoring and high concentrations in flow reactors.^[4] We present a new sensing concept for detection of hydrogen peroxide in a microfluidic flow cell^[5] and demonstrate the application of this sensors.^[6]

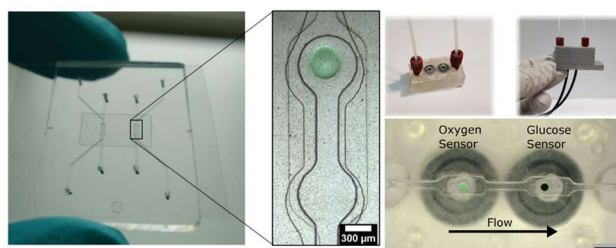


Figure 1. Left: Heart-on-Chip with integrated optical oxygen sensors (green dots). Figure Right: Glucose sensor integrated in a microfluidic flow cell.

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INNOVATIVE PEDAGOGY – CHEMISTRY BOARD GAMES

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The goal of this workshop is to understand the importance and advantages of preparing (together with students) board games with chemical content in chemistry teaching at different levels of education, and to adopt methodological principles that should be used for this purpose. Teachers will gain insights into the selection and adaptation of existing board games and then create a set of their own suitable for use as an additional teaching tool for selected teaching (thematic) units, both in primary and secondary schools.

The introductory part of the workshop will provide a brief overview of the concept of chemical board games and the theoretical concepts that underpin the design of this original and unique teaching tool for each school grade. The central part will present the experiences of the lecturer in these activities with his students (<https://www.chem.bg.ac.rs/predmeti/435B2-en.html>; Instagram: @mnikolic1971), who themselves designed and prepared (by reworking existing) chemical board games. Some of the chemistry board games will be demonstrated (e.g., chemical UNO and other card games, chemical Guess Who?), and their applicability at the appropriate level of curricula and programs will be discussed with the audience. The final part will discuss the advantages of using (self-prepared) chemical board games in everyday chemistry teaching, including greater motivation for students to acquire (with understanding) various chemical content, expressing creativity and developing critical thinking, fostering team spirit and satisfaction in learning chemistry through play, and promoting innovative pedagogy.

Teachers will not necessarily receive brand new competences and/or skills, but rather ideas and guidelines to prepare original supplementary teaching materials, achieving better contact with their students, facilitating the acquisition of assigned chemical content in a fun way, and assessing students' knowledge.

POLYCYCLIC AROMATIC HYDROCARBONS IN PARTICULATE MATTER AND TOTAL DEPOSITED MATTER IN CROATIA

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Air pollution is one of the most pressing issues of today – it is estimated that over 99% of the world's population is exposed to air pollutants at levels exceeding the World Health Organization's guidelines.^[1] Among substances of particular concern is particulate matter (PM) with an equivalent aerodynamic diameter less than 10 and 2.5 μm (PM_{10} and $\text{PM}_{2.5}$). In addition to particle size and PM mass concentration in the air, chemical content plays a key role in determining harmful health effects. Polycyclic aromatic hydrocarbons (PAHs) are a group of compounds well known for their toxic, carcinogenic, mutagenic, and genotoxic effects. In Croatia, levels of PAHs bound to PM have been measured continuously in ambient air for more than 20 years. However, only a limited number of locations have been included in routine monitoring. In addition, scientific research has been carried out, an overview of which will be presented. **The studies** examined seasonal and spatial distribution of PAHs, their origin, correlations with meteorological parameters and other air pollutants, the distribution of PAHs across different particle sizes as well as associated health risks.^[2,3,4] Atmospheric deposition, including both dry and wet deposition, is a key mechanism for the removal of pollutants from the atmosphere and can negatively impact ecosystems and human health. Although EU legislation stipulates the need for measuring PAHs not only in the PM but also in deposited matter, such measurements are extremely rare and, to date, have been conducted at only a few locations in Europe. In the period 2020-2023, a study was carried out in Croatia that involved collecting monthly samples of total (dry and wet) deposited matter (TDM) at 10 locations in Zagreb and its surroundings, providing the first data on PAH levels in TDM for this part of Europe. Differences in deposition fluxes were observed between sampling sites. Data analysis indicated the presence of various pollution sources (biomass burning, petroleum and fossil fuel combustion, traffic emissions). In addition to the characteristics of the sampling site and local sources, PAH levels in TDM were also influenced by the geographical location itself, likely related to differences in precipitation patterns and air flow dynamics.

Acknowledgements. This study is supported by the European Regional Development Fund project KK.01.1.1.02.0007 (Rec-IMI) and the European Union—Next Generation EU project 533-03-23-0006 (EnvironPollutHealth).

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NEW CLASS OF THERAPEUTICS FOR ALZHEIMER'S DISEASE SYMPTOM CONTROL

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Alzheimer's disease, a devastating neurodegenerative disorder, is often linked to a decline in cholinergic signalling.^[1] Current treatments focus on inhibiting cholinesterases – enzymes that break down the neurotransmitter acetylcholine – to boost its levels in the brain. This research explores a novel approach to identifying potential drugs targeting cholinesterase, enzymes recognized as crucial, especially in the later stages of the disease. The strategy for the design involved directly engaging the enzyme's active site in the initial screening, evolution, and selection of promising compounds.^[2,3] For the synthesis, a four-component Ugi reaction, a versatile chemical process, was employed to generate a diverse library of peptidomimetics. New protocols leveraging mechanochemistry and microwave synthesis were developed to optimize the reaction efficiency and yields. To further understand the relationship between a compound's structure and its inhibitory activity (LD_{50} and K_i), advanced computational models were developed. Experimentally measured inhibition constants were correlated with quantum chemically calculated potential energy surfaces (PES) (representations of a molecule's energy landscape). Extensive machine learning was employed to develop regression models capable of predicting compound activity based solely on its PES.^[4] This approach enables a more comprehensive and efficient screening process for identifying promising leads.

Furthermore, methodology utilizes a target-guided synthesis, where the cholinesterase enzyme itself is employed as a template to drive the creation of its own inhibitors. To investigate the binding and all possible interactions of small molecules (including their building blocks) within the enzyme active site, large-scale quantum chemical molecular docking studies were conducted. Findings suggest that in some cases, multiligand binding is possible, potentially leading to enhanced affinity compared to single-ligand interactions. Future work will expand this approach to include larger, more complex heterocycles, aiming to fully unlock the potential of α -acylamino acetamides binding for potential novel Alzheimer's therapeutics.

Acknowledgements. This work was supported by the Croatian Science Foundation under the project number HRZZ-IP-2022-10-9525 and the European Union – Next Generation EU under the project BioMolTox (Class: 643-02/23-01/00016, Reg. no. 533-03-23-0006).

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PHOTOCHEMICAL STRATEGIES FOR THE DESIGN OF CHOLINESTERASE-TARGETING SMALL MOLECULES

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The development of small-molecule ligands targeting cholinesterases (ChEs) remains a central focus in neuropharmacology, particularly for the treatment of neurodegenerative disorders. This research highlights the rational design, synthesis, and biological profiling of diverse classes of photochemically obtained compounds—bicyclo[3.2.1]octadienes and photocyclization products—as reversible inhibitors of acetylcholinesterase (AChE) and butyrylcholinesterase (BChE). The research initially focused on the development of novel inhibitors incorporating the bicyclo[3.2.1]octadiene scaffold, known for its activity on dopamine and serotonin transporters and relevance in CNS disorders.^[1] Utilizing photochemical [2+2]-cycloaddition reaction, a diverse library of polycyclic compounds providing promising candidates for further investigation.^[2] The investigation is also focused on synthesizing reversible cholinesterase inhibitors by photocyclization reaction.^[3] The obtained uncharged and charged naphthoxazole and tienobenzo-triazole scaffolds demonstrated promising dual-target or BChE-selective profiles. Molecular docking studies reveal that π - π stacking and electrostatic interactions play a crucial role in stabilizing their binding within the active sites of cholinesterase enzymes. Collectively, all the findings underscore the therapeutic potential of structurally diverse cholinesterase ligands.

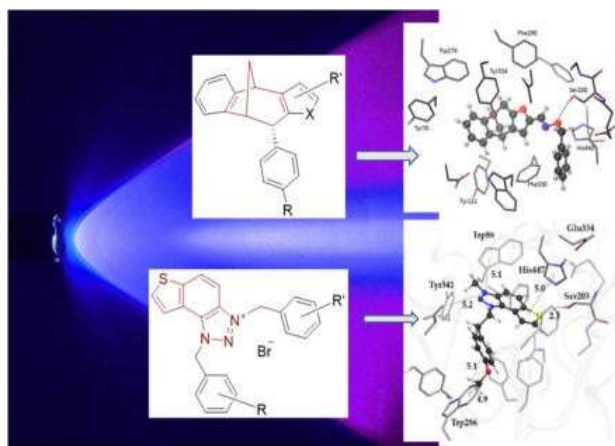


Figure 1. Photochemically obtained bicyclo[3.2.1]octadiene and tienobenzo-triazole scaffolds.

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NEW RECOMMENDATIONS FOR CROATIAN NOMENCLATURE OF INORGANIC CHEMISTRY

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The talk will present the Croatian translation^[1,2] of the IUPAC *Brief Guide to the Nomenclature of Inorganic Chemistry*,^[3] which provides a brief overview of the most important recommendations of the Croatian Chemical Society and the Croatian Society of Chemical Engineers for nomenclature of inorganic chemistry in accordance with the IUPAC recommendations of 2005.^[4] These recommendations are a supplement and partial correction of the previous Croatian recommendations (1995)^[5] which were a translation of the older version (1990) of IUPAC recommendations.^[6] The new recommendations of Croatian nomenclature which will be presented are meant to align the Croatian nomenclature of inorganic chemistry with the current IUPAC recommendations. As many of the changes which have been introduced concern parts of the nomenclature used in primary and secondary education, it is important for chemistry teachers to be acquainted with them. The talk will therefore emphasize all the innovations in the nomenclature of inorganic chemistry which have been introduced. Also, a brief overview of general principles of chemical nomenclature will be given, with emphasis on differences between chemically crucial elements of systemic names, and those which exist primarily for linguistic, grammatical and orthographic reasons.

The universal adoption of an agreed chemical nomenclature is a key tool for communication in the chemical sciences, for computer-based searching in databases, and for regulatory purposes, such as those associated with health and safety or commercial activity. It is therefore expected that during a discussion at the end of the lecture the teachers will actively participate, sharing examples and problems from their own experience.

The talk will hopefully provide guidelines for the Croatian chemical teaching community for the correct usage of nomenclature of inorganic chemistry (and chemical nomenclature in general) in the classroom and beyond.

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BIOCATALYSIS AND PROCESS ENGINEERING IN GREEN PRODUCTION OF NUTRACEUTICALS

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Nutraceuticals, positioned at the intersection of food and medicine, are gaining momentum as functional agents that contribute to disease prevention and health promotion. Their production from renewable sources not only aligns with the principles of green chemistry but also addresses the growing demand for sustainable and naturally derived bioactive compounds. Among emerging production strategies, enzymatic biocatalysis offers a selective, mild, and environmentally friendly alternative to traditional chemical synthesis. Renewable feedstocks—such as plant biomass and agricultural by-products—serve as abundant sources of valuable precursors, which can be transformed into high-value nutraceuticals through tailored enzymatic cascades.^[1]

The integration of reaction engineering into enzymatic process development is essential for optimizing these complex systems. It enables precise control over reaction conditions, substrate flows, and enzyme performance, ultimately ensuring scalability and consistency. Multi-enzyme systems, particularly in one-pot configurations, allow for efficient conversions by minimizing intermediate isolation and maximizing atom economy. The case of raspberry ketone production from birch bark exemplifies this approach: using a two-step enzymatic cascade involving hydrolase and stereoselective alcohol dehydrogenases, the process achieves high yield while employing a renewable, biogenic substrate. Mathematical modeling, enzyme stability profiling, and coenzyme regeneration strategies further enhance process efficiency, offering a viable path toward sustainable nutraceutical manufacturing.^[2]

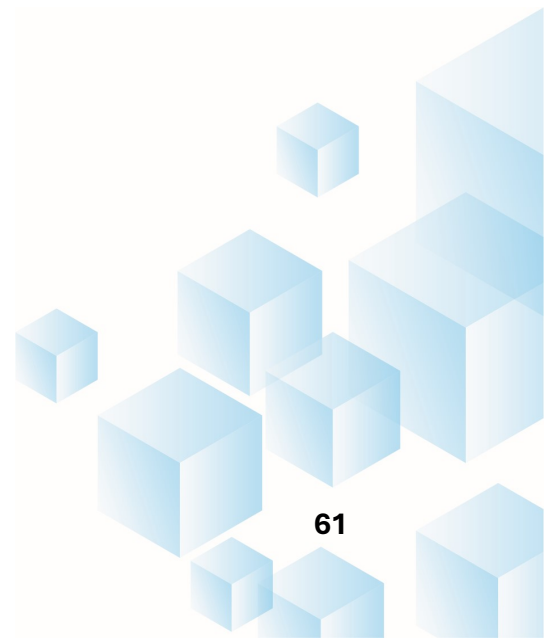
Acknowledgements. This research was funded by the European Union's Horizon 2020 research and innovation programme under Grant Agreement No. 101000560 (RadicalZ).

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SECTION LECTURES



EXPLORING PANTOPRAZOLE–CYCLODEXTRIN INTERACTIONS VIA COFFEE RING IMAGING AND THERMODYNAMIC PROFILING

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The interactions between pantoprazole and cyclodextrins were investigated using both traditional and image-based techniques to assess their potential for formulation enhancement. Isothermal titration calorimetry (ITC) and spectrophotometric titrations revealed the formation of stable inclusion complexes in aqueous media, with thermodynamic data and stability constants confirming strong affinity. These interactions significantly improved the solubility of pantoprazole in its neutral form. Complementing these findings, a novel approach based on the coffee ring effect was employed to visualize the influence of cyclodextrins on pantoprazole's drying behavior. Aqueous solutions of pantoprazole, with and without cyclodextrins, were deposited on glass and analyzed after drying using microscopy and Python-based image analysis. Quantitative descriptors such as ring radii, contour area, and radial intensity were extracted to identify morphological patterns linked to molecular interactions. Clustering analysis suggested distinct stain morphologies for cyclodextrin-containing samples, indicating complexation-related stabilization. Together, these complementary techniques—calorimetry, spectroscopy, and image-based pattern recognition—demonstrate the potential of combining physical chemistry and low-cost visualization methods to probe drug–excipient interactions. This integrative approach enables both mechanistic insight and early-stage screening in pharmaceutical development, supporting more informed and efficient formulation strategies.

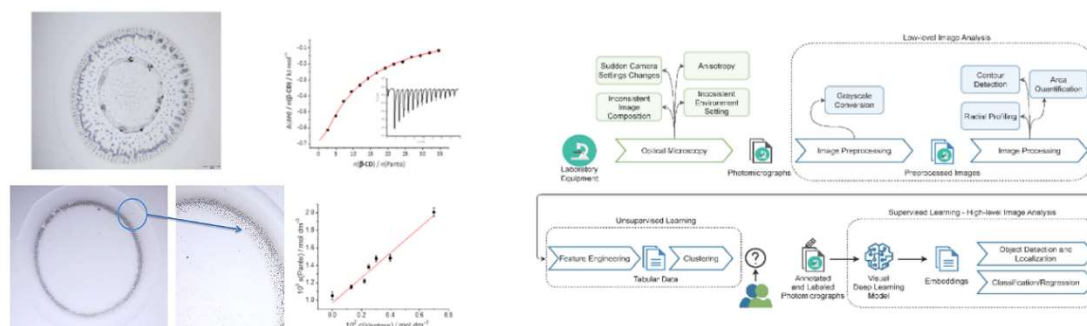


Figure 1. Microscope images of the coffee ring effect (left), ITC and solubility data for pantoprazole–kcleptose systems at 25.0 °C (middle), and schematic of analysis workflow (right).

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

ELECTROSPINNING TECHNOLOGY IN THE DEVELOPMENT OF MEDICAL APPLICATIONS

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Electrospinning is an adaptable and powerful technique for producing nanofibrous membranes with controlled morphology, high surface area, and interconnected porosity—properties that are critical for applications in biomedicine, environmental science, and energy. In addition to its structural tunability, electrospinning allows for the direct incorporation of functional agents into fibers, enabling the creation of bioactive and responsive materials.^[1]

This study focuses on the design and optimization of a custom-built electrospinning apparatus for producing polycaprolactone (PCL) membranes, aiming to advance sustainable polymer processing for biomedical applications. A central composite design (CCD) and response surface methodology (RSM) were employed to optimize key parameters—voltage, flow rate, and tip-to-collector distance—with the goal of tuning membrane thickness, uniformity, and wettability.^[2] Membrane morphology and fiber alignment were characterized using SEM and optical microscopy, while wettability was assessed via droplet absorption tests. FTIR analysis provided insight into fiber structure, confirming the influence of voltage and collector distance on membrane properties, with flow rate showing a lesser effect. The optimized membranes exhibited desirable physical characteristics for biomedical use, including flexibility, porosity, and consistent fiber formation. This work demonstrates the potential of custom electrospinning setups for controlled fabrication of polymeric membranes, offering a sustainable platform for developing functional materials in tissue engineering, wound care, and related fields.

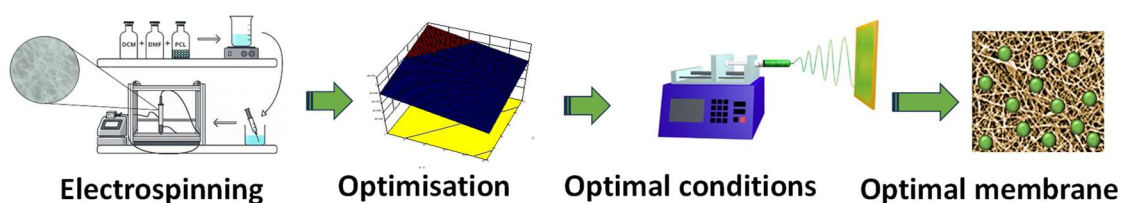


Figure 1. Schematic representation of the electrospinning process.

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

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TRIPYRIDYL PORPHYRINS IN PHOTODYNAMIC THERAPY ON MELANOMA CELLS UNDER THE CoCl_2 -INDUCED HYPOXIA

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Photodynamic therapy (PDT) is based on the creation of oxidative stress, which is used to selectively destroy tumor cells thanks to the local activation of photosensitizer (PS) by light.^[1] Although it has numerous advantages over other therapies, due to its dependence on oxygen, PDT is less successful in hypoxic solid tumors, and melanoma in particular remains a major challenge. Moreover, the hypoxia-inducible factor (HIF) family of proteins helps cancer cells survive in hypoxic conditions and increases their proliferation and metastatic potential.

In our group, we focused on tripyridyl porphyrins as possible photosensitizers in PDT on melanoma, and we use pyridyl nitrogen atoms for quaternization and formation of polar moieties, while we use the fourth *meso*-position of porphyrins for binding lipophilic groups. In this way, we prepare asymmetric amphiphilic structures that enable PS entry into cells.^[2] We recently prepared *N*-methylated pyridiniumporphyrins that were most successful in cellular uptake and PDT, and decided to compare these two groups of PSs in PDT on pigmented (MeWo) and non-pigmented melanoma cells (A375), and on fibroblasts (HDF), in hypoxic conditions (**Figure 1**). Cobalt chloride was used to induce chemical hypoxia, as it is known to stabilize hypoxia inducible factor 1 α (HIF-1 α).^[3]

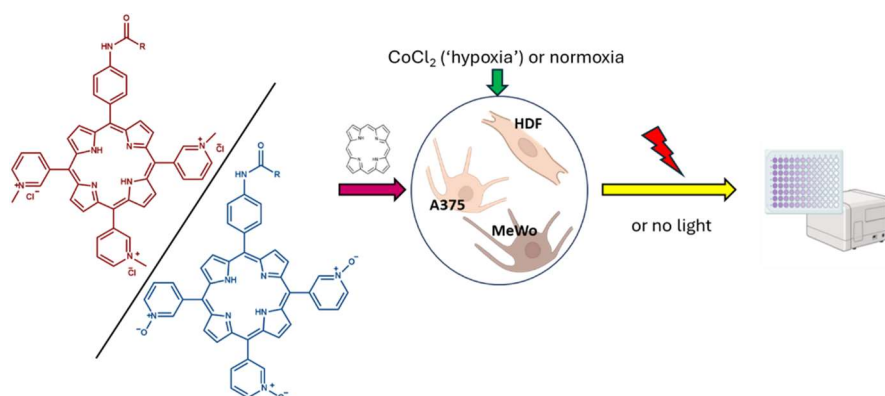


Figure 1. Photodynamic action of *N*-methylated pyridiniumporphyrins and (oxido)pyridylporphyrins under CoCl_2 -induced hypoxia on fibroblasts and melanoma cells

Acknowledgements. This work has been supported by the University of Rijeka's grant assigned to Prof. dr. Nela Malatesti (uniri-iskusni-23-2).

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PHOTOTRUNCATION OF CYANINES

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Cyanine dyes are a class of organic, usually cationic molecules containing two nitrogen centers linked through conjugated polymethine chains. They have been found to be widely used as fluorescent probes for labeling nucleic acids and proteins and as photosensitizers in photodynamic therapy, biosensors, and imaging agents. The synthesis^[1] and reactivity of cyanine derivatives have been extensively investigated for decades but their further synthetic modifications, especially on the polymethine chains, are still a poorly explored area. In conjunction with applications of cyanine dyes in optical imaging and photochemical drug delivery, Schnermann and co-workers described that excitation of heptamethine cyanine (Cy7) in phosphate-buffered saline leads to the formation of truncated (chain-shortened) pentamethine cyanine (Cy5) in small yields (Figure 1).^[2,3] The reported dramatic increase in the phototruncation yield in CAPSO buffer motivated us to perform a deeper study of this reaction and improve the yields. Our mechanistic studies demonstrate that the phototruncation mechanism is a complex photooxidation multi-step process that is related to highly specific buffer constituents.

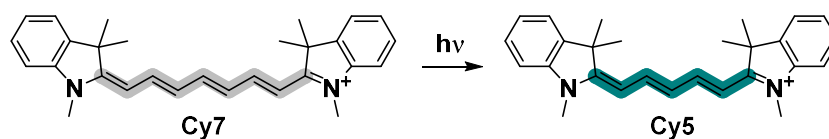


Figure 1. The phototruncation of Cy7 to Cy5.

Acknowledgements. This study was funded by the Marie Skłodowska-Curie Actions under the European Union's Horizon Europe Framework Program grant agreement no. 101149087 (CoeusCy7, G.G.) and the Czech Science Foundation (P.K.: GA23-05111S, and P.S. and J.F.: GA23-07066S). The authors thank the RECETOX Research Infrastructure (no. LM2023069), financed by the Czech Ministry of Education, Youth and Sports for supportive background. This project was also supported by the European Union's Horizon 2020 Research and Innovation Programme under grant agreement no. 857560 (P.K.).

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MODERN APPROACHES TO LASER ABLATION INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY (LA-ICP-MS) ANALYSIS

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Laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) is a highly sensitive microanalytical method for solid sample analysis. It is characterized by low detection limits, high spatial resolution, a wide linear dynamic range, and minimal sample preparation, making it a well-established method for both elemental analysis and mapping. The particular strength of the method lies in its mapping capabilities, which allow detailed visualization of elemental distribution in biological tissues, forensic and geological samples, as well as advanced materials.^[1]

In analytical LA-ICP-MS systems, the beam profile of the laser is typically homogenized to achieve a flat-top shape. However, in practical applications, the shape of the beam—and consequently the geometric profile of the crater—can be described with the 2D super-Gaussian function and quantified using the parameter n , which describes the super-Gaussian order. This parameter has a significant influence on the ablation volume and the sampling efficiency. To improve spatial accuracy and signal quality, a contraction approach was proposed.^[2] By contracting the ablation grid through sub-pixel mapping, this method enhances surface sampling precision, increases pixel density, and ultimately leads to improved spatial resolution and a higher signal-to-noise ratio (SNR).

This study focuses on the characterization of crater geometry to improve image quality by elucidating how various parameters influence analytical outcomes. Given that the complexities of the laser-sample interaction pose significant challenges, an empirical model was developed to investigate the relationship between the super-Gaussian order (n), beam size, and laser fluence. In addition, the contraction approach was applied to a real-life sample to evaluate its effectiveness under practical conditions and to compare the resulting image quality with that of conventional methods.

Acknowledgements. This work has been supported by the Slovenian Research Agency (ARIS), research core funding No. P1-0034 and No. P2-0152. A.H. thanks ARIS for funding her PhD research.

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STABILIZATION AND STRUCTURAL CHARACTERIZATION OF METAGENOMIC ESTERASES FOR ENHANCED BIOPLASTIC DEGRADATION

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Plastic pollution poses a major threat to biodiversity and human health by degrading habitats, contaminating food chains, and disrupting ecosystem functions.^[1] To address this challenge, global efforts have focused on identifying novel enzymes capable of plastic degradation.^[2] Our research focuses on the structural and functional characterization of metagenomic esterases to support their application in bioplastic degradation. Previously, we identified a novel esterase, MGY,^[3] along with more soluble ancestral variants (118, 119, and 121) capable of degrading polylactic acid (PLA) and polycaprolactone (PCL). Among them, variant 119 exhibited the highest stability ($T_m = 84\text{ °C}$). To facilitate 3D structure determination, we engineered a truncated form of 119 (ΔN_{119}) by removing a predicted disordered N-terminal region. To further enhance structural stability and improve crystal packing, we co-purified and co-crystallized the enzyme with phenylmethylsulfonyl fluoride (PMSF), a covalent serine hydrolase inhibitor that reduces conformational flexibility. Size-exclusion chromatography revealed reduced oligomeric heterogeneity in ΔN_{119} compared to full-length 119. Differential scanning calorimetry revealed a lower melting temperature for ΔN_{119} ($T_m = 68\text{ °C}$). Circular dichroism spectroscopy indicated similar secondary structure content ($\approx 20\%$ α -helices, $\approx 30\%$ β -sheets) in both forms. Dynamic light scattering confirmed monodispersity ($PDI < 0.2$), supporting their suitability for structural studies. Crystallization screening using the Oryx8 robot yielded crystals, which were analyzed by single-crystal X-ray diffraction at the XRD2 beamline, Elettra synchrotron (Trieste, Italy). Our results highlight how enzyme engineering and inhibitor-based stabilization can facilitate the structural characterization of dynamic metagenomic esterases. These insights lay the groundwork for developing more robust biocatalysts for bioplastic degradation.

Acknowledgements. This research was funded through National Recovery and Resilience Programme, The Development Research Support (NextGenerationEU), project Enzyme engineering for sustainable recycling of bioplastics (NPOO.C3.2.R2-I1.06.0041).

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CARBONIZED METAL-ORGANIC FRAMEWORKS AS ULTRA-HYDROPHOBIC SOLID TRANSDUCER IN POTENTIOMETRIC POTASSIUM PROBES

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Potentiometric sensors are versatile probes that measure the activity of ions in aqueous samples. Their long-lasting development led to the characteristic, layered design, consisting of a support, electrically conducting leads, solid-contact and the receptor. Recently, solid contact material development received attention, as it was observed that its' character and means of deposition play a crucial role in sensors' response stability and reproducibility¹.

Herein, we compared the applicability of different mechanochemically synthesised cobalt-imidazolate metal-organic frameworks (MOFs) as solid contacts in potassium-selective electrodes (K-ISE). We evaluated the effect of pyrolysis on the solid-contact characteristics, including capacitance and hydrophobicity. Chronopotentiometric measurements provided information on the efficiency of signal transduction: a capacitance value of 1.87 μF jumped to 5.15 μF after pyrolysis. Additionally, the pyrolyzed material exhibited the greatest water contact angle, resulting in the best long-term sensor stability. Finally, the proposed solid-contact materials were drop-cast onto inkjet-printed electrodes to showcase the possibility of integration in printed electronics configurations. It was shown that the presence of MOF-based solid contact significantly improves the electrode response reproducibility.

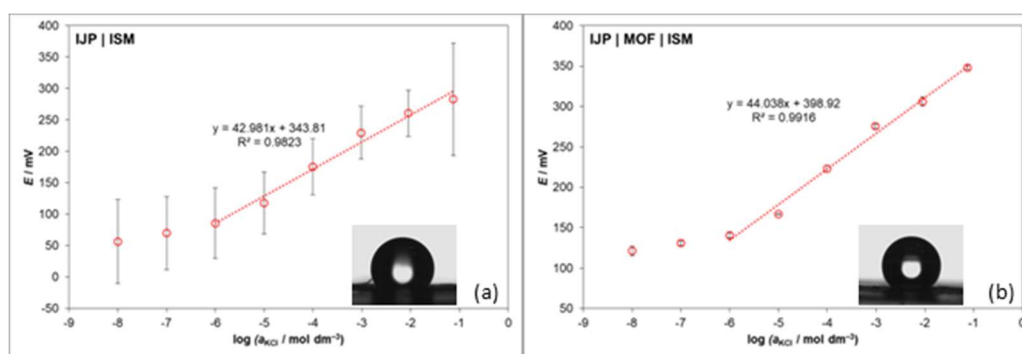


Figure 1. Potentiometric response of inkjet printed electrodes (a) without and (b) with a solid-contact material based on pyrolyzed MOF.

Acknowledgements. This work has been supported by Croatian Science Foundation (grant: UIP-2020-02-9139).

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ANION BINDING BY PHENYLALANINE AND LEUCINE CYCLOPEPTIDES: THERMODYNAMIC AND STRUCTURAL STUDY

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During the past few decades, there has been a growing interest in research of cyclopeptides as anion receptors. These compounds, besides their metabolic stability and bioavailability, exhibit enhanced binding affinity towards substrates compared to their more flexible linear analogs.^[1,2] Many synthesized (pseudo)cyclopeptides show high affinities towards anionic species in organic and aqueous media^[3,4] and some were even capable of transporting anions through the membrane lipid layer.^[5] In this presentation, the anion binding properties of cyclophenylalanine and cycloleucine peptides comprised of 4–6 amino acids in acetonitrile and methanol will be given. In order to elucidate the effect of ring size and amino acid type on the cyclopeptide affinity, and/or selectivity towards selected anions, the stability constants and other thermodynamic parameters of complexation were determined by means of ¹H NMR and microcalorimetric titrations. Furthermore, molecular dynamics simulations of free receptors and their complexes were also performed. This resulted with an insight into structural properties of formed complexes and deeper comprehension of the factors governing the complexation equilibria.

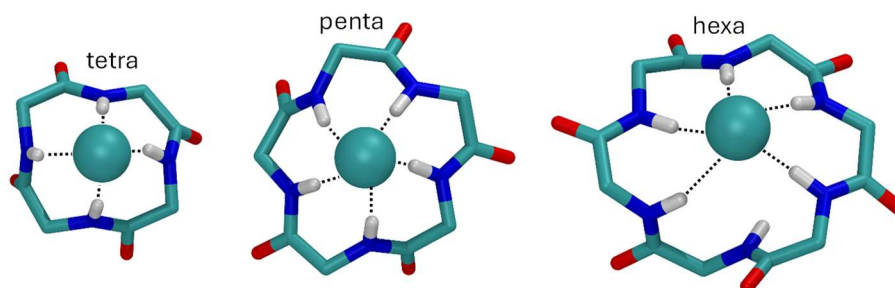


Figure 1. Chloride anion coordination by small cyclic peptides.

Acknowledgements. This work was supported by the Croatian Science Foundation under project IP-2024-05-2012 (CalixCORE) and European Regional Development Fund (project CluK, KK.01.1.1.02.0016)

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AZODIOXY THIN FILMS VIA ON-SURFACE POLYMERIZATION OF AROMATIC DINITROSO COMPOUNDS

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Adsorption of organic molecules on surfaces and formation of thin films is of significant interest for the fabrication of functional materials for applications in electronic devices. Aromatic C-nitroso compounds can dimerize and polymerize on gold surface through azodioxy bonds.^[1] Recent studies revealed the promising electronic properties of aromatic dinitroso-based polymers, which act as organic semiconductors.^[2] This work investigates the polymerization of various aromatic dinitroso derivatives on different solid surfaces. The first part covers the synthesis of novel disulfide-containing nitrosoarenes and their self-assembly and self-polymerization on Au(111) surface.^[3] The second part explores the lateral polymerization of 4,4'-dinitrosobiphenyl on different substrates focusing on the impact of substrates and deposition methods (drop-casting vs. spin-coating) on the morphology and electronic properties of the formed thin films. The prepared films were characterized by different methods, which revealed the formation of azodioxy oligomer or polymer films.

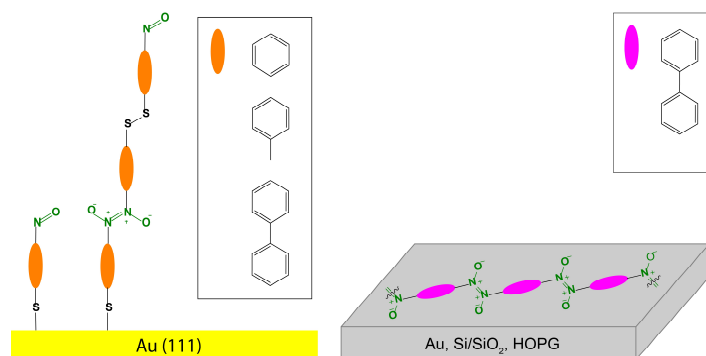


Figure 1. Polymerization of aromatic dinitroso derivatives on solid surfaces.

Acknowledgements. This work has been fully supported by the Croatian Science Foundation under the project IP-2020-02-4467.

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UNCOVERING THE ROLE OF ABCs IN THE SOLID-STATE SUZUKI-MIYAUURA REACTION VIA *IN SITU* RAMAN MONITORING

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Palladium-catalyzed Suzuki-Miyaura cross-coupling of aryl halides with organoboron reagents is one of the simplest and most widely used methods for synthesizing biaryls, which are essential structural motifs in various pharmaceuticals and advanced materials.^[1] As chemistry shifts towards more sustainable and environmentally friendly synthetic strategies, mechanochemical reactions have gained popularity. This solid-state approach offers several advantages, including a broader range of substrates and catalysts, along with the almost complete elimination of solvents.^[2] Despite the potential of these methodologies, detailed insights into the reaction mechanisms remain limited. Optimization of the reaction conditions and pinpointing the exact role of different reaction components are often challenging as most analyses are conducted *ex situ* and cannot reveal real-time reaction dynamics.

Here we present the first comprehensive investigation of the solid-state Suzuki-Miyaura reaction using *in situ* Raman spectroscopy.^[3] Real-time monitoring and systematic variation of the ABCs (Additives, Bases, Catalysts, and substrates) enabled the identification of key factors affecting reaction efficiency. In addition to conventional palladium catalysts, the catalytic potential of various azobenzene palladacycles was evaluated. The obtained results highlight the importance of fine-tuning the ABCs to design efficient solvent-free cross-coupling protocols.

Acknowledgements. This work has been supported by the Croatian Science Foundation under the projects IP-2019-04-9951 (MECHEMFUN) and DOK-2020-01-7515.

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CHIRAL MULTISUBSTITUTED BINOL–CYCLOPENTADIENYL LIGANDS AND THEIR COMPLEXES WITH TRANSITION METALS

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Chiral cyclopentadienyl ligands that are both disubstituted and derived from BINOL are well established in the field of stereoselective organometallic catalysis. These ligands, along with their transition metal complexes, have proven highly effective in a range of stereoselective transformations, including synthetically valuable reactions such as C–H functionalizations and various cyclotrimerizations.^[1]

Despite this success, two major challenges remain: the lack of efficient methods for preparing chiral multisubstituted BINOL–cyclopentadienyl (BINOL–Cp) ligands, and the absence of models explaining how additional substitution on the cyclopentadienyl ring—though empirically confirmed—impacts the stereoselectivity of such transformations.^[2]

This work aims to develop a synthetic method for chiral multisubstituted BINOL–Cp ligands that enables access to these structures in significantly fewer steps. The method also allows for the selective introduction of additional substituents on the five-membered ring in late stages of synthesis.

Special emphasis is placed on the preparation of ligands and their metal complexes whose calculated stereotopographic descriptors—such as buried volume and stereotopographic maps—suggest structural alignment with known systems that have demonstrated high efficiency in model stereoselective transformations.

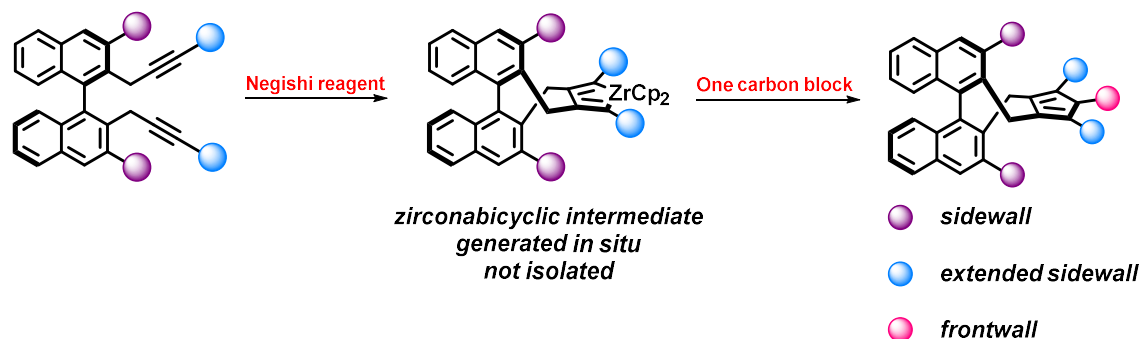


Figure 1. The key step of the proposed synthetic route.

Acknowledgements. This work has been supported by NextGenerationEU (NPOO.C3.2.R2-I1.06.0022).

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SELF-SORTING VERSUS CO-ASSEMBLY: STRUCTURAL INSIGHTS INTO SUPRAMOLECULAR OIL GELS

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Supramolecular oil gels based on low-molecular-weight organic compounds have emerged as promising soft materials due to their ability to immobilize hydrophobic liquids through noncovalent interactions. These systems are of particular interest for applications in materials science, as well as in food and pharmaceutical fields, owing to their tunable properties and the reversibility of the gelation process.

When combining two different gelator molecules, the resulting self-assembled fibrous networks can arise through self-sorting, where each molecule forms its own distinct assembly, or through co-assembly, where both components integrate into mixed supramolecular structures. A major challenge in designing such systems is achieving control over the type of network formed.

In this work, we show that this control can be directed by tuning molecular parameters such as the nature of the chiral units, their molar ratios, and the hydrophobic character of individual components, thus guiding the system toward either self-sorting or co-assembly. The oil gels we investigate demonstrate self-healing properties and high efficiency. These insights offer a strategy for rational design of multicomponent supramolecular gels with tailored properties.

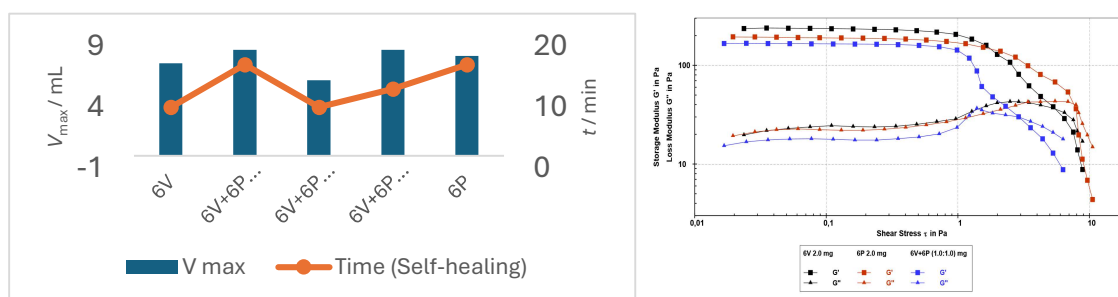


Figure 1. Maximum gelation volume of binary gelator mixtures at different ratios and their self-healing behavior. Viscoelastic properties of the prepared gel mixtures.

Acknowledgements. This work has been supported by the Proof-of-Concept Project under NPOO.C3.2.R3-I1.05.0231: "Innovative Method for Replacing Palm Fat in Complex Food Matrices (INOFAFAT)" and RBI GD1 project "Investigation of Gelator Mixtures for Enhanced Solubility"

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INFLUENCE OF DPP3 INACTIVATION ON ITS INTERACTION WITH THE KELCH DOMAIN OF KEAP1

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Dipeptidyl peptidase 3 (DPP3), a ubiquitously expressed zinc-dependent exopeptidase, has been identified as part of the Keap1 protein interaction network, suggesting its involvement in the cellular response to oxidative and electrophilic stress.^[1] By binding to the Kelch domain of Keap1, DPP3 disrupts the Keap1–Nrf2 regulatory pathway, preventing Keap1-mediated degradation of Nrf2 and thereby enhancing Nrf2's transcriptional activity in the nucleus. Activated Nrf2 promotes the expression of genes involved in the elimination of reactive oxygen species, suppression of inflammation, and detoxification.^[2] While Nrf2 activation is protective in normal cells, its persistent over activation enables tumor cells to evade oxidative stress, resist apoptosis, and enhance proliferation.^[3] Increased DPP3 expression has been associated with tumorigenesis, particularly in breast and colorectal cancers,^[3,4] where it enhances antioxidant responses and supports cancer cell survival through competitive binding to Keap1. Although DPP3's catalytic activity is not essential for its binding to Keap1, the potential impact of peptidase inhibitors on this interaction remains unexplored. The goal of this study was to investigate how enzyme inactivation, through mutation of the catalytically important glutamate residue (E451A) and binding of the inhibitor (IVYPW), affect its interaction with the Kelch domain of Keap1, using both experimental (ITC measurements) and computational (conventional and adaptive steered MD simulations) methods. While experimental results showed that enzyme inactivation enhances interaction with the Kelch domain of Keap1, molecular modeling provided a submolecular explanation for these findings.

Acknowledgements. This work is funded by the European Union – NextGenerationEU, under the project titled “Preliminary study of inhibiting NRF2-dependent transcription by preventing the DPP III – KEAP1 interaction for more effective cancer treatment”

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PHOTOACTIVE PHENYLBORONIC ACID DERIVATIVE: SYNTHESIS AND INTERACTIONS WITH SIALIC ACIDS

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Phenylboronic acid (PBA) derivatives form covalent yet reversible bonds with diols (Fig. 1a).^[1] These specific and pH-dependent interactions enable selective recognition of glycans on the cell surface, triggering a biological response. On the other hand, photoactive compounds are increasingly being used in medicine, especially for controlled drug delivery.^[2] These two functionalities are combined in the novel photoactive PBA-derivative **2**, which was synthesised by azo coupling reaction of naphthol with a diazonium salt of PBA (Fig. 1b). Photophysical parameters of its isomerisation (Fig. 1c) as well as the affinities of its *E* and *Z*-form towards binding with *N*-acetylneuraminic acid have been determined experimentally and by quantum-chemical calculations. The results unveil the potential of this compound as a platform for the development of selective and highly efficient light-activated drug delivery systems.

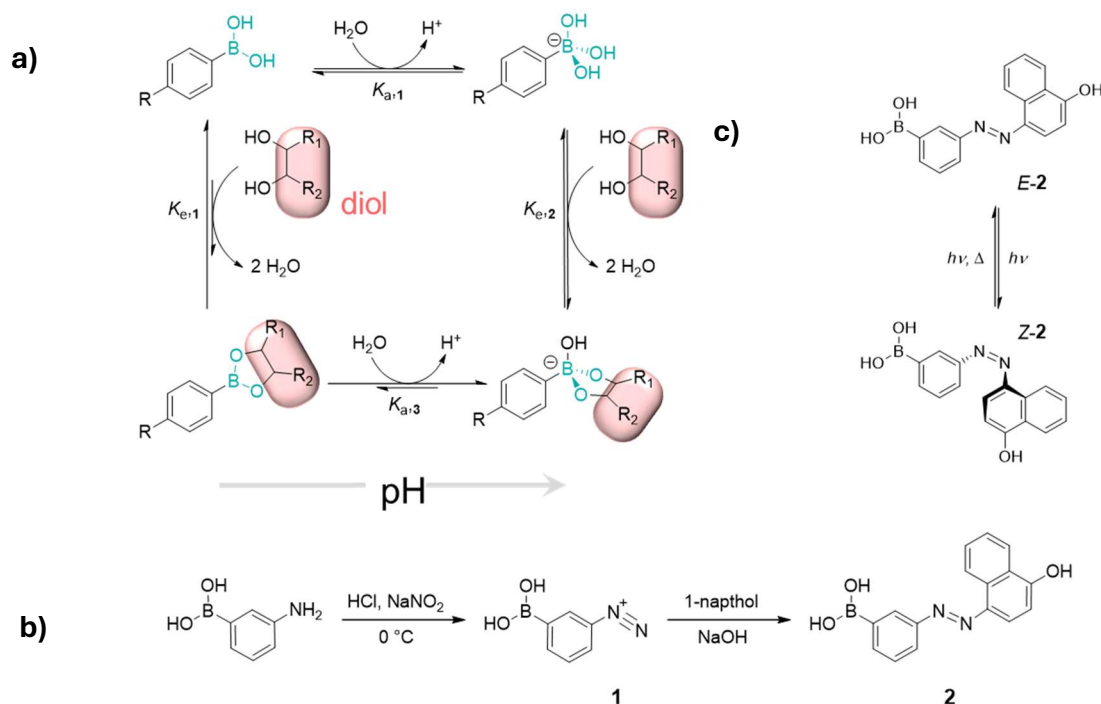


Figure 1. a) Binding of diols to PBA-derivatives *via* boron-ester bond formation, b) synthesis, and c) isomerisation of compound **2**.

Acknowledgements. This work has been supported by the Adris Foundation.

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CAUSAL AI MODELLING OF CHEMICAL PROCESS PLANT

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The concept of “Industry 5.0” is driving significant changes in the production of chemical products and energy, promoting a shift towards a decarbonized and circular economy. Digitalization, robotics, communications, and artificial intelligence (AI) play crucial roles in fostering the development of necessary technological innovations and enhancing intelligent process control. The application of machine deep learning (ML) yields robust, field-neutral solutions for regression prediction objectives, but it is limited in its capacity to address innovative questions that involve causation and counterfactual analysis. Here is presented a application of Bayesian networks (BN) for structural causal modelling (SCM) in the context of Tennessee-Eastman plant (Fig. 1). Main feature of SCM is its capacity to integrate extensive prior structural knowledge derived from fundamental chemical engineering principles with structures inferred from experimental data obtained from manufacturing plants. The developed SCM facilitates forecasting, causal relations, simulation of intervention strategies, and generation of counterfactual inferences essential for process innovations and intelligent process management.

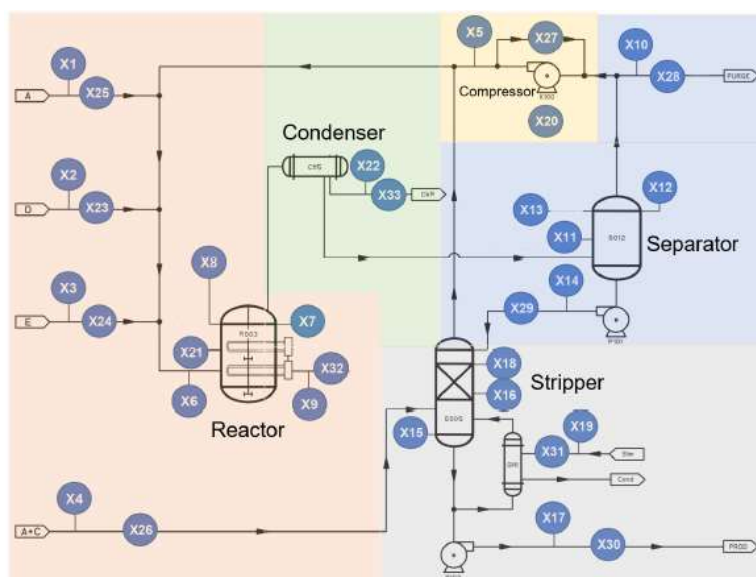


Figure 1. Tennessee-Eastman process scheme

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NICKEL ELECTROCATALYSTS FOR HER: BRIDGING MATERIAL PERFORMANCE AND DATA INTEGRITY

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Hydrogen is emerging as a cornerstone of the global transition to sustainable energy systems as it offers a clean fuel with high energy density that can be produced from water using renewable electricity. Among the various methods of hydrogen production, electrochemical water splitting is particularly attractive due to its scalability and environmental compatibility.^[1] However, the widespread adoption of this technology depends on the availability of efficient, cost-effective electrocatalysts for the hydrogen evolution reaction (HER). Platinum-based catalysts remain the benchmark for HER performance, but their scarcity and high cost are prompting research into alternative materials. Nickel-based catalysts represent a promising class of earth-abundant alternatives,^[2] especially under alkaline conditions.

This work focuses on the development and evaluation of in-house synthesized nickel-based electrocatalysts for HER, emphasizing the crucial role of rigorous data processing, sample preparation and experimental methodology in obtaining reproducible and reliable results. Key aspects such as appropriate sample preparation, optimal film conductivity,^[3] proper iR compensation and consistent data processing protocols are discussed in detail. The importance of these factors is emphasized by a case study using a thin film rotating disc electrode (TF-RDE) setup in alkaline media, where subtle variations in the experimental setup have a significant impact on the catalytic performance metrics. A range of physico-chemical (SEM-EDS, TEM-EELS, XPS, XRD etc.) and electrochemical techniques (CV, LSV, CA, EIS) were used to comprehensively characterize the catalysts to ensure a complete understanding of the structure–activity relationships. This study highlights the need for standardized, transparent reporting practices and reproducible methods to accelerate the development and benchmarking of non-noble HER catalysts.

Acknowledgements. This work has been supported by Slovenian Research Agency (ARIS) through the research funding programs P2-0423, P1-0447, J7-4636, J2-50086, and J7-50227.

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ELECTROCATALYTIC APPROACHES TO HIGH-EFFICIENCY HYDROGEN PEROXIDE GENERATION IN MICROFLUIDIC SYSTEMS

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Hydrogen peroxide (H₂O₂) is a versatile oxidizing agent with applications in pulp and paper bleaching, wastewater treatment, chemical synthesis and energy storage^[1]. Conventional largescale synthesis via the anthraquinone process is energy-intensive, requires scarce platinum group metals (PGMs) and requires the transport of concentrated H₂O₂ – a challenge for safety and logistics^[2]. Electrochemical production via the two-electron oxygen reduction reaction (ORR) in alkaline media has gained attention as a safer and more sustainable alternative. However, its practical application is limited by sluggish kinetics, which necessitates the development of efficient, cost-effective electrocatalysts. While noble metal-based catalysts (e.g. Pd-Au, Pt-Hg) show high performance, their cost and scarcity have increased interest in transition metal and carbon-based materials^[3]. In parallel, scalable electrosynthesis platforms such as fuel cells, membraneless electrolyzers and microfluidic electrochemical flow cells (MEFCs) are being explored^[4]. This study presents a two-plate electrochemical microreactor equipped with a real-time optical sensor system for in situ H₂O₂ quantification. Chronoamperometry was used to evaluate H₂O₂ production at different flow rates, using offline electrochemical measurements for validation. The electrodes were characterized before and after electrochemical measurements using SEM/EDS, FTIR, and XPS to analyze structural and compositional changes.

Acknowledgements. The financial support of the Slovenian Research and Innovation Agency (ARIS) through grants P2-0423, P1-0447, J7-4636, J2-50086, and J7-50227 is gratefully acknowledged.

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APPLICATION OF 3D-PRINTING FOR PRODUCTION OF CERAMIC MONOLITHIC CATALYSTS FOR OXIDATION OF AROMATIC VOLATILE ORGANIC COMPOUNDS

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Due to increasing and more frequent emissions from traffic, numerous industrial and other sources, air pollution is becoming a growing problem, which is given priority in the overall environmental protection strategy. The aim of this work is to prepare 3D-printed ceramic monolithic catalysts for the catalytic oxidation of gaseous mixture of benzene, toluene, ethylbenzene, and xylene, commonly referred to as BTEX. The possibility of using zirconium dioxide (ZrO_2) as a filament for the production of 3D-printed ceramic monolithic carriers was examined using innovative additive manufacturing technology – fused filament fabrication (FFF). The catalytically active layer used was a mixed manganese and iron oxide, applied to the monolithic carriers using the wet impregnation method. The mechanical stability of the prepared catalysts was investigated using ultrasound prior to the measurements in the reactor system. In addition, thorough characterization of the ZrO_2 -based filament and 3D-printed catalyst carriers was performed.^[1] The activity of the prepared catalysts was tested at different temperatures and space times in a monolithic reactor. The obtained results were compared with the results obtained using commercial ceramic cordierite monolithic catalysts with different channel dimensions, as well as with SiO_2 -based monolithic catalysts made by stereolithography.

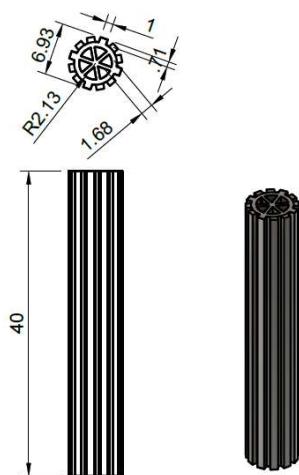



Figure 1. 3D CAD model of the ceramic catalyst carrier – ZDP geometry

Acknowledgements. This work has been supported by the Croatian Science Foundation under the projects IN-PhotoCat (IP-2018-01-8669) and INDIGO (IP-2022-10-8004).

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ULTRASOUND VS. MECHANICAL MIXING IN BATCH CRYSTALLIZATION, COMPARISON OF KEY HYDRODYNAMIC PARAMETERS AND EFFECT ON FINAL PRODUCT

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The role of hydrodynamics in crystallization is multifaceted; it is responsible for reaching the optimal suspension uniformity, and enhanced mass transfer, all of which influence nucleation and crystal growth kinetics. Thus, the focus of this study is to investigate the impact of hydrodynamic conditions on the batch cooling crystallization of borax decahydrate. Experiments were conducted in a 2.65 dm³ double wall batch crystallizer where cooling was performed by Lauda Proline RP855 C X Edition. A classical batch crystallizer in which mixing was performed mechanically was compared with a hybrid system, where mixing was performed by combining mechanical mixing and ultrasonic (US) irradiation. Critical impeller speed with and without ultrasonic assistance was determined. At all investigated conditions, power consumption was determined, as well as the key global hydrodynamic parameter – energy dissipation based on which the characteristics of the flow on the microscale of mixing was estimated according to Kolmogorov theory. Energy dissipation rates were correlated with the metastable zone width (MSZW) to reveal and quantify the shearing effect on nucleation kinetics. Crystal size distribution (CSD) was determined by laser diffraction using Horiba LA300 particle size analyser and crystal morphology was determined by using a Schottky field emission scanning electron microscope (SEM) JEOL JSM-7610FPlus equipped with the Ultim Max 65 energy dispersive spectroscopy detector (EDS) and AZtec software, both from Oxford Instruments. The latter was used to conduct elemental analysis of the surface. The end product agglomeration was inspected by using polarizing microscope BK-POLR. Sample images were taken by Canon EOS 505D and were analysed in Motic Images Advanced 3.2 software. The findings highlight the importance of hydrodynamic optimization in improving crystallization efficiency and product quality. While ultrasonic assistance provided enhanced mixing, it also resulted in altered nucleation kinetics which in turn affected the final product size as crystals were smaller with narrower CSD in sonicated conditions. However, these benefits occurred at significantly increased power consumption. It is also important to emphasise that sonication alone was not able to efficiently suspend particles and that it cannot be used without mechanical mixing in larger volumes if the off-bottom suspension needs to be achieved. This limitation is critical for scale-up, as industrial crystallisers require robust hydrodynamic control to ensure consistent product quality. Overall, these findings underscore the challenges of scaling ultrasonic-assisted crystallization systems, where geometric similarity and power consumption per unit volume may not be enough to maintain hydrodynamic equivalence. The inability of sonication alone to achieve off-bottom suspension in larger volumes suggests that sonotrode(s) must be strategically integrated into larger-scale crystallizers to avoid energy inefficiencies and, consequently, unsuitable product properties.



INTERFACE-TAILORED SEPARATORS *via* ICVD FOR LITHIUM METAL BATTERIES WITH EXTENDED LIFESPAN

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Lithium metal batteries (LMBs), owing to their high energy density, are considered promising candidates for next-generation energy storage systems. However, their practical deployment is hindered by critical issues such as the uncontrollable growth of lithium dendrites and the formation of an unstable solid electrolyte interphase (SEI). In this work, we report a strategy to address these challenges by employing an initiated chemical vapor deposition (iCVD) process to fabricate a highly cross-linked and functionalized polymethacrylic acid (PMAA) coating on polypropylene (PP) separators. The resulting coating features highly oriented carboxyl terminal groups with strong dipole moments, which can donate excess electrons to modulate the degradation kinetics of lithium hexafluorophosphate (LiPF_6). This regulation promotes the formation of a stable SEI enriched with lithium phosphate (Li_3PO_4) and lithium fluoride (LiF), effectively suppressing parasitic reactions on the lithium surface and inhibiting dendrite formation. Electrochemical evaluations demonstrate that the modified separators enable lithium iron phosphate (LFP) batteries to deliver a discharge capacity of 99.1 mA h g^{-1} with a capacity retention of 84.5% after 1000 cycles at a high rate of 10 C. This study highlights the potential of the solvent-free, highly controllable iCVD technique for developing multifunctional separators, paving the way for long-cycle-life lithium metal batteries.

Acknowledgements. This work was financially supported by Ningbo University.



ELECTROLYTE ENGINEERING ENABLES LONG-LIFE IN HIGH-ENERGY-DENSITY LITHIUM METAL BATTERIES


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Lithium metal batteries (LMBs) offer a pathway toward next-generation energy storage due to their exceptionally high energy density. However, their implementation remains challenging, particularly under lean electrolyte conditions, where unstable interfaces and inefficient ion transport severely limit cycling stability. Here, we design a bifunctional ligand-bridged electrolyte (BLBE) by integrating ethyl difluoroacetate (EDFA) into a lithium nitrate/triethyl phosphate matrix. Incorporating EDFA as a dynamic bridging agent drives the formation of interconnected ionic aggregates through synergistic $\text{H}^{\delta+}$ $\text{O}^{\delta-}$ hydrogen bonding with anions and coordination interactions with Li^+ , accelerating interfacial kinetics and suppressing parasitic reactions. The electrolyte further enables weakly coordinating solvents to engage in the solvation sheath via non-classical hydrogen bonding, facilitating the formation of a robust, inorganic-rich solid electrolyte interphase. This design supports high-capacity (13.5 A h) lithium–nickel pouch cells with outstanding cycling stability and delivers an energy density of 600 W h kg^{-1} . These findings demonstrate a viable electrolyte strategy for enabling high-performance lithium metal batteries under practical conditions.

Acknowledgements. This work was financially supported by Ningbo University.



STAINLESS STEEL MEDICAL IMPLANTS SURFACE FUNCTIONALIZATION

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Stainless steel has been widely used for biomedical implants due to its superior mechanical strength, chemical stability, and biocompatibility. However, corrosion remains a major challenge, frequently contributing to implant failure. Surface functionalization represents an effective strategy to improve implant durability and functionality. Surface functionalization is crucial as it can not only enhance corrosion resistance but also improve biocompatibility reducing the risk of adverse biological reactions. Fatty acids, known for their biocompatibility and self-assembling properties, present a promising approach to improve stainless steel implant performance. Conventional fatty acid self-assembled monolayers (SAMs) exhibit limited chemical stability and can be easily detached, diminishing effectiveness over time. By converting SAMs into polymer nanocoatings (PNCs) through radiation-induced crosslinking, their stability and corrosion stability can be substantially enhanced^[1–5].

The aim of this research was to systematically explore and optimize the parameters required for functionalizing stainless steel surfaces with behenic acid to successfully form stable and uniform SAMs. These SAMs were further enhanced through radiation-induced crosslinking, resulting in the formation of PNCs. The stability of the coatings was evaluated in simulated body fluids, under both steady-state and dynamic conditions using a rotating disc electrode and electrochemical techniques. Surface characteristics were analyzed using atomic force microscopy (AFM) and contact angle measurements.

Acknowledgements. This work has been supported by Croatian Science Foundation.

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HARNESSING OPTICAL PROPERTIES OF QUANTUM NOBLE METAL BIO-NANO HYBRIDS

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This lecture explores the distinctive optical and electronic properties of metal nanoclusters (NCs), with a particular emphasis on luminescent noble metal NCs, through two interconnected research avenues: solar energy and biomedical applications. In the quest to advance photovoltaic technologies beyond traditional silicon and emerging perovskite solar cells, Grätzel et al. pioneered the dye-sensitized solar cell (DSSC).^[1] Building upon this foundation, this research integrates natural pigments with noble metal NCs to create bio-nano hybrids. These bio-inspired luminescent nanomaterials show promise for enhancing light absorption, charge transfer efficiency, and overall stability in next-generation photovoltaic systems. Computational quantum chemistry methods, particularly Density Functional Theory (DFT) and Time-Dependent DFT (TD-DFT), are central to designing these advanced nanomaterials for DSSCs, aiming to boost their efficiency and durability. This approach leverages the optical properties of noble metal nanoclusters (e.g., gold and silver) synergistically with eco-friendly organic dyes.^[2,3] Beyond energy applications, noble metal nanoclusters emerge as powerful tools in medical diagnostics, imaging, and biosensing due to their unique quantum effects and outstanding optical properties^[4,5]. This lecture emphasizes an interdisciplinary strategy that merges photophysics, photochemistry and nanotechnology to harness the full potential of luminescent noble metal nanoclusters for advancements in both solar energy conversion and bioimaging technologies.

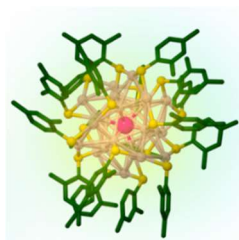


Figure 1. Schematic representation of liganded noble metal NC (adapted from [5])

Acknowledgements. This research was supported by the project STIM – REI, Contract Number: KK.01.1.1.01.0003, funded by the European Union through the European Regional Development Fund – the Operational Programme Competitiveness and Cohesion 2014–2020 (KK.01.1.1.01).

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UNDERSTANDING BATTERY FAILURE MECHANISMS THROUGH STRUCTURE CHANGES DURING OPERANDO XRD MEASUREMENTS

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Global warming, unsustainable usage of fossil fuels and everyday increase in energetic needs of today's modern society, together with the world energy crisis are in a great need for a transition towards sustainable energy systems. Batteries are crucial components in modern technologies, from electric vehicles to portable devices, and their long life and reliability are directly dependent on understanding the mechanisms of their failure.

Among the most significant factors that affect performance degradation in batteries are the structural changes in electrode materials during cycling. This study explains the failure mechanisms of batteries by analyzing structural changes in materials using operando X-ray diffraction (XRD), a technique that allows real-time monitoring of structural modifications during battery operation.^[1] Operando XRD provides insights into the dynamic structural changes that occur during battery cycling, enabling a better understanding of the causes of material degradation, such as crystal lattice breakdown, phase formation, and stress accumulation within the electrodes. Understanding these changes is crucial for optimizing battery design and predicting their lifetime. For operando XRD measurements, home-made 3D printed DANOISE cell in transmission mode was used.^[2]

Results cover from ex-situ XRD measurements of the graphite or LFP electrode in the DANOISE cell, without applied current, to operando XRD measurements in the half-cell, as well as measurements in the full-cell setup with pellet and with coated electrode with mentioned active materials. The aim is to identify specific structural phenomena associated with battery failure, with a focus on improving the performance and stability of future battery materials and technologies. The main accent is on the crystallographic analysis of the operando XRD data, including identification of the phases and sequential refinement in the Fullprof.^[3]

Acknowledgements. The authors greatly appreciate the support of the Ministry of Science, Education and Youth and the Croatian Science Foundation for funding this work. This work is funded by the European Union funds "National plan for Recovery and Resilience" under the number NPOO.C3.2.R3-I1.04.0187.

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UNLOCKING THE POTENTIAL OF IONIC LIQUIDS IN EPOXY RESIN DESIGN AND COMPOSITE PERFORMANCE

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The development of advanced epoxy resin systems has increasingly focused on sustainability, functionality, and performance enhancement. This body of work presents a comprehensive exploration of the design and application of ionic liquids (ILs) as novel and tunable components in epoxy-based composite materials. ILs, due to their structural versatility, low volatility, and potential for tailored chemical functionality, offer unique advantages over conventional curing agents and additives.^[1]

To evaluate the intricate structure–property relationships governing IL-based epoxy systems, a comprehensive range of advanced analytical techniques was employed. Differential scanning calorimetry provided critical insights into curing kinetics and glass transition behavior, while dynamic mechanical analysis and Shore hardness testing illuminated the mechanical performance of the cured networks. Scanning electron microscopy revealed the morphological architecture at the micro-scale, enriching our understanding of phase distribution and interfacial interactions—specifically in systems containing fillers such as cellulose and supported ionic liquid phases (SILPs).

Strikingly, ILs bearing polymerizable allyl groups or DABCO-derived cations, especially when paired with dicyanamide or triflate anions, emerged as frontrunners in promoting rapid, robust curing and mechanical enhancement.^[2] Binary IL mixtures revealed synergistic phenomena, enabling precise modulation of flexibility, rigidity, and thermal resilience.^[3] Systems featuring covalently reactive ILs exhibited superior interfacial adhesion and dimensional stability,^[4,5] while aniline-derived IL formulations struck an elegant balance between latency and structural integrity.^[6]

This investigation transcended conventional formulations by deploying ILs not merely as curing agents, but as functional, chemically integrated constituents within epoxy resin matrices— particularly in the fabrication fiber-reinforced composites incorporating flax or carbon fibers.

Acknowledgements. This research was supported by the National Science Centre (Poland), project SONATA BIS (No. 2017/26/E/ST8/01059).

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PEROVSKITE-BASED ANODES: A NEW HOPE FOR NEXT-GEN LITHIUM-ION BATTERIES

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Lithium-ion batteries are ubiquitous in everyday life, from modern day portable electronics to electric vehicles and emerging stationary storage devices, as a result of high energy and power density, extended longevity and stability, low self-discharge and fast charging. As the battery industry demands for the for safer, more efficient, and sustainable energy storage solutions grows, research into alternative materials is becoming increasingly relevant. Currently, graphite dominates the battery market as anode material, although its intrinsic limitation, in particular irreversible first cycle loss and limited capacity, poses significant challenge to meet the performance of emerging energy storage technology. Metal-organic halide perovskites (MOHPs), widely studied for their optoelectrical properties in photovoltaics, are gradually establishing themselves as anode materials for lithium-ion batteries. Their unique structure, consisting of inorganic and organic layers, facilitates efficient multiple ion storage and transport, thereby expanding their potential as battery materials. As a developing field, research on metal-organic halide perovskites is still limited, nevertheless, studies on lead-based compositions have demonstrated promising potential for anode applications.

In this study, we synthesized tin-based organic metal perovskites with various organic cations including methylammonium, formamidinium, phenethylammonium, as well as inorganic cation cesium, combined with different halide anions such as chloride, bromine and iodine, with the purpose of understanding structure-property relationship and its influence on process of lithium storage. Selected materials were prepared by direct synthesis from tin-halide precursor and organic/inorganic halide salt, followed by antisolvent crystallization with toluene to yield crystal powders. Electrode materials were subsequently prepared using a standard procedure for Li-ion batteries and coated on copper current collectors. Prepared electrodes incorporating perovskite active material were assembled inside the Swagelok cell as a working electrode, while lithium was used as both reference and counter electrode. Electrochemical measurements were conducted using cyclic voltammetry, electrochemical impedance spectroscopy and galvanostatic charge-discharge. Physical characterization of both as-prepared and cycled electrodes, was examined with X-ray diffraction and X-ray energy dispersive spectroscopy to correlate electrochemical results with physical transformation. The obtained results indicate distinct behaviour influenced by the chosen cation and anion. Generally, all materials exhibited high initial capacity values, surpassing conventional graphite electrodes, with stable capacity retention in the following cycles. Even though this discovery offers a promising prospect for advancing lithium-ion technology, further investigation is still needed to elucidate the exact mechanism of lithium-ion storage.

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

THE INFLUENCE OF PREPARATION PARAMETERS ON THE MORPHOLOGY AND FERROELECTRIC PROPERTIES OF METAL-ORGANIC THIN FILMS BASED ON BICYCLIC AMINES

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Ferroelectric materials continue to attract significant interest due to their potential in advanced technologies and the ongoing discovery of new hybrid systems. In this study, we focus on metal-organic complexes, as promising candidates for functional ferroelectric materials. These compounds are interesting since they have the potential to exhibit switchable polarization — property desirable for applications in sensors, memory devices, and nonlinear optics.^[1] The aim is to develop thin films in order to enable their integration into practical devices. Despite its potential, metal-organic thin films have not yet been thoroughly studied. Several methods exist to produce metal-organic thin films such as dip coating, spin coating, drop casting etc. However, many parameters need to be carefully optimized to obtain quality films, such as precursor solution characteristics (concentration, pH, composition of solvents) and other conditions (temperature, relative humidity, withdrawal rate for dip-coating, etc). All these parameters, as well as preparation methods, strongly affect film morphology and properties.^[2] Humidity plays a critical role by influencing structural organization during film formation. In this work, thin films of cinchonine trichlorocobaltate were deposited on Si(100) and ITO-coated glass substrates via dip coating under controlled humidity. Scanning electron microscopy (SEM) analysis revealed that low humidity favors uniform film formation, while higher humidity levels induce morphological changes characterized by nano- and mesoscale pinholes. Optimized parameters yielded homogeneous films suitable for ferroelectric characterization, contributing to the development of novel metal-organic ferroelectric systems.

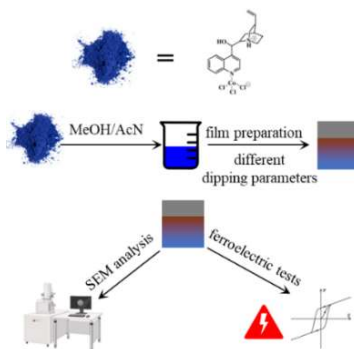


Figure 1. Scheme of research steps.

Acknowledgements. This work has been supported by Croatian Science Foundation (UIP-2019-04-7433). City of Zagreb is gratefully acknowledged.

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IMPROVEMENTS OF TIN HALIDE PEROVSKITE THIN FILMS BY CRYSTALLIZATION MEDIATORS AND PLASMA-ASSISTED CRYSTALLIZATION

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The performance and stability of tin-based perovskite solar cells is highly influenced by the quality of the perovskite crystals and their interfaces with charge-selective contacts. One critical factor in optimizing these materials is the use of crystallization mediators, which play a crucial role in controlling the growth and quality of tin perovskite films. This work focuses on investigating the effects of different precursors, solvents and additives, including various crystallization mediators, on the deposition, crystallization, and overall quality of tin perovskite absorber layers. By examining these processes in detail, the aim is to identify key correlations between material properties and solar cell performance. The ultimate goal is to enhance the efficiency and stability of tin-based perovskite solar cells by developing optimized strategies for plasma-assisted film fabrication and crystallization, contributing to the advancement of this promising photovoltaic technology.

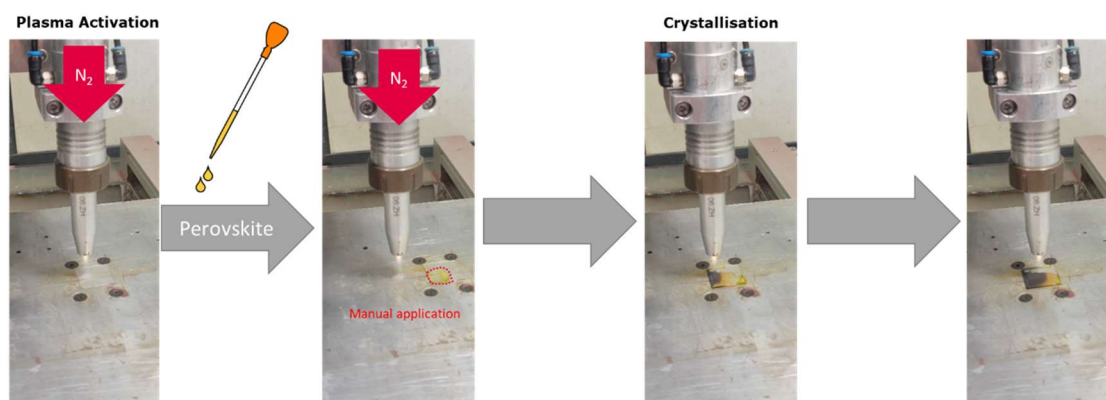


Figure 1. Plasma-assisted crystallization process

Acknowledgements. This work was financially supported by the Horizon Europe project Smartline PV. This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No 101122327.



ENVIRONMENTALLY FRIENDLY LEAD-FREE THIN FILMS FOR HIGH-PERFORMANCE DIELECTRIC CAPACITORS

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We report on the development of sustainable, lead-free dielectric thin films fabricated via a low-cost aqueous chemical solution deposition method for high-energy-density capacitor applications. By strategically combining Bi-based and BaZrTiO₃-derived compositions, we achieved optimized microstructures and phase behaviour at morphotropic boundaries, resulting in significantly enhanced recoverable energy densities (up to 51 J cm⁻³) and efficiencies exceeding 75% at high electric fields (2 MV cm⁻¹). Structural and electrical characterizations reveal excellent stability under varying temperatures and frequencies, as well as outstanding fatigue resistance over 10⁶ cycles. These findings highlight the strong potential of scalable, green-processed thin films for integration in next-generation capacitive energy storage systems, especially in energy-autonomous and miniaturized electronics.

Acknowledgements. This work has been supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No. 817190).

FROM MECHANICAL PROPERTIES TO ATOMIC-LEVEL MECHANISM OF ELASTICALLY FLEXIBLE CRYSTALS

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Mechanically adaptive crystals—those capable of adjusting to a range of external stimuli, including light, heat, and mechanical force—have attracted significant attention in recent decades due to their promising applications in advanced technologies. These applications span optical devices, electronics, wearable technology, and soft robotics.^[1] However, a comprehensive understanding of their mechanical properties and molecular-level movements during mechanical adaptations is essential for their integration into innovative devices. Recently, we explored various families of flexible crystals derived from one-dimensional coordination polymers (CPs) and discovered that they exhibit remarkable adaptive characteristics. Furthermore, we found that intermolecular interactions play a critical role in influencing their mechanical responses, which can range from exceptional pliability to advanced elasticity. To deepen our understanding of these materials' bending capabilities, we aim to investigate the underlying mechanisms driving their flexibility and relate them to the mechanical features.^[2–7] In this study, we examine two novel one-dimensional coordination polymers, $[\text{Cd}(\mu\text{-X})_2(\text{pza})_2]_n$ ($\text{X} = \text{Cl}, \text{Br}$; $\text{pza} = \text{pyrazinamide}$), which exhibit mechanically stimulated elastic flexibility. This unique property enabled us to investigate their elastic characteristics through a variety of methods, including three-point bending tests, atomic force microscopy (AFM), computational techniques, and tensile experiments. Our primary focus, however, was to understand the atomic-level changes that occur during bending from a structural perspective. By mapping the structural alterations at the apex of the crystal bend using micro focus synchrotron radiation ($\mu\text{-SCXRD}$), we identified the first mechanism of elastic bending in coordination polymer crystals. This mechanism contrasts distinctly with those observed in elastically flexible molecular (0D) crystals subjected to mechanical stress and in one-dimensional plastically deformable crystals under quasi-hydrostatic pressure—the only reconfigurable crystal mechanisms identified to date.^[7] In addition, the structural findings were further correlated with mechanical properties, which were explored both experimentally and theoretically.

Acknowledgements. This work has been fully supported by the Croatian Science Foundation under Project IP-2019-04-1242. We gratefully acknowledge the Paul Scherrer Institut, Villigen, CH, for the provision of synchrotron radiation beamtime at beamline X06SA (PXI) at the SLS.

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DEVELOPMENT AND EVALUATION OF NZVI-BASED MATERIALS FOR ARSENATE REMOVAL FROM WATER: ADSORPTION PERFORMANCE

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Nanoscale zero-valent iron (nZVI) is a promising material for remediating contaminated water due to its high surface area and strong affinity for pollutants like arsenate. Its ability for redox reactions supports effective contaminant removal.^[1] However, challenges such as aggregation and oxidation limit its practical use, necessitating surface modification to improve stability and effectiveness.^[2] This study characterises four nZVI types: bare nZVI, nZVI with chelating agents, supported nZVI and nZVI in a polylactic acid (PLA) matrix. Characterisation techniques included isoelectric point determination and scanning electron microscopy (SEM) to evaluate surface properties and morphology. We conducted batch adsorption experiments to assess arsenate removal efficiency across different pollutant concentrations, particle dosages, pH and contact time. The data were analysed with isotherm and kinetic models to clarify contaminant uptake mechanisms. We found that modifying nZVI, particularly its immobilisation in PLA, significantly enhances stability. These findings contribute to ongoing research on optimising nZVI-based materials for effective water purification technologies.

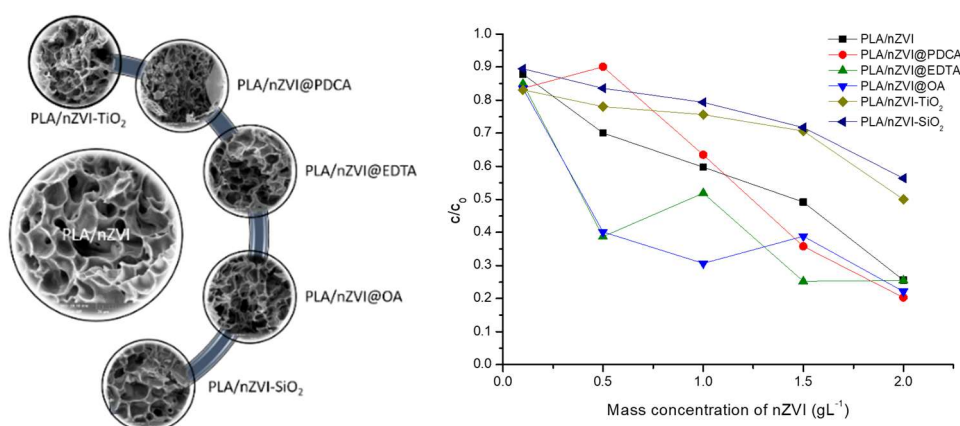


Figure 1. Morphology of biopolymer-based adsorbent and effect of nZVI dosage on arsenate removal efficiency using PLA/nZVI composites.

Acknowledgements. This work has been supported by the Croatian Science Foundation (grant DOK-2021.02).

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EFFECT OF PROCESS PARAMETERS ON REMOVAL OF ACETAMIPRID WITH NANOFILTRATION MEMBRANES

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Increasing use of pesticides, such as acetamiprid (AC), shown on Figure 1^[1] pose significant environmental and health risks through processes like bioaccumulation and biomagnification, most prominently in water sources.^[2] Nanofiltration (NF) is a valuable process for removing substances from aqueous solutions. This study was aimed at optimizing this process by testing the efficiency of AC removal through NF membranes with the molecular weight cut-off of 150-300 Da. Experiments involved 1 mg/L and 5 mg/L AC solutions, with changing pressures (5 bar and 10 bar) and flow rates (2 L/min and 4 L/min). Permeate and retentate samples were taken in 1-hour cycles for each set of conditions. Samples were analysed using high-performance liquid chromatography to assess removal efficiency. The results indicate that changing the pressure and flow rate significantly influences AC removal. The removal efficiency of a 1 mg/L AC solution at 5 bar equals 48.10 % at 2L/min and 64.87 % at 4 L/min. The same 1 mg/L solution with the pressure raised to 10 bar shows an efficiency improvement to 65.95 % at 2 L/min and 74.09% at 4 L/min. In conclusion, AC removal by nanofiltration improves at higher pressures and flow rates.

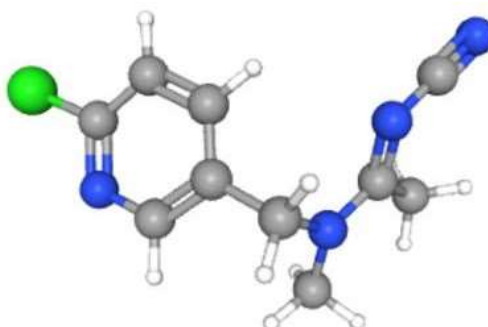



Figure 1. Acetamiprid structure^[1]

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



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INTEGRATED APPROACH TO TEACHING RADIOACTIVITY: CONNECTING CHEMISTRY AND PHYSICS FOR BETTER UNDERSTANDING

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Understanding abstract concepts like radioactivity can be challenging for students. Since chemistry and physics overlap in the final gymnasium year, we adopted an integrated teaching approach—coordinating content across both subjects to deepen students’ understanding through practical and interdisciplinary work. This also created space for enriched learning experiences: Viewing materials such as Chernobyl, The Mystery of Matter (E3), and BBC’s Elements: Radioactives to discuss historical, scientific, and safety aspects of nuclear energy, Dice experiment simulating radioactive decay, helping students discover half-life principles independently, Geiger counter activity to detect radioactivity in everyday objects and spark critical thinking, Field trip to the Krško Nuclear Power Plant to apply theoretical knowledge in a real-world context, supported by structured worksheets. Discussions on environmental impacts of nuclear energy, engaging students less confident in science through broader societal perspectives.

This interdisciplinary model fostered active participation and multi-angle exploration of radioactivity. Students showed greater accuracy and deeper understanding on assessments compared to previous years, affirming the method’s success.

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LEGO PHOTOMETER AS A TOOL FOR STUDYING CHEMICAL REACTION KINETICS

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The crystal violet (CV) reaction with hydroxide ions (Figure 1a) is a commonly used model system for studying chemical kinetics in education, as it allows simple monitoring of changes in the concentration of a colored reactant via (spectro)photometry.^[1] Although photometers are standard lab equipment, their cost often limits availability in educational settings. In this work, a method for studying the kinetics of the CV + OH⁻ reaction is described, utilizing a simple and inexpensive photometer constructed by students from LEGO bricks, LEDs, and a voltmeter (Figure 1b), following the concept introduced by Kvittingen et al.^[2] The device uses identical LEDs as both light source and detector, with absorbance calculated from the voltage measured across the detector LED.

Although the reaction follows second-order kinetics, it was carried out with a large excess of OH⁻ ions, allowing application of a pseudo-first order model. Measurements were performed at three OH⁻ concentrations to determine the second-order rate constant. Despite the simple setup, the results showed surprisingly good agreement with those obtained using a professional UV-Vis spectrophotometer. This educational and accessible approach was developed as part of the chemistry task for the *European Olympiad of Experimental Science* (EOES 2025), aiming to enhance understanding of spectrophotometry and kinetics while promoting low-cost STEM tools.

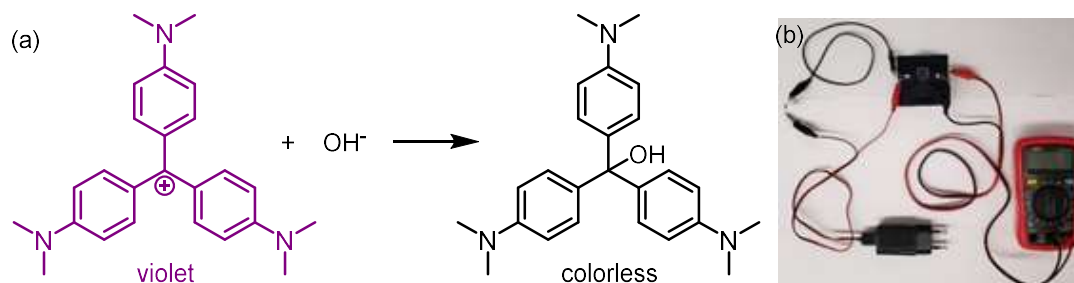


Figure 1. (a) The chemical reaction used for the kinetic study, (b) the LEGO photometer.

Acknowledgements. This work was carried out with funding from the Ministry of Science, Education, and Youth, designated for the organization of the European Olympiad of Experimental Science 2025.

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DIFFERENTIATED TEACHING OF CHEMISTRY

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Differentiated teaching is one of the forms of teaching that relies on differences in learning styles, methods and speed. In the strictest sense, differentiation consists of the teacher's efforts to respond to differences among students.

The idea's originator, Carol Ann Tomlinson, defines it as taking into account individual learning styles and levels of readiness for learning before making the actual preparation for the lesson, or as an approach to teaching that meets the different needs of students.^[1]

In the teaching of chemistry, this form of work is applied in terms of adapting the teaching methods and forming different types of tasks to check the adoption of the outcomes of the knowledge level from basic adoption to critical thinking.

Students are divided into homogeneous groups according to their interests and abilities, and the lessons are adapted to their interests, learning style and willingness to learn. One group consists of pupils who demonstrate excellent or very good knowledge and have an interest and ability to absorb more complex content. They're used for multi-level tasks and complex problem-solving. The other group is the students who show mediocre knowledge, and the benefits of this approach to learning for them are that they're more engaged, they're more expressive, they're more active, they're seeking clarification. In the end, both groups adopt the same outcomes, but in slightly different ways.

Through the lecture, different types of assignments and learning styles would be shown to suit the needs of the groups. It would also show the results of a survey of the opinions of pupils involved in this way of working.

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GREEN CHEMISTRY IN HIGH SCHOOL EXPERIMENTS

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Green chemistry (GC) is a scientific field developed to reduce or eliminate the use and generation of hazardous substances.^[1] Studies show that incorporating GC into chemistry education can enhance student motivation.^[2] Burmeister et al. propose several models for integrating sustainability, including the application of GC principles in laboratory practice.^[3] This presentation outlines how GC experiments have been integrated into high school chemistry textbooks and teaching practices in Croatia. Several textbooks now include dedicated GC chapters with corresponding experimental activities. Additional materials have been presented at educational conferences and through project platforms. Various strategies help implement GC principles in school laboratories, such as shifting from macro- to micro-scale experiments, substituting hazardous chemicals with safer alternatives, or using solvent-free techniques like mechanochemistry. More advanced approaches involve students in experiment design, encouraging them to apply GC principles and reconsider chemical use. For instance, as part of an inquiry-based learning approach, students first produce hydrogen through a conventional laboratory reaction between aluminum and hydrochloric acid. While effective, this method generates chemical waste and relies on non-renewable resources. Students then critically evaluate the process using Green Chemistry principles—particularly *Principle 1 (Prevention)*, *Principle 3 (Less Hazardous Chemical Syntheses)*, and *Principle 7 (Use of Renewable Feedstocks)*. Guided by these principles, they redesign the experiment to utilize a reversible fuel cell, enabling hydrogen production from water via electrolysis. This not only reduces environmental impact but also deepens students' understanding of sustainable practices in chemistry. By shifting responsibility for method development from teacher to student, the activity fosters critical thinking, problem-solving, and a greater appreciation of environmentally responsible science. More specific examples of experiments reflecting these strategies will be presented.

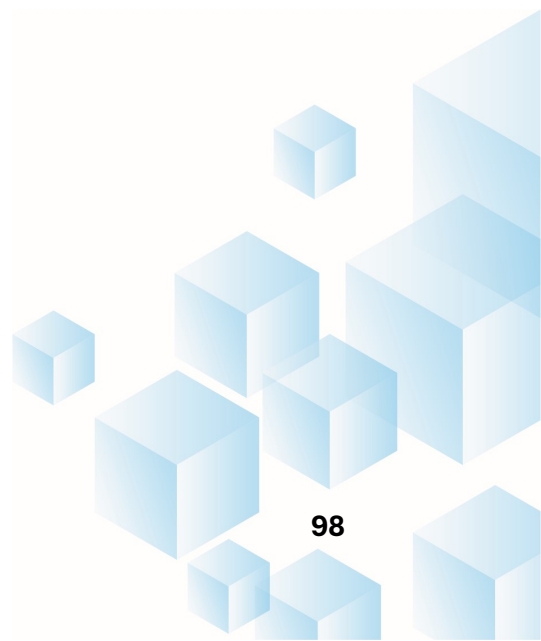
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POSTERS

CHEMISTRY



EMERGENCE OF DIAMONDROID CLUSTERS IN HELIUM NANODROPLETS

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Diamondoids are cage hydrocarbons useful as building blocks in the design of new materials.^[1] They can be selectively functionalized and recently the field further expanded to diamondoid covalent assemblies, molecules composed of several diamondoid cage subunits connected by a heteroatom.^[2] Non-covalent interactions are known to have a significant effect on spontaneous self-assembly of diamondoid derivatives, especially intermolecular London dispersion interactions between the cages. To gain more insight into the fundamental properties of these compounds, we explored diamondoid agglomeration in helium nanodroplets (HNDs) since that is a good medium for characterizing weakly-bound supramolecular clusters.^[3,4] We confirmed that for derivatives of low polarity (hydrocarbons and ethers)^[3] dispersion is indeed the main driving force for molecular organization in HNDs, while introduction of more polar functional groups to diamondoid scaffolds^[4] resulted in the emergence of more complex nanostructured supramolecular networks. A combination of experimental and computational techniques provided us with a clearer picture of the forces driving the diamondoid self-organization processes,^[5] which is important for their future application in nanotechnology.

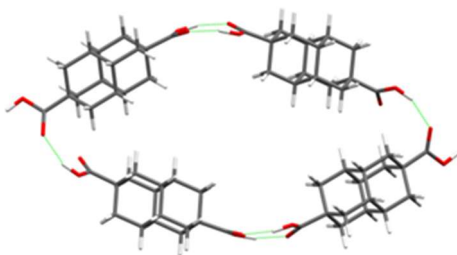


Figure 1. Computed networks of 4,9-diamantanedicarboxylic acid molecules.

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DEUCRAVACITINIB TABLET DOSAGE FORMS: ACHIEVING ANALYTICAL EXCELLENCE THROUGH A NOVEL HPLC-DAD METHOD

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Approved for treating moderate to severe plaque psoriasis in adults, deucravacitinib is a selective oral allosteric tyrosine kinase 2 inhibitor with a novel mechanism of action. Given its administration as a 6 mg tablet once daily, this study aimed to develop and validate a high-performance liquid chromatography (HPLC) method for quantifying deucravacitinib in pharmaceutical form.

Chromatographic analysis was performed on an Agilent 1260 HPLC system equipped with a diode-array detector (DAD), using a Poroshell 120 SB-C18 column (3.0 × 100 mm, 2.7 µm; Agilent Technologies, Santa Clara, CA, USA) maintained at 30.0 ± 0.1 °C. Isocratic elution was employed with a mobile phase composed of ultra-pure water (75 %) and acetonitrile (25 %), acidified with 0.1 % formic acid at a flow rate of 1.0 mL/min. The injection volume was 5 µL. Quantification was carried out at 254 nm (4 nm slit width), while the full UV spectrum (200–600 nm) was recorded.

Method validation followed the International Council on Harmonisation (ICH Q2 (R2)) guidelines.^[1] The calibration curve demonstrated linearity over the concentration range of 10–100 µg/mL ($r = 0.9997$), with a limit of detection (LOD) of 3.06 µg/mL and a limit of quantification (LOQ) of 9.26 µg/mL. Accuracy was assessed through recovery studies at three concentration levels (10, 50, and 100 µg/mL), with recoveries ranging from 96.4 % to 101.5 % and relative standard deviations (RSDs) below 2.3%. Precision was confirmed by intraday and interday analysis of six replicate samples (50 µg/mL), yielding RSDs from 0.14 % to 0.59 %. Stability testing demonstrated high stability of deucravacitinib standard solutions: 100.4 % after 8 hours at room temperature, 99.4 % after 3 days at 4 °C, and 99.5 % after 7 days at –20 °C. Robustness testing revealed minimal variations in results when small changes were made to column temperature (±2 °C, deviation <0.43%), flow rate (±0.05 mL/min, deviation <3.28 %), and mobile phase composition (±1 %, deviation <2.28 %).

In conclusion, the developed HPLC-DAD method is accurate, precise, robust, and suitable for the routine determination of deucravacitinib content in tablet dosage forms.

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NATURAL COMPOUNDS AS LAG-3 INHIBITORS IN CANCER IMMUNOTHERAPY

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LAG-3 is a membrane protein found on T and B lymphocytes and NK cells. Its inhibition stops the activation of immune system cells. Some cancers overexpress LAG-3 ligand — MHCII— which, when in contact with the immune system, cause its inhibition. For this reason, drugs targeting the LAG-3 protein are becoming the focus of an increasing number of research groups.^[1]

Currently, the main known inhibitors are based on monoclonal antibodies, which are extremely effective but also expensive to produce and problematic to administer. The discovery of the first small molecule inhibitor will be a milestone on the path to discovering a cheaper, orally available drug.^[2]

Compounds naturally occurring in plants are an interesting set of molecules to search for potential protein inhibitors. If a sufficiently active inhibitor is discovered, further testing in animals or humans is easier and faster to conduct, as these compounds are often widely used in folk medicine. Furthermore, their often optimal pharmacokinetic properties make active natural compounds a good starting point for optimizing the structure of the inhibitor. In this case, the initial optimization of a number of physicochemical properties that the drug must meet has already been done by nature.

Among the compounds tested, a group of flavonoids proved to be particularly interesting, characterized by their ability to block interactions between LAG-3 and MHCII proteins (IC₅₀) at a concentration of approximately 20 μM. They also activated the immune system response in cell studies. The cytotoxicity, which occurred on higher concentrations has been abolished by developing appropriate formulation. It is interesting to note that changing the position of substituents strongly affects their ability to block LAG-3/MHCII interactions in cells, suggesting high selectivity and opening possibilities for SAR and QSAR studies.

Acknowledgements. This work has been supported by the National Science Center of Poland as part of the OPUS grant “Innovative small molecule inhibitors targeting LAG-3 and the MHCII complex for cancer immunotherapy” (grant number UMO-2024/53/B/NZ7/02801).

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DEVELOPMENT AND VALIDATION OF A FLOW INJECTION METHOD FOR THE DETERMINATION OF ASCORBIC ACID IN PHARMACEUTICAL PREPARATIONS

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Ascorbic acid (AA), commonly known as vitamin C, is a water soluble compound that shows acidic properties as well as reducing properties due to the endiol group in its structure. Since it cannot be synthesized by the human body, ascorbic acid must be ingested with food or supplements. Consequently, there is a need to develop a selective, simple and accurate method for the determination of ascorbic acid in pharmaceutical preparations.

Flow injection analysis (FIA), the first generation of flow analysis introduced by Ruzicka and Hansen, is a powerful instrumental analytical technique for pharmaceutical analysis.^[1] The advantages of this technique are its simplicity, cost-effectiveness, high throughput capacity and flexibility. As an environmentally friendly technique, requiring small amounts of samples and reagents, FIA reduces chemical waste and lowers analytical costs.

The new flow method utilizes a rapid redox reaction in which AA reduces the Cu(II)-neocuproine complex to Cu(I)-neocuproine with maximum absorbance at 458 nm. The optimization of the experimental conditions and the parameters of the manifold was performed by the univariate method using a simple two-stream single reagent manifold. The reagent prepared in Britton-Robinson buffer solution (pH = 3) was merged with a sample (500 µL) and injected into a carrier stream of distilled water at a confluence point, where the streams are combined. A linear calibration curve was established in a concentration range of AA from 6.0×10^{-7} to 4.0×10^{-5} mol L⁻¹ with the regression equation $y = 6932x + 0.0025$ ($R^2 = 0.9989$). The new FIA method is sensitive with an LOD of 1.8×10^{-7} mol L⁻¹ of AA at a sampling rate of 60 samples per hour. This new FIA method offers a sensitive, simple and rapid approach for the determination of ascorbic acid in pharmaceutical preparations. Furthermore, FIA method is precise (RSD 0.9 %) and accurate (recovery in the range of 95.5 % to 101.5 %).

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SHORTENING THE LINKER-DISTANCE IN BINOL-DERIVED CYCLOPENTADIENE LIGANDS

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Cyclopentadienyl (Cp) ligands are fundamental components in organometallic chemistry and have been extensively utilized in a wide range of transition metal-catalyzed transformations.^[1] Despite their broad utility, the development of Cp-based ligands for stereoselective catalysis has been hindered by the challenges associated with introducing substituents that can exert precise control over the coordination environment.^[2] Most stereochemically directed Cp ligands incorporate a BINOL-derived moiety tethered to the Cp ring.^[3] In the present study, we report the design and synthesis of a new class of structurally simple, C_2 -symmetric Cp ligands, in which the Cp unit is directly fused to a binaphthyl scaffold. This rigid framework is expected to provide enhanced stereocontrol in catalytic applications. The synthetic approach relies on a zirconium-mediated cyclization of chiral diynes, as illustrated in Figure 1. The synthesis, structural features, and preliminary applications of these ligands in asymmetric catalysis are discussed herein.

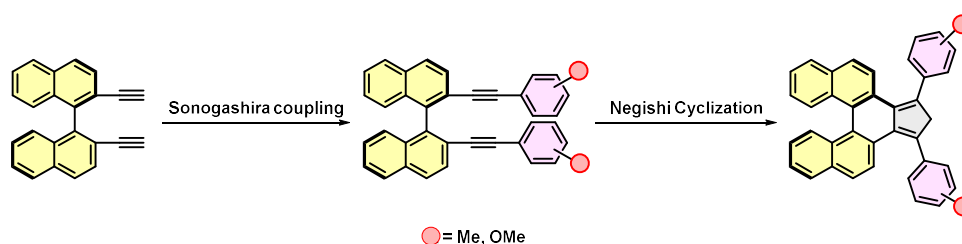


Figure 1. Conceptual design of the chiral Cp ligands.

Acknowledgements. This work was supported by the NextGenerationEU project NPOO.C3.2.R2-I1.06.0022.

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FMOC SOLID-PHASE SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF C-GLYCOPEPTIDES

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The incorporation of non-proteinogenic amino acids (NPAAs) into peptides is a well-established strategy to modulate their secondary structure and improve physicochemical properties. Previous studies suggest that both the number and distribution of NPAAs within the peptide sequence can significantly influence peptide conformation and intermolecular interactions.^[1]

We hypothesize that sterically demanding carbohydrate moieties bound directly to the C α atom of C-glycosyl α -amino acids can stabilize certain secondary structures, depending on their number, stereochemistry and positional arrangement within the peptide sequence. To investigate this, we developed a robust and highly diastereoselective strategy for the preparation of C-glycosyl- α -amino acid monomers that is compatible with a wide range of carbohydrate substrates.^[2] These building blocks were subsequently incorporated into peptides using Fmoc-based solid-phase peptide synthesis (SPPS). The resulting C-glycopeptides (Figure 1) were purified by RP-HPLC and structurally characterized by 1D and 2D NMR spectroscopy and CD spectroscopy.

This study systematically evaluates the effects of structural variations and incorporation patterns of C-glycosyl α -amino acids on peptide conformation through non-covalent interactions. We demonstrated that stereochemistry, glycosylation pattern, and positional arrangement of these amino acids predictably influence the stabilization of the secondary structure.

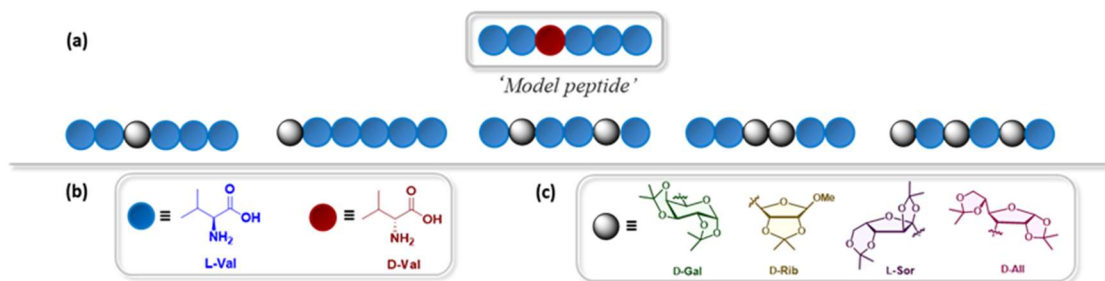


Figure 1. (a) Hexapeptides incorporating C-glycosyl α -amino acids synthesized by Fmoc-based solid-phase peptide synthesis. (b) Proteinogenic α -amino acids. (c) C-glycosyl donors.

Acknowledgements. This work has been supported by the Croatian Science Foundation (IP-2022-10-9617).

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MACHINE LEARNING PREDICTION OF CHOLINESTERASE INHIBITION BY α -BENZOYLAMINO ACETAMIDES

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Alzheimer's disease is a progressive neurodegenerative disorder characterized by significant cognitive impairment and memory loss.^[1,2] This major global health concern is often linked to the cholinergic hypothesis, which proposes that a decline in acetylcholine signaling contributes to cognitive decline. Acetylcholine is a crucial neurotransmitter for learning, memory, and attention, and its activity is regulated by the enzymes acetylcholinesterase (AChE) and butyrylcholinesterase (BChE). Because Alzheimer's disease involves neuronal degeneration and reduced acetylcholine production, cholinesterase inhibitors are used to increase acetylcholine levels and mitigate symptoms.

To link experimentally measured reversible inhibition of AChE and BChE to the theoretical potential energy surfaces (PES) of the compounds, we developed inhibition/PES regression models. An extensive machine learning procedure for the generation and subsequent cross-validation of multivariate linear regression models with a linear combination of original variables as well as their higher-order polynomial terms was performed.^[3] The best-performing models have been identified and will be presented. These activity/PES models can be used for accurate prediction of activities for new similar compounds based solely on their PESs, which will enable wider screening and guided search for new potential leads. Our results demonstrate that α -benzoylamino acetamides represent a promising scaffold for the further optimization of novel cholinesterase inhibitors.

Acknowledgments: This work was supported by the Croatian Science Foundation under the project number IP-2022-10-9525: *Target-guided synthesis of cholinesterase inhibitors supported by machine learning*.

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DEVELOPMENT OF LC-MS/MS METHOD FOR SIMULTANEOUS DETERMINATION OF THIAMINE, FOLIC ACID, AND NIACIN IN FERMENTED MILK SUPPLEMENTS CONTAINING PROBIOTIC BACTERIA

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The probiotics are typically defined as live microbial food additives that, when consumed in sufficient quantities, confer health benefits to the host.^[1] Lactic acid bacteria (LAB), most commonly species from the *Lactobacillus* genus, along with *Bifidobacterium* species are among the most commonly used starter cultures for the fermentation of a wide range of foods. Their application enhances the safety, shelf life, nutritional value and overall quality of fermented products.^[2] Although many LAB strains are auxotrophic for certain vitamins, laboratory studies suggest that *Lactobacillus* and *Bifidobacterium* strains possess the ability to synthesize water-soluble vitamins, particularly those from the B-vitamin group.^[3,4] This characteristic is especially valuable because consuming LAB-fermented foods can serve as a dietary source of vitamins.^[4]

In this study, our goal was to develop an extraction protocol and sensitive LC-MS/MS quantification method for determination of thiamine, folic acid and niacin from a fermented milk food supplements containing *Lactobacillus acidophilus*, *Lactobacillus casei*, *Lactobacillus rhamnosus* and *Bifidobacterium lactis*. Simultaneous determination of more water-soluble vitamins in one method is challenging due to the diverse structures and chemical properties of these compounds, their trace amounts of vitamins present, the complexity of the matrix, and additional issues such as light and heat instability, as well as solubility limitations. Various solvent mixtures have been tested for the extraction of analytes and the best results were obtained in LLE extraction with 0.5 M TFA and hexane followed by protein precipitation. The analytical recoveries, determined using the internal standard addition method before and after extraction, were found to be satisfactory for all three analytes. Samples were analyzed on the Agilent QQQ LC-MS/MS in multiple ion monitoring (MRM) mode. The solvents used for the chromatographic analysis were 0.1 % FA in water and acetonitrile with gradient elution performed on Zorbax XDB C18 with flow rate of 0.3 mL/min.

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QUANTITATIVE DETERMINATION OF THE CHIRAL COMPOUNDS IN THE SEA FENNEL ESSENTIAL OIL USING GC-MS/MS

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Sea fennel (*Crithmum maritimum* L.) is one of the most widespread perennial, facultative halophytes with a great ability to survive in saline environments and a well-developed mechanisms of adaptation to the Mediterranean climate.^[1] Sea fennel essential oil is characterised by a high content of limonene and significant amounts of sabinene, γ -terpinene and terpinen-4-ol. This work aimed to develop and validate a method for quantification of limonene, sabinene, sabinene hydrate and terpinen-4-ol enantiomers, as well as achiral γ -terpinene.

Gas chromatography hyphenated with tandem mass spectrometry (GC-MS/MS) is a suitable technique for qualitative and quantitative determination of volatile constituents in essential oils. Chiral standards of (1R, 5R)-(+)- and (1S, 5S)-(-)-sabinene, (R)-(+)- and (S)-(-)-limonene, (R)-(-)- and (S)-(+)-terpinen-4-ol, as well sabinene hydrate and γ -terpinene were purchased for the preparation of the standard solutions using hexane as a solvent. Gas chromatography was applied to separate these compounds using a chiral CycloSil-B column and was optimized by changing the oven temperature program and the carrier gas (helium) flow. A triple quadrupole mass spectrometer, in MRM scan mode, was used to monitor specific fragmentation reactions (quantifier and two qualifiers for each compound). Mass spectrometry was optimized by determining the collision energy with nitrogen for each MRM transition. The developed method was validated according to the ICH guidelines and tested parameters were range, linearity, limit of detection, limit of quantification, accuracy, precision, specificity and system suitability.^[2]

The presented procedure was applied in the analysis of *C. maritimum* essential oil, showing that only (R)-(+)-limonene was present while (S)-(-)-limonene was not detected. Only one enantiomer was quantified in the case of sabinene, sabinene hydrate and γ -terpinene. On the contrary, both enantiomers of terpinen-4-ol were identified with a higher amount of (S)-(+)-terpinen-4-ol compared to subsequently eluting (R)-(-)-terpinen-4-ol.

Acknowledgements: This work has been supported by the PRIMA program (supported by EU) under project SEAFENNEL4MED.

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NUCLEOFUGALITY OF PHENYLSULFINATE LEAVING GROUP IN AQUEOUS ACETONE AND AQUEOUS ETHANOL

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Understanding the reactivity of organic compounds and the structural factors that influence it is of fundamental importance in organic chemistry. The ability to predict reaction rates is particularly valuable when handling compounds during synthesis, purification and storage. The assessment of the solvolytic reactivity of compounds can reliably be estimated using the Mayr equation.^[1]

$$\log k (25\text{ }^{\circ}\text{C}) = s_f(E_f + N_f) \quad (1)$$

In the equation (1), k is a first-order rate constant, whereas N_f and s_f are nucleofuge-specific parameters that define the heterolytic reactivity of a leaving group (nucleofuge) in some solvent. On the other hand, the E_f value refers to the heterolytic reactivity of an electrofuge and it does not depend on solvent. Using reference benzhydryl electrofuges with defined E_f parameters,^[1] it is possible to determine N_f and s_f values of leaving groups of various structures and functionalities over a very wide range of reactivity.^[1,2,3] In order to determine the nucleofugality parameters of the phenylsulfinate leaving group in aqueous acetone and ethanol, a series of benzhydryl phenylsulfonates were synthesized and rate constants for solvolyses of substrates in 60 % acetone and 60 % ethanol (v/v) at 25 °C were measured using the conductometric method. The nucleofuge-specific parameters (N_f and s_f) of phenylsulfinate were determined from $\log k/E_f$ plots using the E_f values of the reference benzhydryl electrofuges as defined by equation (1). Determined N_f parameters of phenylsulfinate allow comparison of heterolytic reactivity of this leaving group with reactivities of other leaving groups on the nucleofugality (N_f) scale. In addition, as in the case of other substrates bearing different leaving groups, rate constants and half-lives for solvolyses of various phenylsulfonates in aqueous acetone and ethanol at 25 °C can be predicted according to Equation (1) using existing E_f values^[1,4] of corresponding electrofuges.

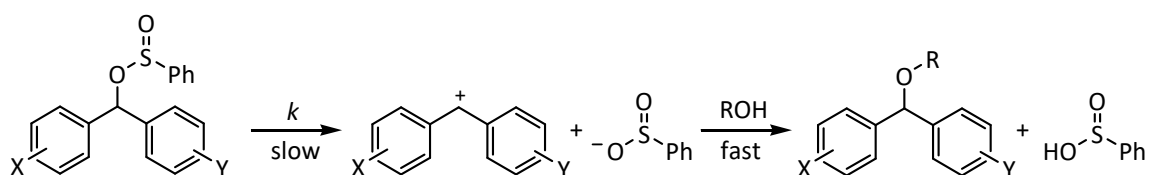


Figure 1. Solvolysis of substituted benzhydryl phenylsulfonates

Acknowledgements. This work has been supported by the University of Zagreb.

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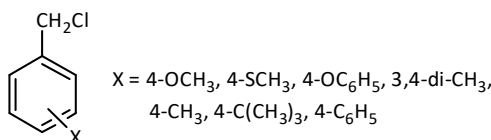
DUALITY IN S_N1 AND S_N2 MECHANISMS IN REACTIONS OF BENZYL CHLORIDES WITH AMINES UNDER SOLVOLYTIC CONDITIONS

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Reactions of unhindered primary benzylic substrates with various nucleophiles might be expected to proceed through a concerted S_N2 displacement mechanism. However, as has been previously reported, these substrates react with some amine nucleophiles in aprotic solvents (nonsolvolytic conditions) simultaneously via both stepwise S_N1 and concerted S_N2 mechanisms if they are substituted by strong electron-donating substituents and contain very good leaving groups, such as tosylate and bromide.^[1,2,3] In this study we set out to investigate the mechanism of the nucleophilic displacement reactions of activated benzyl derivatives bearing a moderately good leaving group (i.e., chloride) with piperidine (a strong nucleophile) and pyridine (a weak nucleophile) under solvolytic conditions (that is in a protic solvent). For that purpose, reaction rates at different concentrations of the mentioned nucleophiles were measured in 80 % aqueous ethanol (v/v) at 60 °C using the conductometric method.



Reactions of all activated benzyl chlorides with piperidine (a strong nucleophile) in aqueous ethanol followed the rate law in equation (1) with a nucleophile-independent term k_1 and a nucleophile-dependent term k_2 , indicating the duality of nucleophilic substitution mechanism. In addition, the Yukawa-Tsuno treatment of measured rates has confirmed that concurrent S_N1 and S_N2 pathways occur in the reaction with solvent and piperidine.

$$k_{\text{obs}} = k_1 + k_2[\text{Nucleophile}] \quad (1)$$

Kinetic analysis further indicated that the most activated benzyl chlorides (X = 4-OCH₃ and 4-SCH₃) in the presence of pyridine (a weak nucleophile) reacted only with solvent by the S_N1 mechanism. On the other hand, the nucleophilic displacement under solvolytic conditions of the less activated substrates in the presence of pyridine were shown to proceed simultaneously through the both concurrent mechanisms.

Acknowledgements. This work has been supported by the University of Zagreb.

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CONFORMATION AND SUPRAMOLECULAR STRUCTURES OF *N*-HETEROCYCLIC HYBRIDS BASED ON 1,2,3-TRIAZOLE AND QUINOLINE

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Quinoline is a key structural component in a variety of compounds with diverse applications, several of which exhibit strong cytostatic activity through multiple mechanisms, including DNA intercalation, apoptosis, abrogation of cell migration and others.^[1,2] Additionally, the 1,2,3-triazoles became the heterocycle of choice in drug discovery, due to their favourable pharmacokinetic and safety profiles, hydrogen-bonding capability, moderate dipole moment, rigidity and stability under in vivo conditions.^[3] Based on these considerations, we have synthesized 6-phenylquinoline derivatives featuring a trifluoromethyl group at the C-2 position, along with either an unsubstituted (**1**) or a *p*-halogen-substituted (**2-4**) phenyl-1,2,3-triazole moiety (Figure 1). We succeeded to obtain single crystals of all compounds and their structures were determined by X-ray diffraction. Structures of non-substituted and *p*-chloro-substituted derivatives **1** and **2** were presented recently.^[4] Herein, we will compare supramolecular structures of **3** and **4** with previously presented structures in order to determine how such small change in the molecular structure, *i.e.* replacement of hydrogen atom at C-4 position of the phenyl ring with halogen atoms, can affect their supramolecular assembling. Conformation of structures **3** and **4** will be also compared with **1** and **2**.

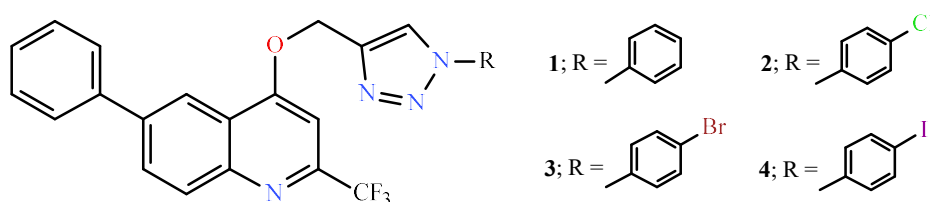



Figure 1. Molecular structures of the *N*-heterocyclic hybrids based on quinoline and 1,2,3-triazole moieties

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DEVELOPMENT OF A DYE INGRESS TEST COMPARABLE TO MICROBIAL INGRESS FOR ASSESSING CONTAINER CLOSURE INTEGRITY

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The role of a pharmaceutical product's primary packaging is to protect the drug from outside contaminants, enabling safe storage and transportation to patients. Defects in the packaging can have serious implications, potentially causing the drug to leak from the container, exposing the drug to external contaminants, moisture, and oxygen, thus affecting the product's sterility and stability. To ensure an adequate packaging system, leak testing is highly important during the development of new products and in stability studies, which assesses the integrity of the packaging across the entire shelf-life of the drug. Because of the limitations associated with sterility testing (microbial ingress method), the use of various physical tests for confirming container-closure integrity (CCI) have been proposed.^[1] One of these tests is a dye ingress method, which is performed under vacuuming conditions and is based on spectrophotometric measurements to determine the absence/presence of dye in vials. Positive control or defect creation methods most often include inserting a needle through the package wall or stopper since it represents an easy and inexpensive approach for creating larger size defects useful for test method feasibility studies.^[2] However, positive controls for sterile products should be close to the microbial ingress limit of detection, which is about 20 μm .^[3]

In this study we have investigated two most used leak standards, pre-pulled glass micropipettes and fused-silica microcapillaries. The investigation included the use of different dyes, surfactant concentration, vacuum level and dwell time, ambient pressure dwell time, and different position and length of leak standards. Micropipette leaks with orifice diameter yielded good results under mild vacuum level and shorter dwell time, whereas microcapillaries with nominal diameters yielded significantly lower leak rates. Vacuum condition and dwell time had to be significantly higher and longer to achieve positive results with the use of microcapillaries. In addition, the length of microcapillaries had a great influence on dye ingress in tested vials. In conclusion, this study demonstrated that improved sensitivity and repeatability were achieved with micropipettes using standard vacuum parameters of 270 mbar for 10 minutes and ambient pressure dwell time of 30 minutes, attributed to the orifice's minimal depth, which eliminated the impact of path length. Although determining the sensitivity of a method is challenging, usage of pre-pulled glass micropipettes as a leak standard makes the dye ingress method a reliable and time-efficient test method for evaluating container closure integrity.

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INNOVATIVE GELLED EMULSIONS FOR GENERAL USE

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Low molecular weight organic gelators are molecules capable of forming unidirectional self-assembled aggregates through no-covalent interactions and consequently preventing the flowing properties of the solvent used. These patent protected gelators show remarkable gelation efficiency in vegetable oils and emulsions, a thermal and mechanical stability, self-healing properties, a long period of stability and controlled simultaneous delivery of hydro and liposoluble bioactives. One such gelator is *N*-butyloxalamido-L-phenylalanine amide (4-P) where the molecules are connected by strong intermolecular hydrogen bonds between planar oxalamide units.

The rheological measurements performed on the gelled w/o emulsions of the chiral oxalamide compounds showed similar or even better viscoelastic properties compared to the vegetable oil gels. Figure 1. b) shows the amplitude sweep test of oil gels that contain 0.05, 0.1, 0.2, 0.5 and 1.0 wt% of 4-P gelator. Storage modulus (G') values of the gels were in the range from 50 to 55000 Pa. An increase in the concentration of the 4-P gelator led to higher yield point values, ranging from 2 to 40 Pa, and a lower loss factor ($\tan \delta$), confirming that the gel containing 1.0 wt% of 4-P gelator shows the highest structural ordering.

The research focused on the behavior of the ambidextrous 4-P gelator under varying water contents, as well as the determination of the rheological properties and morphology of w/o emulsions.

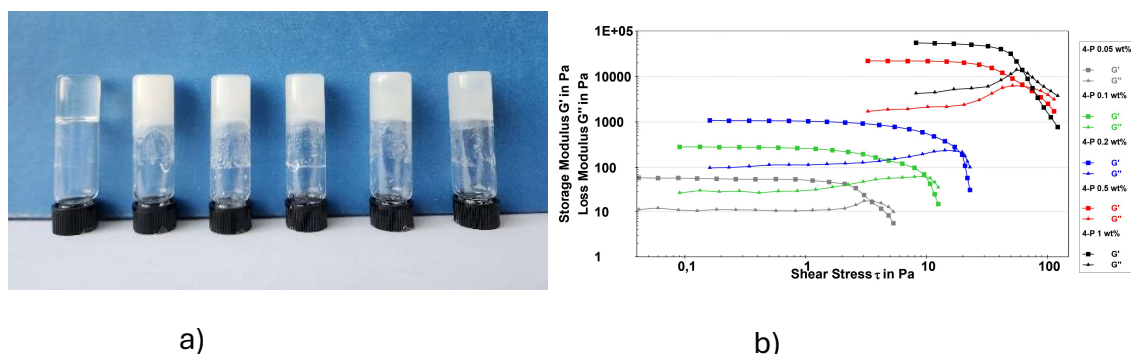


Figure 1. a) 4-P gels of sunflower oil at 0.2 wt% with different amounts of water (10–50 % H₂O); b) Amplitude sweep test of oil gels that contain 0.05, 0.1, 0.2, 0.5 and 1.0 wt% of 4-P gelator.

Acknowledgements. This work has been supported by the Proof-of-Concept Project under NPOO.C3.2.R3-11.05.0163: “Innovative gelled emulsions for general use (InoGEM)”

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BINDING OF CARBOXYLATE ANIONS BY (THIO)UREA-CALIX[4]ARENES

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Urea and thiourea macrocycles remain central to modern anion receptor design, offering strong, directional H-bonding and sophisticated supramolecular behaviour.^[1] In our recent work we have demonstrated that (thio)urea-calix[4]arenes exhibit multiple advantageous features: high affinity for various anions in acetonitrile,^[2] controllable supramolecular dimer assemblies based on interactions with its carboxylic-calixarene counterpart,^[3] and ion-pair binding displaying positive cooperativity.^[4] In each case we devoted extensive efforts to perform detailed thermodynamic description of the systems. This included detection of higher-stoichiometry complexes and characterisation of several coupled processes, like proton transfer, ion-pairing and salt precipitation.

In this study, we focused on the influence of structural variation among carboxylate anions (benzoate, acetate, fumarate, maleate) on the binding affinity of the investigated (thio)urea-calixarenes (Figure 1) in acetonitrile. Complexes of different stoichiometries (1:1, 2:1, 1:2) were observed and their stabilities were determined or assessed using UV, NMR, and ITC titrations. Special attention was devoted to the possibility of proton transfer from the receptor to the negatively charged guest, as well as from the water (present in the solvent) to the highly basic anions (maleates).

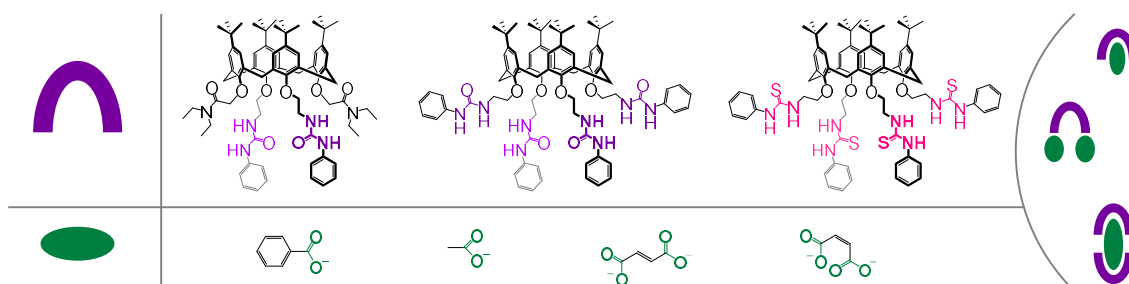


Figure 1. (Thio)urea-calixarenes and carboxylate anions investigated in this study.

Acknowledgements. This work has been supported by the Croatian Science Foundation (projects MacroSol: IP-2019-04-9560, and CalixCORE: IP-2024-05-3012).

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THE MECHANOCHEMICAL SYNTHESIS OF Co(III)-AMMINE HETEROPOLYOXOMOLYBDATES $[X_xMo_mO_y]^{n-}$ (X = Al, Si, Ge or Te)

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Polyoxometalates (POMs) represent a large and structurally diverse class of metal-oxo clusters characterized by their rich structural topology and wide range of chemical and physical properties. The versatility in terms of their size, structure and redox activity makes them attractive candidates for numerous applications, including homogenous and heterogenous catalysis, biomedicine, and material sciences. A significant subclass of POMs comprises polyoxomolybdates (POMos), anionic molybdenum oxoclusters formed through the condensation of $\{MoO_4\}$ units. POMos containing exclusively molybdenum centers are classified as isopolyoxomolybdates, $[Mo_mO_y]^{n-}$, whereas those incorporating an additional p-, d- or f-block metal heteroatom (X) are known as heteropolyoxomolybdates, $[X_xMo_mO_y]^{n-}$. The self-assembly of molybdate ion, $[MoO_4]^{2-}$, and its transformation into higher-nuclearity species, as well as their crystallization into ionic POMo structures is governed primarily by a combination of hydrogen bonding and electrostatic interactions. Complex cations have proven exceptionally useful in POMo synthesis: beyond simply balancing the charge, they participate in supramolecular interactions that guide the condensation of $\{Mo_mO_y\}$ units, either by forming labile coordination complexes or through hydrogen bonding with reaction intermediates. These interactions contribute to templating, stabilization of polyoxomolybdate frameworks, and influence their reactivity, structural diversity, and supramolecular organization. In this work, we employed a mechanochemical synthesis approach involving liquid-assisted ball milling followed by vapor-assisted aging to prepare heteropolyoxomolybdates with aluminium, silicon, germanium, and tellurium as heteroatoms. We investigated reaction systems comprising molybdate ion, malonic acid, cobalt(III) complex cation ($[Co(en)_3]^{3+}$, $[Co(C_2O_4)(en)_2]^+$, $[Co(NH_3)_6]^{3+}$ or $[Co(C_2O_4)(NH_3)_4]^+$) and a source of the selected p-block metal ion (Al^{3+} , Si^{4+} , Ge^{4+} or Te^{6+}). By conducting the reactions in the solid state and varying the Co(III)-ammine complex cations along with heterometal ion used, we successfully isolated several new $[X_xMo_mO_y]^{n-}$ species, as well as identified some of the reactions intermediates. All products were structurally characterized in means of single-crystal and powder X-ray diffraction.

Acknowledgements. This work has been supported by the Croatian Science Foundation (HRZZ) under the project IP-2022-10-7368 (MOCASS).



DEVELOPMENT AND CHARACTERIZATION OF A 1,8-NAPHTHALIMIDE-BASED FLUORESCENT PROBE FOR HYDROGEN SULFIDE DETECTION IN HUMAN BLOOD SERUM

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H₂S is an environmental pollutant, a colorless, flammable, and toxic gas with high toxicity. A concentration of 500 ppm of H₂S can cause respiratory disorders whereby the lethal dose of H₂S is 1000 ppmv. Moreover, H₂S is involved in immune response, signal transduction, and energy production, while endogenous H₂S plays a role in various physiological functions, including regulating blood pressure, neurotransmission, anti-inflammatory effects, vasodilation, antioxidation, and apoptosis.^[1] Due to these facts, developing precise methods for monitoring and determining H₂S is very important. A large number of methods for H₂S detection have been developed, including gas chromatography, colorimetric assays, and fluorescent probes. The advantage of fluorescent probes is their non-destructive and sensitive nature, which is very important for selective determination of H₂S.^[2] The aim of this work implied the design of 1,8-naphthalimide based fluorescent probe containing azide group as recognition group for H₂S detection. Prepared fluorescent probe was characterized using ¹H, ¹³C NMR spectroscopy, and elemental analysis. Fluorescence spectra measurements were carried out, and several influences on fluorescence intensity were investigated, including pH, time dependence, selective response, and influence of H₂S concentration. Finally, prepared fluorescent probe was successfully applied to detect H₂S in a human serum sample whereby the accuracy of the H₂S determination was confirmed with the standard addition method.

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MONITORING AND CHARACTERIZATION OF SUBVISIBLE PARTICLES IN PHARMACEUTICAL PRODUCTS USING MICRO-FLOW IMAGING (MFI)

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Pharmaceutical formulations are developed with strict controls to minimize particulate matter, classified into visible and subvisible particles. The detectability and visibility thresholds depend on particle composition and testing conditions, with subvisible particles typically ranging from 2 – 100 µm.^[1] As a critical quality attribute, subvisible particles require monitoring throughout product development. Pharmacopeial methods, such as light obscuration (LO) and microscopic particle count tests, are commonly used for particle quantification. However, flow imaging techniques, like Micro-Flow Imaging (MFI), enable detailed particle characterization by capturing individual microscopic images, providing insights into particle size distribution (PSD) and concentration at specified thresholds.^[1,2] This study explores the operating principles of the MFI instrument and demonstrates how morphological particle parameters can enhance classification and characterization of subvisible particles in pharmaceutical products.

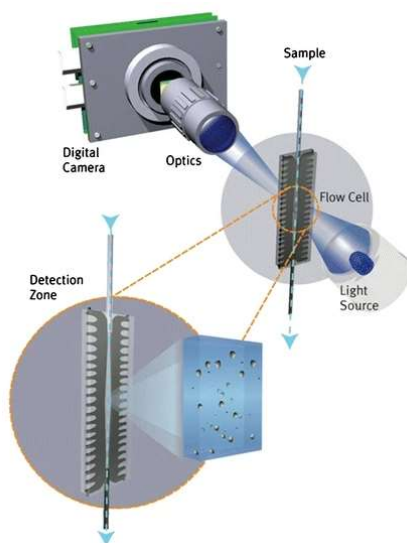


Figure 1. Micro-flow imaging instrument configuration

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SYNTHESIS OF α -NICOTINOYLAMINO ACETAMIDE DERIVATIVES AS BUTYRYLCHOLINESTERASE INHIBITORS

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Acetylcholinesterase (AChE) and butyrylcholinesterase (BChE) are important targets in the treatment of neurodegenerative diseases such as Alzheimer's and Parkinson's disease.^[1] *N*-acylamino amides^[2] have been reported to show noteworthy cholinesterase inhibitory activity. Thus, we synthesized novel *N*-acylamino nicotinamides by employing the Ugi multicomponent reaction^[3] with nicotinic acid, paraformaldehyde, isobutylamine, and *tert*-butyl isocyanide. The Ugi reaction was performed using microwave irradiation, solvent-free ball milling, liquid-assisted grinding (LAG) with a small amount of solvent, and conventional methods. Subsequent quaternization^[4] of the nicotinamide pyridine nitrogen with benzyl or substituted benzyl bromides was also achieved using both microwave and conventional techniques. The resulting compounds were characterized using standard analytical methods (NMR, FTIR, HRMS) and their purity confirmed by HPLC. The synthesized α -nicotinoylamino acetamide derivative exhibited BChE inhibitory activity ($IC_{50} = 2.1 \text{ mM} \pm 0.3 \text{ mM}$), while its quaternary derivatives showed much stronger inhibition in micromolar and submicromolar range, measured using the Ellman method.^[5]

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

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SUBSTITUENT EFFECTS ON THE REGIOSELECTIVITY OF THE FERROCENOYLATION OF PURINES

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In the development of new biomolecules based on conjugates of ferrocene and nucleobases, the focus is on mimicking the parent structure of nucleosides and preserving the potential biological activity of the prepared compounds. In these bioconjugates, ferrocene is usually bound as an *N*-substituent to a nitrogen-containing base, and the site at which it is bound determines the biological properties of the compound itself. In our previous research on the preparation of organometallic ferrocene derivatives, the regioselectivity of these reactions, which included both pyrimidine and purine bases, was tested. The bioconjugates were prepared by the reaction of ferrocenoyl chloride with the deprotonating agent sodium hydride in dimethylformamide. This reaction is regiospecific for pyrimidine derivatives with the formation of only *N*1 isomers,^[1] whereas purine derivatives exhibit different regioselectivity of the *N*7 and *N*9 isomers formed. By using a suitable substituent at the C6 position in the purine ring, the ratio of the isomeric products *N*7 and *N*9 can be adjusted, i.e. the regioselectivity of the ferrocenylation reaction can be modulated.^[2] In the continuation of research on pyrimidine derivatives, NaH was replaced by Et₃N and DMF by CH₃CN, leading to the formation of *N*1,*N*3 derivatives in addition to *N*1-copulates.^[3]

The research in this presentation is related to purine derivatives, focusing on the regioselectivity under the above-mentioned reaction conditions and the effect of substituents at the C2 and C6 positions (Fig. 1). Regioselectivity is monitored *in situ* during the reaction using NMR techniques and isolation of the final products.

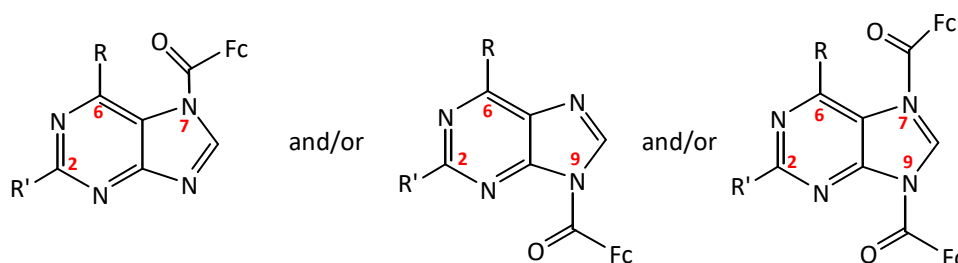


Figure 1. Reaction products of ferrocenylation of derivatives of purine bases (Fc = ferrocenyl).

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COORDINATION-DRIVEN SELECTIVITY: TERNARY COPPER(II) BIPYRIDINE COMPLEXES WITH ANTITUMOR POTENTIAL

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Coordination compounds of transition metals with heterocyclic nitrogen ligands, such as 2,2'-bipyridine, have been the subject of intense research in recent years due to their structural diversity, chemical stability and biological activity, including antitumor activity. In particular, copper(II) complexes are characterized by their involvement in oxidative stress, their potential cytotoxicity and their relatively low toxicity towards healthy cells compared to classical cytostatics.^[1,2] This work describes the synthesis and characterization of novel ternary copper(II) complexes obtained from copper(II) nitrate and chloride in the presence of 2,2'-bipyridine as an auxiliary ligand. After synthesis, the complexes were subjected to detailed structural characterization by FT-IR and UV-Vis spectroscopy and single crystal X-ray diffraction. The thermal properties and stability were investigated by thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). The biological evaluation includes in vitro cytotoxicity tests against the human liver cancer cell line HepG2, with a focus on selectivity against tumor cells. Comparison of the results will identify structural characteristics that contribute to both biological activity and thermal stability, making these complexes promising candidates for further development as copper-based anticancer agents.

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STRATEGIC DESIGN OF PORPHYRIN-BASED POROUS ORGANIC POLYMERS FOR CO₂ CAPTURE: A COMPUTATIONAL STUDY

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An increase of carbon dioxide (CO₂) in nature has prompted researchers to design effective and selective functional materials for CO₂ capture. In previous studies, we investigated azo-linked porphyrin-based porous organic polymers (POPs), which are promising candidates for CO₂ capture due to nitrogen-rich functionalities which could facilitate interactions with CO₂. Additionally, the variety of linear and trigonal spacers allows for fine-tune of CO₂ adsorption abilities.^[1] Our research has progressed computationally with the implementation of sterically hindered and functionalized spacers as units that are connected to porphyrin building blocks through azo linkages, forming 2D frameworks. Crystal structures were optimized using periodic DFT methods in the CRYSTAL23 program. These optimized structures were subjected to grand-canonical Monte Carlo (GCMC) simulations in the RASPA program and adsorption isotherms were compared. The distribution of CO₂ molecules within the examined structures was visualized, and the obtained data was compared with the results of the electrostatic potential analysis. Based on the findings, we identified potential candidates for selective CO₂ capture and further examined the stability and CO₂ adsorption at different neighboring stacking configurations.^[2] Finally, the calculated CO₂ uptake values were compared with experimental data. These results demonstrate that periodic DFT calculations and GCMC simulations can be used to analyze, compare and predict CO₂ adsorption properties of POPs.

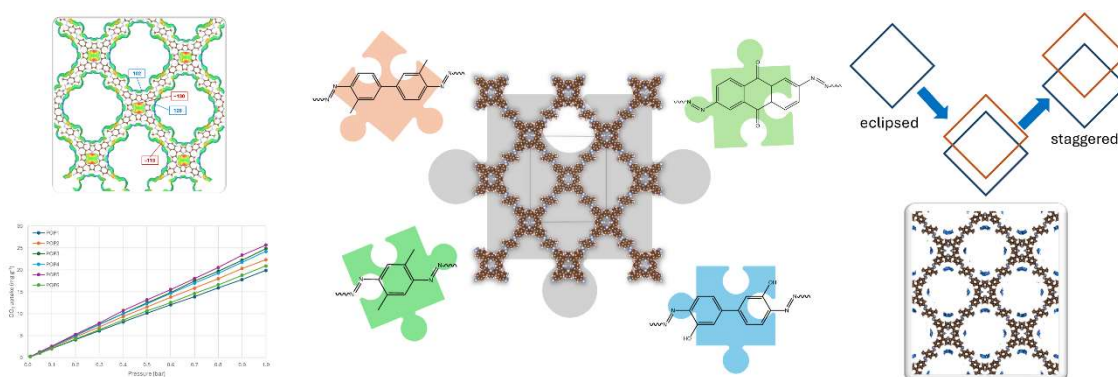
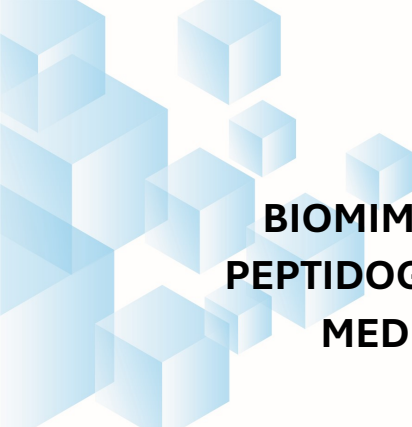


Figure 1. Strategic design of porous organic polymers for CO₂ capture.

Acknowledgements. This work has been fully supported by Croatian Science Foundation under project IP-2020-02-4467.

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BIOMIMETIC NANOMATERIALS FUNCTIONALIZED WITH PEPTIDOGLYCAN MONOMER: STUDYING CARBOHYDRATE-MEDIATED INTERACTIONS FOR BIOMEDICAL USE

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Biomimetic nanomaterials, which mimic the structure and function of natural biological systems, represent a versatile platform for a broad range of biomedical applications, including targeted drug delivery and the investigation of host–pathogen interactions.^[1] Peptidoglycan (PG), a major component of bacterial cell walls, plays a pivotal role in bacterial viability and in activating the host innate immune response. Due to its absence in higher organisms, PG represents a prototypical pathogen-associated molecular pattern (PAMP) recognized by pattern recognition receptors (PRRs). The peptidoglycan monomer (PGM), GlcNAc-MurNAc-L-Ala-D-isoGln-mesoDAP(ε-NH₂)-D-Ala-D-Ala, isolated from *B. divaricatum*, has demonstrated significant biological activity and serves as a promising molecular scaffold for the development of novel immunomodulatory and antimicrobial agents.^[2]

This study focuses on the design and synthesis of biomimetic nanomaterials functionalized with PGM and the investigation of their interactions with lectins. Liposomes and gold nanoparticles functionalized with PGM were prepared to enable multivalent glycan presentation for targeted interaction with specific lectins, aiming to elucidate structure–activity relationships. To explore these interactions, complementary label-free biophysical techniques, including isothermal titration calorimetry (ITC) and surface plasmon resonance (SPR), were employed to determine binding kinetics and thermodynamic parameters. The results will deepen our understanding of how nanoscale glycan organization influences specific lectin interactions, thereby enhancing our insight into host–pathogen dynamics and directly supporting the development of novel antimicrobial and immunomodulatory strategies based on biomimetic nanomaterials.

Acknowledgements. This work has been supported by Croatian Science Foundation (IP-2018-01-6910).

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ELECTROCHEMICAL STUDY OF NOVEL HYDRAZIDE MACROCYCLIC COMPOUNDS

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Macrocyclic hydrazides represent a group of compounds with donor atoms capable of forming multiple non-covalent interactions with host species. The hydrazide group also displays tautomerism depending on the solvent and pH, which can be used to optimize electrochemical properties. The herein presented hydrazide macrocycle, was prepared using a hydrazine derivative of pyridine-2,6-dicarboxylic acid and dialdehydes previously prepared by our group.^[1] The structural features of the prepared compound was investigated using FT-IR, NMR, and MS spectroscopy. The cyclic voltammetry was used to study the electrochemical properties in Tris-HCl buffer.^[2] In cyclic voltammograms recorded at three different pH values (pH = 7, 8, and 9), one oxidation peak (A1) of the investigated macrocyclic compound was observed, corresponding to the oxidation of NH groups. The oxidation peak current decreased with successive scans at all investigated pH values, indicating that the oxidation product of the macrocyclic compound is adsorbed at the glassy carbon electrode surface. It was observed that the oxidation peak potential of the investigated compound decreases with an increase in the pH value from $E_{p,a} = 0.91$ V (at pH = 7) to $E_{p,a} = 0.85$ V (at pH = 9).

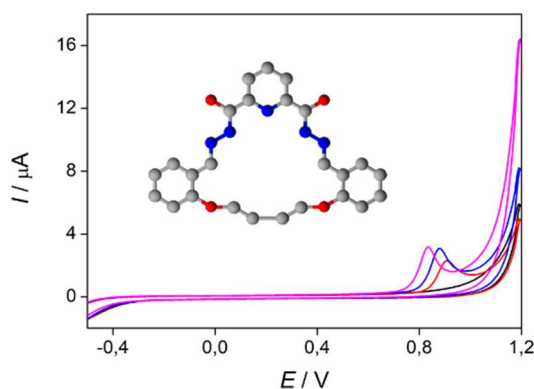


Figure 1. Cyclic voltammograms of Tris-HCl buffer (—) and macrocyclic compound recorded in Tris-HCl buffer: pH = 7 (—), 8 (—), and 9 (—). Scan rate, $\nu = 100$ mV/s. Inset figure shows presumed structure of macrocyclic compound.

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ENANTIOSELECTIVE TRANSITION METAL CATALYSIS WITH SELF-ASSEMBLED HOST-GUEST SYSTEMS

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Coordination cages with transition metals are advanced supramolecular structures with broad potential in catalysis, sensing, molecular recognition, and selective extraction.^[1] Their properties depend on the metal centers and ligand design, allowing fine-tuning of geometry and function. These cages often contain multiple metal nodes capable of catalyzing various reactions. A key feature is their ability to encapsulate chiral guests, which can induce chirality in the host via noncovalent interactions, enabling enantioselective catalysis. However, no examples have yet shown the metal centers themselves acting as catalytic sites influenced by chiral guests.^[2,3]

In this study, a series of achiral 1,3,5-benzenetricarboxamide based phosphine ligands framework were designed and synthesized (Figure 1.). These ligands possess C_3 -symmetric geometry, promoting self-assembly and facilitating the formation of supramolecular architectures. Furthermore, achiral and chiral guest molecules were prepared to explore non-covalent interactions within the system. Various transition metal complexes with e.g. Pd(II), Pt(II), Rh(I), and Zn(II) were prepared and characterized having different metal-to-ligand ratios. Rhodium-based complexes demonstrated a clear capacity for guest-to-metal chiral induction upon interaction with chiral guest molecules. All synthesized compounds were characterized using a suite of analytical techniques, including NMR, IR, MS and UV-Vis spectroscopy. A series of catalytic hydrogenation reactions of model substrates were carried out using the in-situ prepared rhodium complexes in the presence of chiral guest molecules. Enantiomeric excess of the hydrogenation products was determined by gas chromatography on chiral stationary phase.

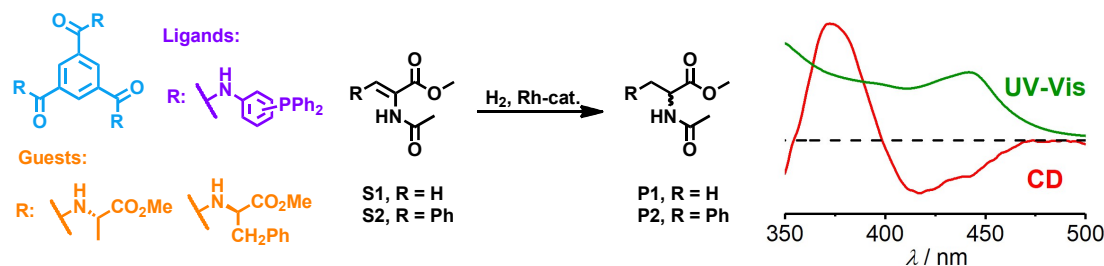


Figure 1. Ligands, guests, model reactions, and CD/UV-Vis spectra indicating chiral induction at rhodium cation.

Acknowledgements. This work was supported by The Croatian Science Foundation project Cage Cat (IP-2022-10-8456) and doctoral scholarship to Filip Grdović (DOK-NPOO-2023-10-4846).

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3D PRINTED ION SELECTIVE ELECTRODES FOR POTASSIUM ION DETERMINATION

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Ion-selective electrodes (ISEs) are widely used analytical tools for the determination of specific ions in complex matrices due to their simplicity, selectivity, and low cost.^[1] Recent developments in materials science and digital fabrication have opened new opportunities for redesigning ISEs using modern manufacturing techniques.^[2] Among these, 3D printing offers a modern and flexible approach that allows for rapid prototyping, customization, and scalable production of electrochemical sensors. This shift in fabrication methodology opens new possibilities for designing cost-effective and high-performing ISE systems.^[3] In this study, we present a novel application of 3D printing in the development of ISE for the determination of potassium ions, featuring improved functionality and a simplified membrane composition. The electrodes were fabricated using masked stereolithography (MSLA), a high-resolution resin 3D printing technique that uses an LCD screen to selectively cure each photopolymer layer. Our electrodes consist of three main components: potassium tetraphenylborate, silver sulfide or graphite, and industrial ABS. All measurements were performed in a 0.1 M solution of KNO₃. Membranes were tested both without and with the addition of ZnO nanoparticles, and the results demonstrated that the incorporation of ZnO NPs significantly improved the slope of the calibration curve. Also, membranes containing graphite instead of Ag₂S as charge transfer material showed high responsiveness, with potential readings stabilizing within 3 to 7 seconds over a concentration range between 4.88×10^{-5} mol L⁻¹ and 1.00×10^{-2} mol L⁻¹. Our results demonstrate a near-Nernstian behaviour, with slopes approaching the theoretical value of -59.2 mV per decade for monovalent cations and correlation factors exceeding 0.99. To ensure accuracy and reproducibility, each membrane was tested five times, confirming consistent and reliable electrode responses. The ion-selective membranes feature a simple and cost-effective design, avoiding the need for multiple complex components. In addition to their reliable analytical performance, the electrodes can be easily fabricated in large quantities using additive manufacturing techniques, offering a cost-effective and scalable solution. Moreover, they exhibit excellent long-term stability, with a functional lifetime exceeding one year.

Acknowledgements. This work has been supported by HrZZ MOBOL-2023

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COMPARISON OF MICROSTRUCTURAL AND MAGNETIC PROPERTIES OF RADIOLYTICALLY SYNTHESIZED FERROXYHYTE AND MAGNETITE NANOPARTICLES FOR MAGNETIC HYPERTHERMIA TREATMENT

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In the past decade, interest in magnetic hyperthermia has increased considerably. This method of cancer treatment exploits the greater sensitivity of tumor tissues to heat compared to healthy tissues by using thermal energy generated from the relaxation of superparamagnetic nanoparticles in an external alternating magnetic field—namely, Néel and Brownian relaxation mechanisms. Effective hyperthermia requires raising the tissue temperature to between 41 °C and 45 °C, which can activate various cellular responses. The heating efficiency is commonly quantified using the specific absorption rate (SAR), defined as the amount of energy converted to heat per unit mass of magnetic material per unit time. SAR depends on both the amplitude and frequency of the applied magnetic field.^[1]

In this study, we examined the effects of phase composition and particle morphology of different iron-oxide nanoparticles on SAR values in different dispersing media. Feroxyhyte and magnetite nanoparticles were synthesized through γ -irradiation of deoxygenated precursor solutions containing Fe(III), 2-propanol, and DEAE-dextran hydrochloride (M.W. 500,000). Gamma irradiation of aqueous solutions generates hydrated electrons (e^-_{aq}), serving as the primary reducing agent to convert Fe(III) to Fe(II) with 2-propanol acting as a scavenger of oxidizing hydroxyl radicals. This method avoids the use of toxic and environmentally harmful chemical reducing agents.^[2] Spherical magnetite nanoparticles were obtained by irradiating a 20 % Fe/polymer (w/w) solution at 50 kGy, while feroxyhyte nanodiscs were produced from a 5% Fe/polymer (w/w) solution irradiated at 75 kGy (higher reducing conditions). The resulting particles were washed and dried. Feroxyhyte nanoparticles were further annealed in a hydrogen atmosphere to produce magnetite nanodiscs. Scanning electron microscopy (SEM) revealed distinct morphological differences between the nanoparticle types. The reduction degree, given by the $[Fe^{2+}]/([Fe^{2+}]+[Fe^{3+}])$ ratio, was measured using UV-VIS spectrophotometry with the 1,10-phenanthroline method. X-ray diffraction (XRD) confirmed the presence of magnetite or feroxyhyte phases depending on the irradiation dose. Mössbauer spectroscopy and SQUID magnetometry verified the superparamagnetic behavior of the nanoparticles and showed that their magnetic properties were influenced by all examined parameters. SAR measurements, conducted across a range of frequencies and field strengths, indicated that both the iron oxide phase and nanoparticle morphology play a significant role in determining heating efficiency.

Acknowledgements. This work was supported by the Croatian Science Foundation under the project number HRZZ-IP-2022-10-3687 (RadMagnNanoHyperT)

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DIMERIC METALLOSURFACTANT WITH ZINC: PHYSICOCHEMICAL PROPERTIES IN SOLUTION AND APPLICATION AS ANTIBACTERIAL COATING

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Unlike conventional single-chain surfactants, dimeric surfactants are made up of two amphiphilic moieties covalently linked by a spacer group.^[1] Combining metal ions and surfactants can yield unique compounds—metallosurfactants. In this work, the dimeric metallosurfactant, bis(*N,N*-dimethyl-*N*-dodecyl)ethylene-1,2-diammonium tetrabromozincate (II), denoted as (12-2-12)[ZnBr₄] was synthesized.^[2] The conductometry and tensiometry measurements showed that (12-2-12)[ZnBr₄] displays enhanced physicochemical properties compared to the precursor surfactant. In combination with alginate, (12-2-12)[ZnBr₄] was then used to prepare coatings on stainless steel surfaces by airbrushing. Scanning electron microscopy was used for surface imaging of the coatings, while surface roughness was determined by profilometry. Peel-off and scratch tests were also conducted to evaluate the adhesion and cohesion of the coatings. SEM images showed that the stainless-steel surfaces were only partially covered, exhibiting an island-like morphology. Furthermore, peel-off test results indicated that the coatings adhered well to the substrate surface, and scratch test results revealed that the coatings could withstand a continuously increasing load of up to 20 mN. Additionally, preliminary antibacterial tests showed promising results.

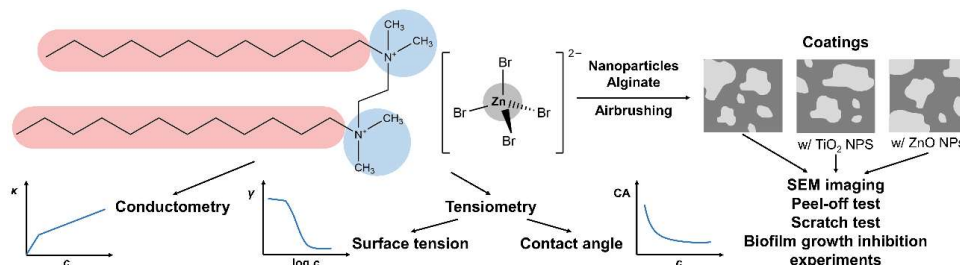


Figure 1. Graphical abstract.

Acknowledgements. This work has been financially supported by the European Union's Horizon-RIA project, Surface Transfer of Pathogens (STOP), Grant agreement ID: 101057961 and Croatian Science Foundation project IP-2024-05-3668, MSurf-*n*-SWIM.

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MULTILIGAND DOCKING OF THREE-MEMBERED HETEROCYCLES IN THE ACTIVE SITE OF BUTYRYLCHOLINESTERASE

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Butyrylcholinesterase (BChE) is increasingly recognized as a key enzyme in the later stages of Alzheimer's disease, where its activity rises to compensate for the decline in acetylcholinesterase.^[1] This study explores the binding of a series of small heterocycles—in this case, 3-membered rings—within the active site of BChE using quantum chemical molecular docking techniques. These heterocycles are investigated as building blocks for larger and more complex molecules.

Docking was performed in multiple phases: initially, each ligand was docked individually, and its binding energy was estimated. This was followed by multiligand docking simulations with two or more, the same or different, small molecules simultaneously docked into the active site. This approach aims to investigate the overall potential for synergistic effects and multiple occupancy, while also finding the best spatial arrangement within the extended active site.^[2] To ensure a comprehensive exploration of spatial binding possibilities, configurational sampling for up to 100,000 different configurations was performed for each combination of ligands. Following this, parallel processing of output data was performed, including geometry optimizations and binding energy calculations. The results suggest that stable multiligand binding of these small molecules is possible within the BChE active site, with certain configurations displaying potentially enhanced affinity compared to single-ligand binding. Future work will include testing combinations of larger heterocycles to evaluate cooperative or competitive interactions.

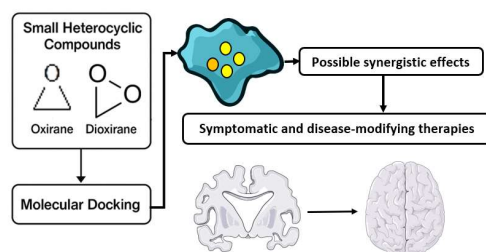


Figure 1. Workflow of a multiligand quantum chemical molecular docking study of three-membered heterocycles into the BChE active site.

Acknowledgments: This research was funded by the Croatian Science Foundation, grant: *Target-guided synthesis of cholinesterase inhibitors supported by machine learning* (IP-2022-10-9525).

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ADSORPTION OF POLY(*N*-ETHYL-2-VINYLPYRIDINIUM BROMIDE) ON SILICA NANOPARTICLES AND FLAT SURFACES

Nanoparticles have already been applied in various fields, including food, drug and cosmetic industry, catalysis, medicine, and environmental protection.^[1,2] Among them, silica and titania nanoparticles are most commonly used due to their wide availability and the variety of sizes and shapes. Depending on their application, it is important to study how nanoparticles interact with simple salts as well as with synthetic and natural oligomers and polymers.^[3] In this study, we investigated the adsorption behavior of the synthetic polymer poly(*N*-ethyl-2-vinylpyridinium bromide) (PE2VP) on both silica nanoparticles and flat surfaces (SiO₂ films on silicon wafers). We observed that the maximum surface concentration of PE2VP increased by approximately 20% when the salt concentration was raised by two orders of magnitude. Simultaneously, the adsorption constant increased by three orders of magnitude. For flat surfaces, the thickness of the silica layer (ranging from 2 nm to 160 nm) did not significantly affect the thickness of the adsorbed polymer layer. Instead, the adsorption was more strongly influenced by factors such as the surface cleaning method and the duration of the adsorption process.

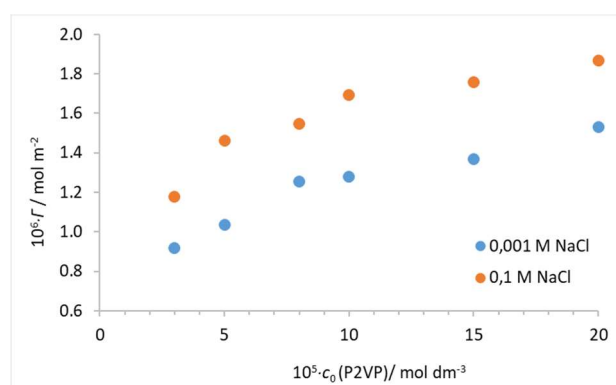


Figure 1. Adsorption isotherm of PE2VP on silica nanoparticles ($\gamma(\text{SiO}_2) = 1 \text{ g dm}^{-3}$) at $\text{pH} \approx 11$, $\theta = 25^\circ \text{C}$ and two different NaCl concentration.

Acknowledgements. This work has been supported by Croatian Science Foundation (HRZZ) under the project “Physical chemistry of processes at mineral/(poly)electrolyte solution interface” IP-2020-02-9571.

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EFFECT OF CHLORIDE IONS ADSORPTION ON THE SERS ACTIVITY OF SILVER NANOPARTICLES

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Silver nanoparticles (AgNPs) have been widely studied for their remarkable plasmonic properties, which enable their use in diverse applications such as chemical sensing, biomedical imaging, and catalysis.^[1,2] Among these, their role in surface-enhanced Raman scattering spectroscopy (SERS) is especially prominent, as they are known to be among the most effective nanostructures for Raman signal enhancement due to their ability to support strong localized surface plasmon resonances.^[3]

In this study, silver nanoparticles modified with adsorbed chloride ions were synthesized and evaluated as SERS-active substrates. Chloride ions are known to influence nanoparticle behavior by affecting aggregation, surface charge, and molecular adsorption. Those factors are closely tied to SERS performance.^[4] The SERS activity of these modified nanoparticles was tested using standard model molecule rhodamine 6G. By varying the amount of adsorbed chloride ions, it was examined how surface modification impacts both the enhancement of Raman signals and the underlying surface interactions. Key physicochemical characteristics, particularly the electrokinetic potential, were analyzed to assess changes in surface properties and colloidal stability.

This work underscores the importance of controlled surface chemistry in tuning the performance of silver-based SERS substrates. The study contributes to the ongoing development of reliable, sensitive, and customizable nanomaterials for future analytical and diagnostic applications.

Acknowledgements. This work has been supported by the Croatian Science Foundation under the project IP-2020-02-9571.

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NITROSAMINE IMPURITY RISK ASSESSMENT IN OPHTHALMIC PHARMACEUTICAL PRODUCT

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Nitrosamines in pharmaceutical products have recently become a major concern for regulatory authorities due to their potential carcinogenicity, leading to stringent requirements for risk assessment and analytical testing.^[1] This study presents a comprehensive evaluation of nitrosamine formation risks in an ophthalmic formulation containing two active pharmaceutical ingredients (APIs) – dorzolamide hydrochloride (**1**) and timolol maleate (**2**) (Figure 1), where *N*-nitrosamines related to the structures of these active substances can potentially be formed. The potential formation of *N*-nitroso Timolol and *N*-nitroso Dorzolamide was assessed, by considering the presence of the potential nitrosatable amine moiety in the two APIs' structures, as well as the possibility of *N*-nitrosomorpholine formation during the API synthesis. All formulation components, including excipients, purified water, packaging, as well as the manufacturing process were evaluated, revealing that there are no significant contributors to the nitrosamine impurities formation. Developed analytical methods were validated to quantify the relevant nitrosamines. Analytical methods were developed and validated to detect the presence of the targeted nitrosamines and to quantify them if their presence is confirmed above the LOD levels of the instrument abilities. Results showed that *N*-nitroso Timolol was below the limit of quantification (LOQ), while *N*-nitroso Dorzolamide was detected at a level of 10 % of the established specification limit for this targeted nitrosamine, indicating an acceptable safety margin. These findings underscore the importance of the integrated risk assessments combined with experimental data to ensure the quality and safety of pharmaceutical drug products (human medicines) in the light of nitrosamine contamination concerns.

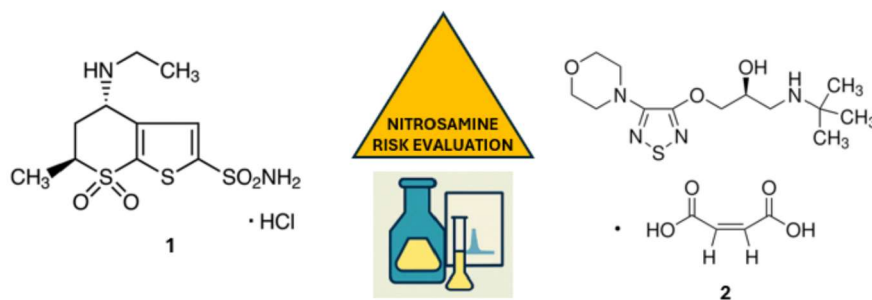


Figure 1. Active pharmaceutical ingredients in this work.

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SOLVOLYTIC REACTIVITY OF TRIPHENYLPHOSPHONIUM SALTS

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Quaternary phosphonium salts (QPSs) are a fundamental class of organophosphorus compounds, which have been applied as important reagents in synthetic chemistry.^[1] Although, organic phosphonium salts are electrophilic species and the positive charge on phosphorus could enhance the electrophilicity or acidity of its substituents because of the inductive effect, the substituent on the phosphorus can act as a nucleophile for the construction of C-C bond while initiated by another appropriate nucleophile.

Nucleofugalities (the leaving group abilities) of triphenylphosphine (Ph_3P) in various solvents have been derived from the $\text{S}_{\text{N}}1$ solvolysis rate constants of the corresponding ferrocenylphenylmethyltriphenylphosphonium salts (Figure 1) by applying the *Linear Free Energy Relationship (LFER)* equation: $\log k (25^\circ\text{C}) = s_f (E_f + N_f)$.^[2] In this equation k is a first order rate constant for $\text{S}_{\text{N}}1$ reaction at 25°C , s_f (the slope of the $\log k/E_f$ correlation line) and N_f (nucleofugality, the negative intercept on the abscissa of the $\log k/E_f$ correlation line) are nucleofuge specific parameters, while E_f is the electofugality parameter of the corresponding ferrocenylphenylmethyl cations determined earlier.^[3]

On the nucleofugality scale developed in line with *LFER* equation triphenylphosphine is the weakest neutral nucleofuge (the poorest neutral leaving group). Because of solvation in the reactant ground state, the reactivity of triphenylphosphonium salts slowly decreases as the polarity of the solvent increase. The impact of the phenyl group in ferrocenylphenylmethyl cations on stabilization of the positive charge is balanced by the α -ferrocenyl group and due to the rate effect of the substituents on the phenyl ring is suppressed.

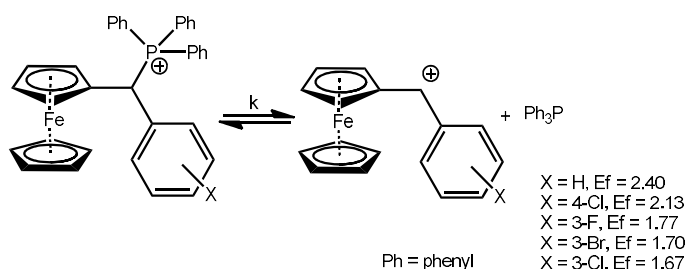


Figure 1. Solvolysis of ferrocenylphenylmethyltriphenylphosphonium salts.

Acknowledgements. This work has been supported by the University of Zagreb.

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COMPARISON OF THE NUCLEOFUGALITIES OF THE NEUTRAL LEAVING GROUPS

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The first step in solvolytic reactions that follow the S_N1 route involves the heterolytic cleavage of the carbon-leaving group (LG) bond and formation of the carbocation intermediate (electrofuge) and the free leaving group (nucleofuge). Nucleofugalities or the leaving group abilities have been derived from the S_N1 solvolysis rate constants of the corresponding substrates by applying the *Linear Free Energy Relationship (LFER)* equation: $\log k (25\text{ }^\circ\text{C}) = s_f (E_f + N_f)$.^[1] From the $\log k$ versus E_f plots (LFER equation) using of the corresponding benzhydryl and ferrocenylphenylmethyl neutral and positively charged substrates, the nucleofuge specific parameters (N_f and s_f) of large number of the anionic and neutral leaving groups were determined.^[1–3]

Up to now, the least reactive neutral nucleofuges on the nucleofugality scale developed in line with *LFER* equation have been pyridines (Figure 1). Given that the difference in N_f of one unit corresponds approximately to a reactivity difference in an order of magnitude, triphenylphosphines are less reactive leaving groups than pyridines by about an order of magnitude of three. Because of their low reactivity, numerous triphenylphosphonium salts are more stable in various solvents under normal conditions by comparison with corresponding sulfonium and pyridinium salts.

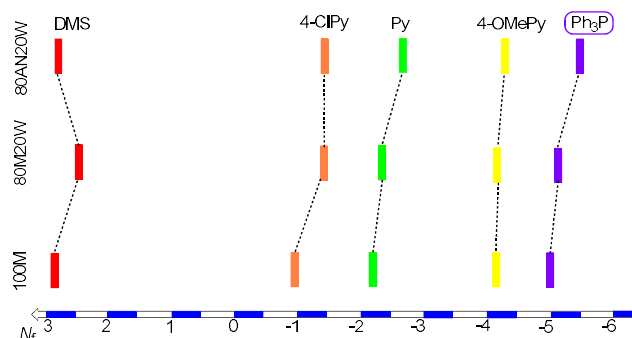


Figure 1. Comparison of the nucleofugalities of some neutral leaving groups in various solvents. Binary solvents are given as v/v; AN = acetonitrile, M = methanol, and W = water. DMS = dimethylsulfide.^[2] Py = pyridine.^[3]

Acknowledgements. This work has been supported by the University of Zagreb.

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DESIGN AND ANTIMICROBIAL ACTIVITY OF POLYALLYLAMINE-*N*-HYDROXYSUCCINAMIDE CONJUGATES

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Amine containing polymers such as polyallylamine proved to be biologically active^[1] and are known as gene vectors or as antimicrobial materials,^[2] still cytotoxicity can be an issue. Recent studies included succinylation of polyallylamine, however sometimes with complete loss of antimicrobial activity.^[1] Two novel polymer conjugates comprised of an *N*-hydroxysuccinamide conjugated to polyallylamine hydrochloride (PAA), were prepared via aminolysis of *N*-hydroxysuccinimide (NHS) in aqueous conditions at pH > 9. NHS was added in molar ratios of 1:1 (n-PAA1) and 1:10 (n-PAA10) relative to PAA (Figure 1).

The PAA derivatives were characterized using NMR and IR spectroscopy, and charge analysis was performed by potentiometric and polyelectrolyte titration. n-PAA10 showed antimicrobial activity against *Staphylococcus Aureus* and *Pseudomonas Aeruginosa*, with MIC values ranging from 0.08 to 0.016 mg/mL.

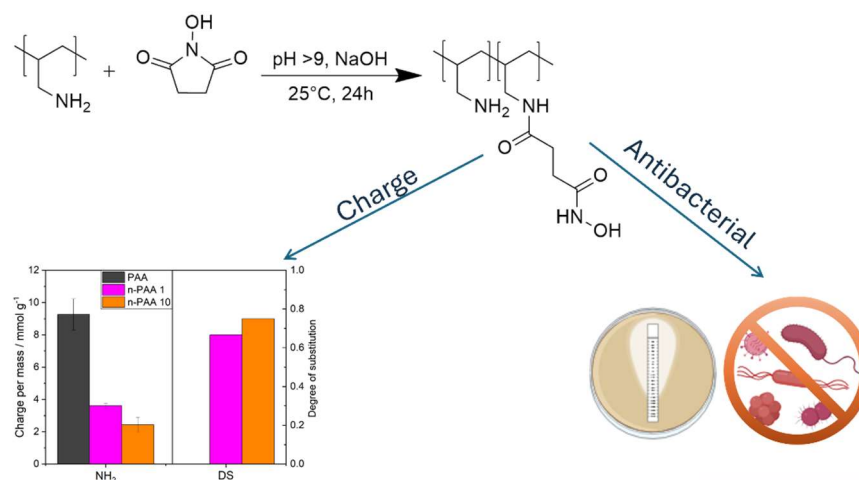


Figure 1. Preparation and investigations on polymer conjugates within this work.

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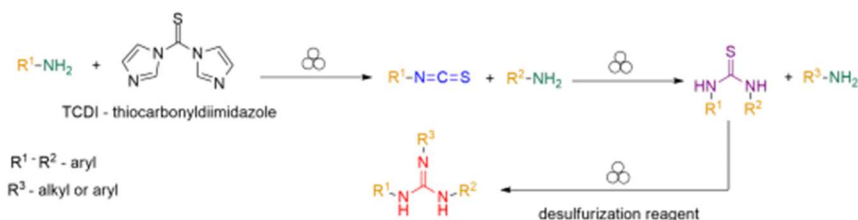
MECHANOCHEMISTRY AS A GREEN ROUTE TO TRISUBSTITUTED GUANIDINES

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Mechanochemistry was recognized by IUPAC in 2019 as one of the top ten emerging technologies in chemistry that will change the world. Today, mechanochemistry is acknowledged as a sustainable and solvent-free alternative to traditional synthesis.^[1,2] Guanidines are fascinating molecules well known because of their superbasicity and ability to form hydrogen bonds. Mercury-based reagents are often used as desulfurization reagents in guanidine synthesis. However, the toxicity of these reagents is a serious drawback. This reason inspired us to replace it with safer metal salts, such as iron, copper, silver or bismuth as a greener alternative.^[3-5] The aim of this study is to investigate the mechanochemical route to trisubstituted guanidines with potential application in anion sensing.



Scheme 1. General reaction scheme.

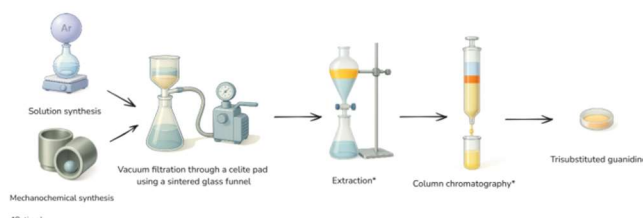


Figure 1. Schematic representation of the general synthetic procedure for the preparation of trisubstituted guanidines.

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

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ECOTOXICITY ESTIMATION OF IMIDAZOLE-BASED IONIC LIQUIDS: THE EFFECT OF ALKYL SIDE CHAIN LENGTH

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Imidazole derivatives are important compounds in heterocyclic chemistry due to their various biological activities, which have led to the development of many commercial drugs and pesticides. However, in the field of plant protection, only a limited number of these compounds have been approved by the European Commission due to their potential negative ecological impacts.^[1] Imidazole-based ionic liquids (ILs) are popular in both chemistry and industrial processes because of their simple preparation, numerous modification possibilities, thermal stability, good water solubility, and low vapor pressure. Nevertheless, there are concerns regarding their environmental accumulation and the risks related to the aquatic and non-target species toxicity.^[2] A rational approach using computational methods is recommended when designing ILs with specific properties in order to fine-tune their molecular structure for desired purpose. In this study, we estimated ecotoxicological parameters for a series of proposed imidazole ILs, changing the length of the alkyl side chains attached to the imidazole ring (Figure 1). As anticipated, longer alkyl chains reduced water solubility and increased lipophilicity of the ILs. Other observed properties, including pesticide-likeness, toxicity to algae and daphnia, toxicity to earthworms, bioconcentration, and persistence in water, sediment and soil, suggest that the optimal alkyl side chain length for this type of imidazole ILs is four carbon atoms.

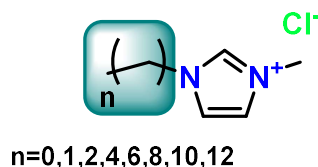



Figure 1. General structure of proposed imidazole-based ionic liquids

Acknowledgements. This work has been supported by the Croatian Science Foundation project “Innovative Approaches in the Development of Imidazoles for Plant Protection”, under the project number HRZZ-IP-2024-05-6164.

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VARIABILITY, COMPOSITION, AND CHEMICAL PROFILING OF LAVENDER EXTRACT FROM CROATIA OBTAINED WITH SUPERCRITICAL EXTRACTION

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Lavender is one of the most appreciated aromatic plants, with high economic value in food, cosmetics, and other industries. The innovative and green approaches like microwave, and subcritical water or CO₂ extraction, significantly reduces energy consumption, shortens extraction time, and enhances both the yield and quality of essential oils and other plant extracts. These benefits firmly establish supercritical CO₂ extraction as a highly sustainable extraction technology – green technology.^[1,2]

The aim of this study was to determine the variability in the chemical composition and quality of Lavanda Gdinj and Trilj extracts, derived from lavender flowers (*Lavandula angustifolia* and *Lavandula hybrida* [*intermedia*]) produced using supercritical CO₂ extraction. The study focused on analyzing the volatile compounds in the supercritical extracts through gas chromatography-mass spectrometry (GC-MS) to assess their commercial suitability. The results revealed the chemical composition of the extracts, highlighting variations between the two varieties, with particular attention to key aromatic compounds such as linalool, linalyl acetate, and borneol, which are known for their biological activity. The study discussed differences in volatile compound content. This research demonstrates the potential of lavender extracts as high-quality products obtained using the green technology of supercritical CO₂ extraction.

Acknowledgements: The work is the result of the Faculty of Chemistry and Technology, University of Split, Croatia, institutional project titled “NATURELAB: research and innovation in natural chemical compounds,” as well as the Institution for Research and Knowledge Development of Nutrition and Health (CEKOM 3LJ), funded by the European Regional Development Fund under grant number KK.01.2.2.03.0017.

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FLUORESCENCE “WITHOUT FLUOROPHORES”: INVESTIGATING CATION COMPLEXATION BY CALIXARENES

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Among many potential and realized applications of calixarenes, a variety of their fluorescent derivatives have been proposed as sensitive receptors for diverse species.^[1] Nevertheless, it has been believed that these macrocycles cannot be used as effective fluorescent sensors without incorporating luminescent moieties in their structures.^[2] In this work, however, it was proven that rather simple calix[*n*]arene derivatives (*n* = 4, 6, Figure 1) with no intentionally introduced fluorophores can be successfully employed for fluorimetric cation sensing due to their intrinsic fluorescence. Although the luminescence of these compounds was low to moderate, the cation-binding induced fluorescence changes were shown to be substantial. That allowed for the quantitative monitoring of the corresponding complexation reactions in water, methanol, and acetonitrile by spectrofluorimetry, at much lower concentrations than those typically required by other commonly used techniques. It also enabled the determination of quite high complex stability constants by means of direct fluorimetric titrations, thereby avoiding time- and material-consuming competitive experiments which inevitably introduce additional uncertainty into the resulting equilibrium constant values. To find out the relation between the fluorescence responses upon cation binding by calixarene **2** and its monomeric structural component **4**, the cation complexation by the latter compound was studied as well. In addition, the results of excited-state lifetime measurements and quantum chemical calculations provided insight into the emission mechanisms and explained the differences between photophysical properties of the ligands and their cation complexes.

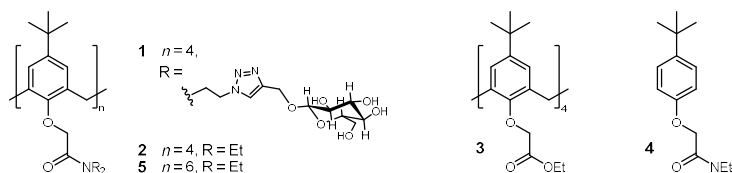


Figure 1. Structures of investigated calixarenes.

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

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POLYMORPHISM AND MECHANICAL BEHAVIOR IN MOLECULAR CRYSTALS: A COMPUTATIONAL STUDY

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Molecular crystals have played a central role in the development of electronics, photonics, and materials science due to their unique electronic and optical properties.^[1] However, their broader use and commercialization are often constrained by mechanical fragility and other performance limitations. These challenges have driven the search for next-generation molecular materials with improved performance and tunable properties. Crystal engineering offers a powerful approach, enabling the rational design and synthesis of molecular crystals by manipulating crystal packing and intermolecular interactions. A better understanding of these structural factors enables the fine-tuning of properties to suit specific applications. Special attention is given to polymorphism, where compounds with identical chemical compositions adopt distinct crystal packing arrangements, resulting in distinct mechanical behaviors.

For example, 4-bromophenyl 4-bromobenzoate exhibits two polymorphs – one brittle and one elastic – highlighting the significant impact of packing variations on mechanical response.^[2] This study investigates the relationship between crystal structure and mechanical properties in *para*-halogenated phenyl benzoates using periodic DFT calculations implemented in the CRYSTAL23 program. A series of derivatives with different *para*-substituted halogens were examined to assess how minor structural modifications influence molecular packing and mechanical behavior. Optimized crystal structures and interaction energies along specific crystal planes were analyzed, followed by virtual tensile tests to evaluate elastic responses. The 3D shapes of Young's modulus and the 2D cross-sections perpendicular to specific crystal directions further enhance our understanding of the structural features leading to mechanically pliable materials.

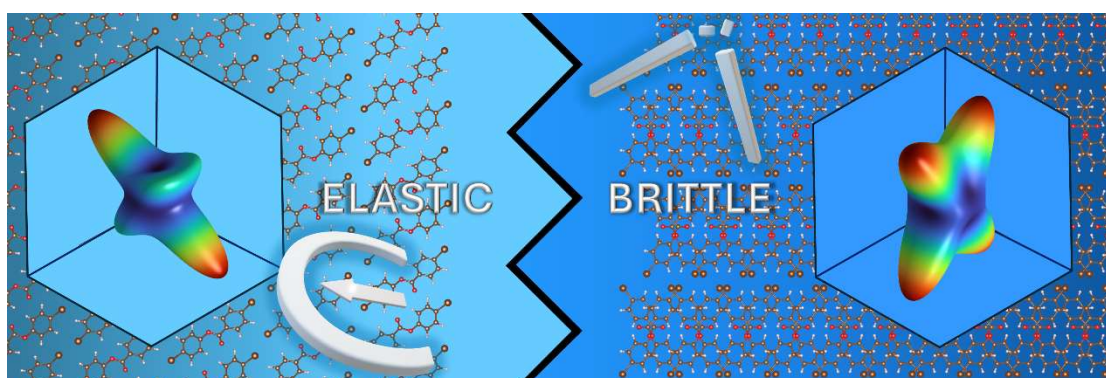


Figure 1. 3D representations of Young's modulus for two polymorphs: elastic and brittle.

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DEAROMATIVE [3+3] ANNULATION FOR THE CONSTRUCTION OF POLYCYCLIC SKELETONS

Robert Junior Kolman and Matija Gredičak

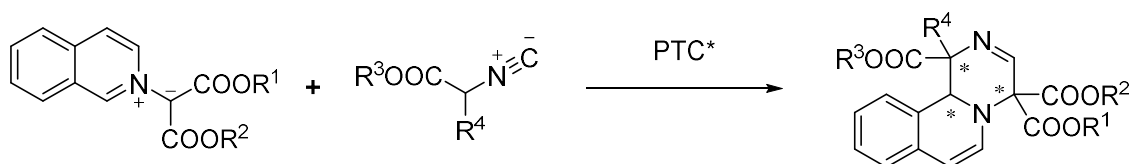
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Among the top 200 small molecule drugs by retail sales in 2024, 71 of them contain polycyclic skeletons.^[1] Usually, synthesis of these structures includes multiple-step routes and expensive starting materials. On the other hand, aromatic compounds as cheap and readily available bulk chemical feedstock provide direct access. Traditionally, reactions of aromatic compounds are restricted by their aromaticity and are limited to reactions where it is preserved. Dearomatization reactions allow for escape from these restrictions and forging of sophisticated three-dimensional molecular topologies. By taking inspiration from known drugs and bioactive natural products, organocatalytic asymmetric dearomatization (OCADA) reactions are being developed.

Azomethine ylides are readily employed in 1,3-dipolar cycloadditions for the construction of highly substituted heterocycles.^[2] Usually, azomethine ylides are generated from α -iminoesters during the reaction course. On the other hand, their isoquinolinium derivatives are bench stable chemicals. In 2011, Carillo, Vicario *et al.* reported enantioselective [3+2] cycloaddition of isoquinolinium methylides with α,β -unsaturated carbonyl compounds.^[3] We aim to develop chiral PTC (phase-transfer catalyst) mediated OCADA [3+3] cycloaddition reactions between isoquinolinium methylides and α,α -disubstituted isocyanides for the construction of quinolizidine-type polycyclic skeletons (Scheme 1).

Starting materials were prepared through known procedures. Isoquinolinium ylides were obtained by reaction of isoquinoline with α -halocarbonyl compounds and subsequent deprotonation. Isocyanides were obtained from the corresponding aminoacids, through esterification, amine formylation and formamide dehydration.



Scheme 1. Chiral PTC mediated OCADA [3+3] cycloaddition between isoquinolinium methylides and α,α -disubstituted isocyanides.

Acknowledgements. This work has been supported by Croatian Science Foundation, project “Natural product-inspired organocatalytic dearomatization strategies”, IP-2022-10-5184.

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MECHANOCHEMICAL SYNTHESIS OF 1,2,3-TRIAZOLES VIA COPPER(I)-CATALYSED 1,3-DIPOLAR CYCLOADDITION: A GREEN APPROACH TO ANTIGUNGAL AGENTS

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Mechanochemistry represents a promising green alternative to conventional synthetic methods, offering solvent minimization, and enhanced reaction efficiency.^[1] In this work, the synthesis of 1,2,3-triazole derivatives was achieved via copper(I)-catalysed 1,3-dipolar cycloaddition under mechanochemical conditions. The reactions were carried out using terminal alkynes and azides bearing coumarin, quinazolinone, and quinolinone scaffolds. Several catalytic systems and solvent combinations were screened, including both classical and deep eutectic solvents. The optimal conditions involved copper(II) sulfate pentahydrate and sodium ascorbate in an ethanol–water mixture (1:5), affording high yields within 60 minutes of grinding. Several 1,2,3-triazole derivatives were synthesized and subsequently evaluated for their antifungal activity, highlighting the potential of this sustainable synthetic strategy in the development of bioactive heterocycles.

Antifungal activity was determined according to the method described by Kovač et al. (2017).^[2] Briefly, *Aspergillus flavus* NRRL 3251 was cultured on a rotary shaker at 200 rpm for 72 hours at 29 °C in YES medium (2 % yeast extract and 6 % sucrose, pH 5.8). The tested compounds were applied at final concentrations of 0, 0.01, 0.1, and 1 µg mL⁻¹. Antifungal efficacy was expressed as a percentage of inhibition, with a concentration-dependent reduction in dry mycelial weight observed. Complete inhibition of *A. flavus* growth was achieved at the highest concentration tested.

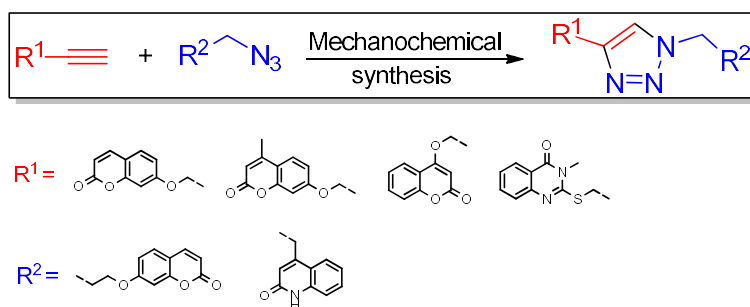


Figure 1. Mechanochemical synthesis of 1,2,3-triazoles via 1,3-dipolar cycloaddition.

Acknowledgements. This work has been supported by project POC (NPOO.C3.2.R3-I1.05.0174).

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IDENTIFICATION AND FUNCTIONAL CHARACTERIZATION OF METAGENOMIC ESTERASES FOR BIODEGRADATION OF BIOPLASTICS

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The widespread use of synthetic plastics, combined with their high stability and resistance to degradation under natural conditions, has led to significant environmental pollution.^[1] In response to this ecological concern, biobased polyesters have been proposed as sustainable and biodegradable alternatives to fossil fuel-derived plastics.^[2] In this study, we analyzed three candidates of esterases from metagenomic databases that have the potential to degrade aliphatic polyesters. To optimize protein expression in *E. coli* BL21(DE3), expression was performed at two temperatures: 28 °C and 15 °C. SDS-PAGE analysis revealed higher expression levels at 15 °C. All three proteins were purified using affinity chromatography on Ni-NTA agarose. Protein yields were quantified to determine the most efficiently expressed esterase, which was then produced on a larger scale, yielding approximately 3.7 mg of purified protein. The enzymatic activity of this esterase was tested on two aliphatic biopolymers—polylactic acid (PLA) and polycaprolactone (PCL). Activity was observed only against the PLA. Size-exclusion chromatography further revealed that the enzyme predominantly exists in a monomeric form in solution. Following the biopolymer assays, the esterase's activity was evaluated using small ester substrates. Although this enzyme requires further optimization, particularly in terms of solubility and catalytic efficiency—through enzyme engineering, our findings highlight the vast potential of uncharacterized esterases in metagenomic resources. These enzymes may represent a valuable source for developing more robust and efficient biocatalysts for bioplastic degradation.

Acknowledgements: This research was funded through National Recovery and Resilience Programme, The Development Research Support (NextGenerationEU), project Enzyme engineering for sustainable recycling of bioplastics (NPOO.C3.2.R2-I1.06.0041).

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BIOLOGICAL ACTIVITY OF NEW FERROCENYLPYRIMIDINE DERIVATIVES OF CURCUMIN

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Pyrimidine-based derivatives as a class of *N*-heterocyclic compounds have been extensively researched for their therapeutic and medicinal properties.^[1] Curcumin, a naturally occurring polyphenol, also has many biological benefits, but due to its low bioavailability, it is usually structurally modified to improve its stability, bioavailability and pharmacological activity.^[2] On the other hand, ferrocene, as an organometallic compound with high lipophilicity and stability, favourable redox properties and low toxicity, represents an attractive core for conjugation with bioactive natural products, often leading to an improvement in their biological properties and activities.^[3] Against this background, the aim of this study was to investigate the antiproliferative activity of ferrocenylpyrimidine derivatives of curcumin **C1-C5** synthesized by multicomponent Biginelli reactions on two cancer (human breast cancer cells MCF-7 and mouse hepatoma cells Hepa1-6) and two normal (human keratinocytes HaCaT and hamster ovary cells CHO-K1) cell lines. Strong growth inhibition in MCF-7 and Hepa1-6 cells after 48h of **C1** exposure was confirmed with MTT method with significant antiproliferative effects in concentrations ≥ 10 μ M. Derivative **C1** vs. **C2-C5** proved to be the most toxic towards cancer cell lines (IC_{50} – 20.55 μ M (MCF-7) and 15.60 μ M (Hepa1-6), respectively). Nevertheless, it is important to observe extensive cytotoxicity in normal cells as well.

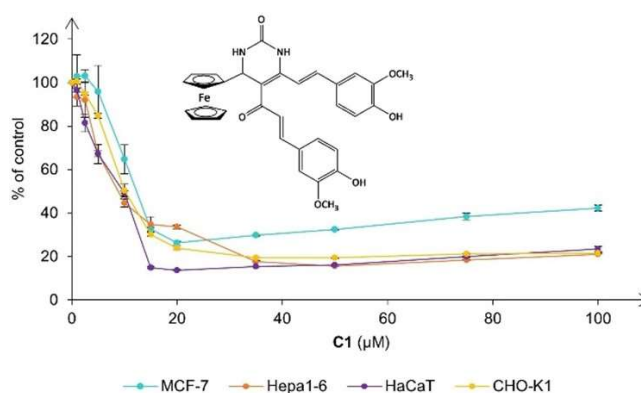



Figure 1. Antiproliferative activity of synthesized ferrocenylpyrimidine derivative of curcumin **C1** on two cancer (MCF-7 and Hepa1-6) and two normal (HaCaT and CHO-K1) cell lines.

Acknowledgements. This work has been supported by the Croatian Science Foundation under the project number HRZZ-IP-2020-02-9162.

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SPECTROSCOPIC CHARACTERIZATION OF (–)-EPICATECHIN-LIPID INTERACTIONS IN A MASLD MODEL

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Metabolic dysfunction-associated steatotic liver disease (MASLD) is characterized by excessive lipid accumulation in the liver, which can progress to more severe conditions such as steatohepatitis (MASH), fibrosis, and liver cancer. Also, MASLD affects various organs and regulatory pathways, increasing the risk of type 2 diabetes, cardiovascular disease, and chronic kidney disease.^[1,2] The aim of this study was to evaluate the preventive and therapeutic effects of (–)-epicatechin, a green tea polyphenol, on an *in vitro* model of hepatic steatosis using HepG2 cells. Fourier-transform infrared (FTIR) spectroscopy was used to analyze structural and biochemical changes in HepG2 cells following treatment with (–)-epicatechin. Pure sodium oleate, (–)-epicatechin, and untreated cells were analyzed to identify characteristic absorption bands. Additionally, the effects of different concentrations of (–)-epicatechin were examined in sodium oleate-treated cells under both preventive and therapeutic conditions. The FTIR analysis revealed spectral changes in (–)-epicatechin-treated cells, indicating interactions between (–)-epicatechin and lipids. In the therapeutic model, the highest concentration of (–)-epicatechin led to the disappearance of bands associated with unsaturated lipids, while in the preventive model, (–)-epicatechin appeared to promote the breakdown of sodium oleate.

These findings suggest that (–)-epicatechin may modulate lipid metabolism in liver cells in a concentration-dependent manner, highlighting its potential in the prevention and treatment of MASLD. In this regard, FTIR spectroscopy proved to be a valuable method for monitoring these biochemical changes.

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SYNTHESIS AND BIOLOGICAL ACTIVITY OF NEW BENZOXAZOLINONE-COUMARIN HYBRIDS

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Coumarin hybrids have emerged as a promising class in medicinal chemistry due to their diverse biological activities, including anticancer, antibacterial, antiviral, and antifungal properties. In addition to established coumarin hybrids featuring cores such as quinoline, imidazole, thiazole, indole, and triazole, novel derivatives incorporating coumarin and 2-benzoxazolinone scaffolds are being developed.^[1] The 2-benzoxazolinone core, in particular, represents an attractive scaffold for drug development due to its weakly acidic nature and balanced lipophilic and hydrophilic properties, which facilitate structural modification and support a wide range of biological activities.^[2]

In this study, we prepared benzoxazolinone-coumarine hybrids linked via an ethyl spacer in order to evaluate their antitumor and antiviral potential. The synthetic route involved the cyclization of 2-aminophenol to 2-benzoxazolinone using 1,1'-carbonyldiimidazole, followed by nitrogen alkylation with dibromoethane under basic conditions to yield *N*-bromoethyl-2-benzoxazolinone. This intermediate was subsequently reacted with 4-hydroxycoumarin and 7-hydroxycoumarin to afford the target hybrids. The structures were confirmed by ¹H- and ¹³C-NMR spectroscopy, and compounds were subjected both antitumor and antiviral evaluations. The most potent antitumor activity was observed for the compound bearing a 5-chloro substitution on the benzoxazolinone ring and a 4-trifluoromethyl group on the coumarin moiety. Notably, the highest antiviral activity was exhibited by the hybrid with the same benzoxazolinone substitution and an unsubstituted coumarin ring.

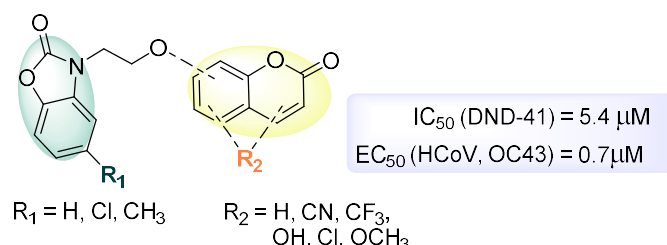


Figure 1. Designed and synthesized coumarin-benzoxazolinone hybrids

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

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ANTIPROLIFERATIVE ACTIVITY OF NOVEL BENZIMIDAZOLE-COUMARIN HYBRIDS

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Both benzimidazole and coumarin hold a prominent position in medicinal chemistry.^[1,2] Our previous research has focussed on the synthesis and biological evaluation of 5(6)-substituted benzimidazole hybrids.^[3] Here we present new 5(6)-substituted benzimidazole-coumarin hybrids linked by a phenoxy-ethoxy linker. Besides the 5(6) benzimidazole substituents, additional derivatisation was achieved by introducing a methyl group at C4 of the coumarin and a bromo or methoxy substituent at C2 of the phenoxy residue. The newly synthesised compounds were tested on one non-tumour (MRC-5) and five tumour cell lines (HeLa, CaCo-2, HL-60, THP-1 and HuT78). The methoxy 5(6)-substituted benzimidazole hybrid, featuring a methoxy group at the C2 position of the phenoxy ring and a methyl group at the C4 position of the coumarin moiety, exhibited the highest selective activity against leukemia and lymphoma cell lines.

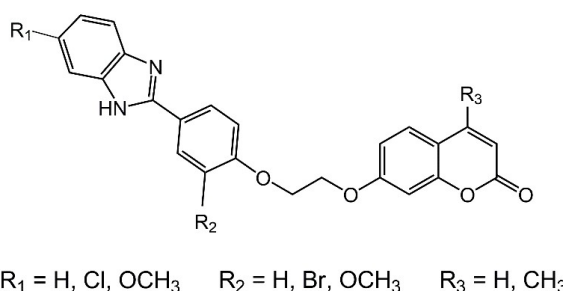


Figure 1. Novel coumarin benzimidazole hybrids.

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SYNTHESIS OF ARGININE HYDROXAMATE – A POTENTIAL INHIBITOR OF AMINOACYL-tRNA SYNTHETASE

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Arginine derivatives, such as arginine hydroxamate, have attracted considerable attention due to their potential as enzyme inhibitors and therapeutic agents.^[1] Although a wide range of methods for synthesizing hydroxamic acids exists, the preparation of arginine hydroxamate and its derivatives has been relatively unexplored. Synthetic approaches to these compounds often rely on peptide coupling techniques, which typically result in low yields of the desired products.^[2,3] This limitation is likely due to the unique structure of arginine, particularly the presence of the guanidinium group on its side chain.

In this work, we report the synthesis of arginine hydroxamate from L-arginine hydrochloride using different peptide coupling methodologies. In order to improve yield and purity while minimizing side reactions, our work also focuses on two additional strategies: (i) the use of mono- and triply-protected arginine derivatives in the condensation step, and (ii) the application of different hydroxylamine-donating agents. Using these approaches, we successfully synthesized arginine hydroxamate. The synthesized arginine hydroxamate was characterized by NMR spectroscopy and mass spectrometry, confirming its structure. As an additional confirmation of the presence of a hydroxamic functional group in the product molecule, a quantitative test with Fe³⁺ ions was performed.

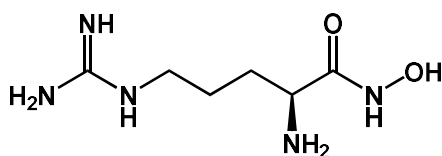


Figure 1. Structure of L-arginine hydroxamate.

Acknowledgements. This work is supported by the Croatian Science Foundation under the project number IP-2022-10-1400.

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A NEW GENERATION OF POLYMER INCLUSION MEMBRANES WITH SUPERIOR PERFORMANCE

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Membrane separation using **non-porous extracting liquid membranes** is a promising alternative to traditional solvent extraction, driven by environmental and economic benefits. These membranes significantly reduce or eliminate the need for large volumes of organic diluents and extractants, thus reducing environmental pollution and making the use of costly and highly selective extractants more feasible. They also offer faster and simpler separation compared to separation based on conventional solvent extraction by enabling simultaneous extraction and back-extraction at the membrane/solution interfaces with the feed and receiving aqueous solutions. These simultaneous processes make them suitable for **on-line industrial separation**. Enhancing their stability and transport rates will further boost industrial adoption. Key types of liquid membranes for industrial separation include **bulk liquid membranes (BLMs)**, **emulsion liquid membranes (ELMs)**, **supported liquid membranes (SLMs)**, and **polymer inclusion membranes (PIMs)**. Among these, **PIMs** are a recent development, offering superior stability and versatility in comparison with SLMs, being the most frequently used liquid membranes, and demonstrating significant potential for industrial applications in the selective separation of both metallic and non-metallic species.^[1,2] This research is focused on the fabrication and study of PIMs with improved characteristics which are expected to make PIM-based separation a commercially viable "Green Chemical" technology which will be an attractive alternative to conventional solvent extraction technologies that dominate industrial separation at present. The critical difference between these PIMs and those used at present is the incorporation of a supporting structure, consisting of glass fibres. The newly developed PIMs were composed of 55–60 wt% base polymer (i.e., (poly(vinyl chloride) (PVC), cellulose triacetate (CTA) or poly(vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP)), 40 wt% of the commercial anion-exchange extractant Aliquat 336 and 0–5 wt% glass fibres. Their mechanical, long-term stability and transport properties for SCN[−] as model target chemical species were studied for different concentration of the glass fibres and different polymers with the aim of selecting the optimal polymer and glass fibre composition.

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DIARYLETHENE-BASED PHOTOSWITCHES: PHOTOCHEMICAL BEHAVIOR AND BIOMOLECULAR INTERACTIONS

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Photochromic molecules like diarylethenes can undergo reversible structural changes upon light irradiation, enabling precise control over molecular properties. This switchable behavior makes them attractive for applications in electronics, data storage, and light-regulated biological systems. Their ability to modulate interactions with biomolecules such as nucleic acids and proteins offers potential for designing responsive probes and therapeutics.^[1]

In this study, three diarylethene-based photochromic compounds (Figure 1) were subjected to comprehensive spectroscopic characterization. Initial fluorescence measurements revealed very low fluorescence yields, prompting a shift toward UV/Vis absorption studies. The compounds were analyzed in both methanol and Na-cacodylate buffer, where the dynamics of ring-closing and ring-opening processes were monitored over time. Particular attention was given to the photochemical fatigue resistance through repeated switching cycles. UV/Vis titrations of the closed-ring isomers with polynucleotides and bovine serum albumin (BSA) were performed, allowing for the determination of binding constants. The closed-ring forms exhibited three distinct temporal stability profiles, as revealed by UV/Vis kinetic measurements. Additionally, circular dichroism (CD) titrations were conducted using various DNA structures, including three G-quadruplexes and one duplex. Thermal melting experiments were also performed for both open- and closed-ring forms with DNA and RNA to assess structural stability and interaction modes. These results enhance our understanding of diarylethene–biomolecule interactions and highlight their potential for use in light-responsive systems and sensors.

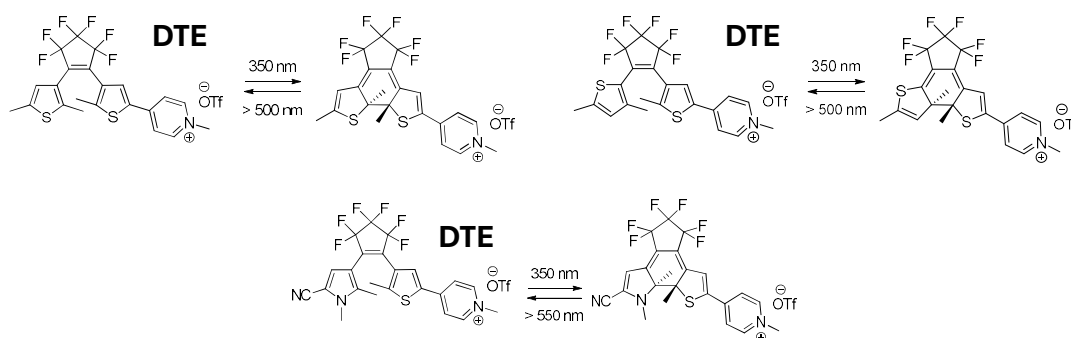


Figure 1. Structures of diarylethene-based photochromic compounds.

Acknowledgements. This work has been supported by the Croatian Science Foundation under the project number HRZZ IP-2022-10-9829.

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NOVEL BIOACTIVE QUATERNARY QUINUCLIDINE PEPTIDOMIMETICS

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Bioactive chemical compounds, such as quinuclidine derivatives, are recognized as entities with a broad spectrum of biological activities, including in the field of neurodegenerative diseases. Accordingly, they are used in the treatment of Alzheimer's and Parkinson's diseases.^[1–3] In this work, one novel quinuclidine peptidomimetic was synthesized. Reactions were performed using standard synthetic techniques and a microwave-assisted Ugi multicomponent reaction.^[4] 3-Aminoquinuclidine was used as the amino component, benzyl isocyanide as the isocyanide component, paraformaldehyde as carbonyl component and benzoic acid as the acid component. A series of eight new quaternary derivatives were prepared by quaternization of the quinuclidine nitrogen atom with methyl iodide, benzyl bromide and selected, differently *para*-substituted benzyl bromides. These structural modifications were designed to define parameters influencing biological activity, particularly interaction with cholinesterases. Prepared compounds were characterized by melting point determination, infrared spectroscopy, mass spectrometry, and 1D/2D NMR. Finally, the inhibitory potential of all prepared compounds toward the enzyme butyrylcholinesterase from horse serum (EC 3.1.1.8) was determined using the Ellman method.^[5]

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

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COMPLEXATION REACTIONS OF SOFT METAL CATIONS WITH CALIX[4]ARENE DERIVATIVES CONTAINING SULPHUR AND GLUCOSE FUNCTIONALITIES

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Calixarenes are a class of supramolecular ligands that can be readily functionalized to give very efficient and even selective receptors for various ionic and neutral chemical species^[1] Among them, those functionalized with sulphur-containing groups are efficient binders of low-charge density and soft metal cations.^[2] Additionally, development of neutral water-soluble calixarene-based receptors for cations^[3] is of great interest for the detection and extraction of toxic metal ions in aqueous media. In the scope of this work, calix[4]arene derivatives **L1** and **L2** (Figure 1) were synthesized and their binding affinities towards soft metal cations in water were investigated by means of isothermal titration calorimetry, spectrophotometry, and NMR spectroscopy. The obtained results were discussed regarding the structural characteristics of the ligands as well size and charge density of the cations.

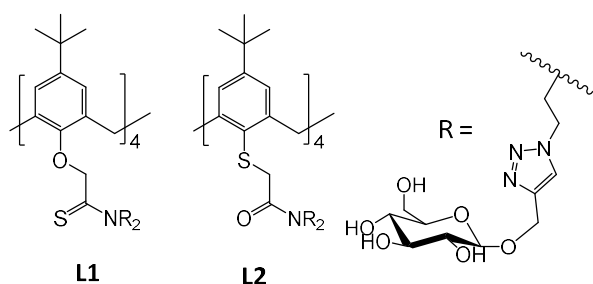


Figure 1. Structure of calix[4]arene derivatives **L1** and **L2**.

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 Regional Development Fund (infrastructural project CluK, grant number KK.01.1.1.02.0016).

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MECHANISTIC STUDY OF AMINOBIIPHENYL PHOTOCAGES

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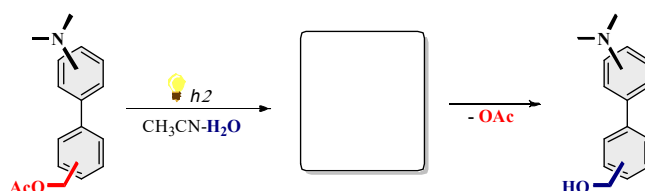
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Photocages (photochemically cleavable protective groups) are increasingly used in biological studies because of their non-invasiveness and spatiotemporal controllability. However, their reactive intermediates, and photoproducts may have phototoxic effects on some targets in biological substrates, which can lead to undesired effects. In order to reduce the possibility of the formation of toxic intermediates and photoproducts, the development of new photocages, as well as the understanding of their mechanism, is extremely important.^[1]

In our research group, the synthesis and photoreactivity of aniline^[2] and aminonaphthalene^[3] photocages have been investigated. The investigation of the photochemical reaction mechanism of aniline photocages revealed that the decaging takes place heterolytically, giving the carbocation as intermediate.^[2] On the contrary, the decaging mechanism for aminonaphthalenes involves homolytic cleavage on the singlet excited state surface and formation of radical species, which may not be benign for biological applications.^[3] Further investigation led to the development of different substituted aminobiphenyl derivatives (Scheme 1) which react more efficiently in releasing carboxylates ($\Phi_R = 0.04$ – 0.37) than aminonaphthalenes ($\Phi_R = 0.01$ – 0.22).

To understand the sparse and limitation of the use of aminobiphenyl photocages, the mechanism of the decaging reaction was studied by fluorescence spectroscopy and laser flash photolysis (LFP).



Scheme 1. The photolysis of aminobiphenyl photocages.

Acknowledgements. This work has been supported by HrZZ-IP-2019-04-8008 and HrZZ-IP-2024-05-8565.

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PHOTOSWITCHABLE CUCURBIT[7]URILS

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Self-assembled monolayers (SAMs) with photoresponsive functionality were constructed on gold surfaces through the use of host–guest complexes incorporating cucurbit[7]uril (CB[7]). In this system, CB[7] functions as a universal anchoring motif, binding to the gold substrate via one of its portals, while the opposite portal captures a photoresponsive molecular rod bearing a pyridinium–adamantyl recognition element. To showcase the flexibility of this modular design, four different molecular rods were synthesized. In solution, the supramolecular CB[7] complexes^[1] maintained the intrinsic light-responsive behavior of the original rods, undergoing reversible isomerization with minimal influence from complexation and demonstrating excellent fatigue resistance. Once immobilized on surfaces, the resulting monolayers preserved their photoactivity, as confirmed by the light-triggered isomerization of a representative diarylethene derivative. These findings highlight the promise of CB[7]-mediated architectures in developing stable, switchable molecular interfaces and devices.

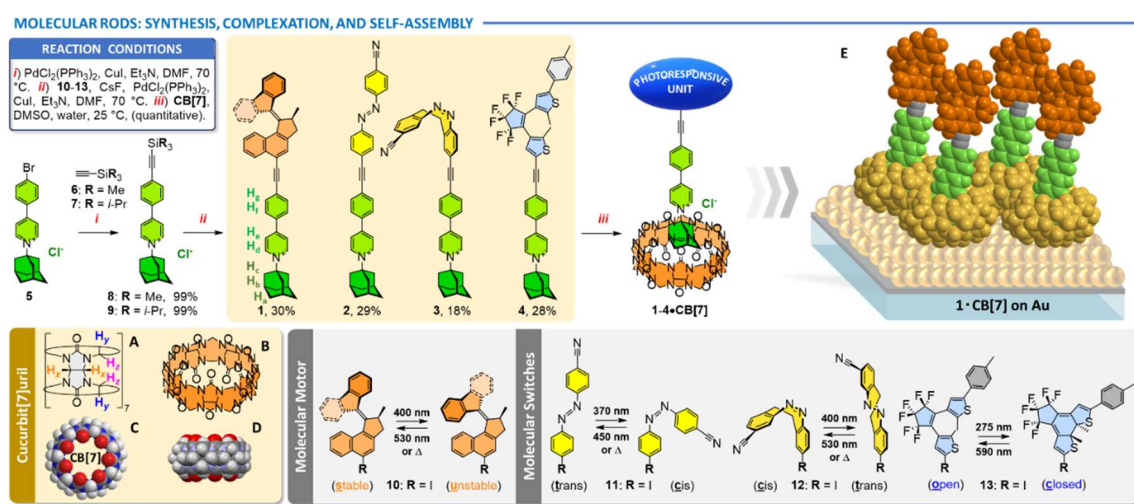


Figure 1. Synthesis of molecular rods **1-4** and their reaction with **CB[7]** leading to supramolecular complexes **1-4·CB[7]**. **CB[7]**: a schematic representation (A), chemical structure (B), and top (C) and side (D) view on a space-filling model. Idealized visualization of **1·CB[7]** on a gold surface (E).

Acknowledgements. This work was supported by the Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic (RVO: 61388963), Czech Science Foundation, and the Ministry of Education, Youth and Sports (grant number: LTAUSA19120).

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SYNTHESIS AND EVALUATION OF (OXIDOPYRIDYL)PORPHYRINS IN PHOTODYNAMIC THERAPY

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Porphyrins are organic dyes that can meet a large number of criteria required for photosensitisers (PSs) in photodynamic therapy (PDT), such as absorption in the visible part of the EM, efficient triplet excited state formation and production of singlet oxygen ($^1\text{O}_2$) and other reactive oxygen species (ROS).^[1] PDT is a promising approach in cancer treatment due to minimal invasiveness, high selectivity and fewer side effects, and a low likelihood of developing resistance, but one of its limitations is dependence on molecular oxygen ($^3\text{O}_2$). Given that the microenvironment in cancer is often hypoxic, especially in melanomas and solid tumors, it is necessary to develop PSs that will be able to produce ROS by different mechanisms depending on the local $^3\text{O}_2$ concentration.^[2]

We have recently shown both high cellular uptake and phototoxicity of amphiphilic AB₃ *N*-methylated pyridiniumporphyrins conjugated with fatty acids (**Figure 1** (left), R = C₁₃H₂₇ or C₁₇H₃₅) on melanoma cells (amelanotic A375 and melanotic MeWo) and fibroblasts (HDF).^[2] We prepared their *N*-oxide analogues (**Figure 1** (right)) to evaluate their potential as hypoxia-activated prodrugs, and here we present a study of their properties by absorption and fluorescence spectroscopy, laser flash photolysis (LFP), time-correlated single photon counting (TC-SPC) and determination of $^1\text{O}_2$ /ROS production. Cellular uptake, localisation, and (photo)cytotoxicity in different melanoma cell lines and fibroblasts under conditions of normoxia and hypoxia (induced by CoCl₂) will be compared between these two groups of PSs.

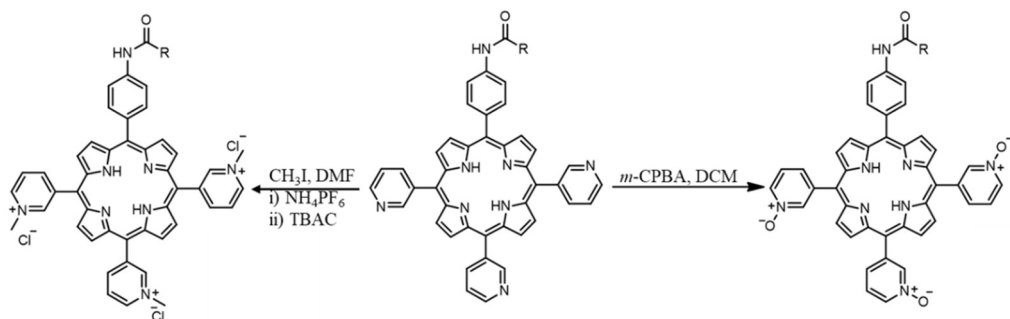


Figure 1. Synthesis of *N*-methylated pyridiniumporphyrins (left) and (oxido)pyridylporphyrins (right) from 5-amidophenyl-10,15,20-tri(3-pyridyl)porphyrins (general structure in the middle).

Acknowledgements. This work has been supported by the University of Rijeka's grant assigned to Prof. dr. Nela Malatesti (uniri-iskusni-23-2).

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DESIGN AND DEVELOPMENT OF QUINAZOLINE WHITE LIGHT EMITTERS FOR LIGHTNING APPLICATION

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In this work, we combine experiment and theory in the design and development of new quinazoline chromophores with targeted properties, *i.e.* white light emitters for application in White Organic Light-Emitting Diode devices.^[1] The heterocyclic structure of quinazoline allows for various structural modifications that can be achieved by different synthetic routes, allowing the spectroscopic properties to be tuned. First, we selected four commercial quinazoline compounds based on our previous work^[2] and determined the optical and photophysical properties both in solution and in the solid state (fluorescence quantum yield and lifetime, colour coordinates according to the CIE 1931 colour system (fr. Commission Internationale de l'Éclairage))^[3] as well as quantum chemical DFT calculations (protonation sites, emission spectra, excited state deactivation pathways). Based on the obtained results, we then designed the new compounds with the targeted properties of white light emitters, which should be achieved by the mechanisms of intramolecular charge transfer and excited-state intramolecular proton transfer. Finally, we synthesised and characterised new compounds to confirm the prediction. The structure-property relationship is discussed for both commercial and novel compounds.

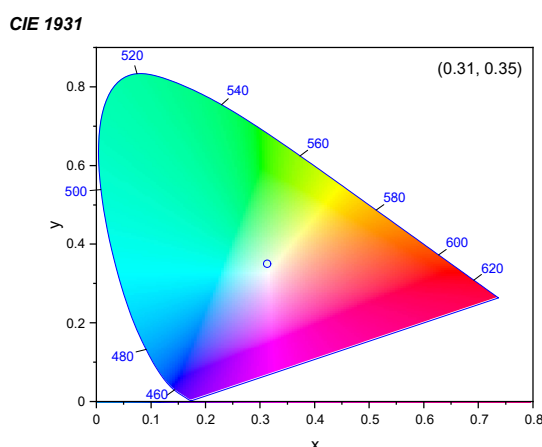


Figure 1. CIE 1931 coordinates for quinazoline compound with 2 equiv. of trifluoroacetic acid in MeOH.

Acknowledgements. This work was supported by the Ruđer Bošković Institute grant KP3-25, under Objective 3.2 of the EU-funded National Recovery and Resilience Plan (NRRP).

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ESSENTIAL OIL AND HYDROSOL COMPOSITION OF *Globularia alypum* L. FROM CROATIA

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Shrubby globularia (*Globularia alypum* L.) is a heliophilous, xerophilous and thermophilous plant species indigenous to the Mediterranean region.^[1] It is a medicinal plant that has been used in the Mediterranean folk medicine since ancient times.^[2] The objective of this study was to compare the essential oil and hydrosol composition of Croatian *G. alypum* collected from two nearby locations on the Konavle cliffs. Gas chromatography–mass spectrometry (GC–MS) analyses of essential oils obtained by hydrodistillation revealed that the major constituents belonged to the groups of aliphatic carboxylic acids (45.72–61.34 %) and oxygenated monoterpenes (18.39–31.80 %). The major carboxylic acid was hexadecanoic (palmitic) acid, followed by tetradecanoic (myristic) and oleic acid, while linalool, borneol and 1,8-cineole (eucalyptol) were found as the major oxygenated monoterpenes. The GC–MS analyses of the remaining hydrosols showed high relative contents of phenols (53.87–55.10 %), with eugenol (4-allyl-2-methoxyphenol) and *p*-vinylguaiacol (2-methoxy-4-vinylphenol) being the major components. These compounds, which were also present in the analyzed essential oils, but in much smaller relative amounts (<2.5 %), may contribute to the recorded biological activities of *G. alypum* such as antimicrobial, antidiabetic, anti-inflammatory, and antioxidant.^[3,4] Volatile components may also add to the beneficial effects of skincare products, and at the same time possibly serve as their preservatives and perfumes.^[4,5] However, it should be noted that compounds such as linalool and eugenol may cause allergic reactions (allergic contact dermatitis) and are among the 26 fragrances that need to be labelled on cosmetic products according to the EU Cosmetics Regulation when their concentration exceeds 0.001 % in leave-on products and 0.01 % in rinse-off products.^[6]

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SYNTHESIS AND BIOLOGICAL ACTIVITY OF NOVEL METHOXY AND HYDROXY SUBSTITUTED PYRIDINE BENZAMIDES

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Nitrogen heterocycles are one of the most significant substructures in medicinal chemistry and rational design of potential drugs. Pyridine and its derivatives possess wide range of biological activities owing partially to their properties like polarity, basicity, and possibility for hydrogen bond-forming important for interactions with biological targets.^[1] The structural similarity of pyridines with naturally occurring nucleotides allowed their optimization to get more selective molecules which could play a crucial role in the function of biologically important molecules. Herein we present the synthesis of methoxy and hydroxy substituted *N*-(pyridine-2-yl)-benzamides to investigate their biological potential. Starting from methoxy substituted benzoyl-chlorides and 2-aminopyridines, methoxy substituted benzamides were synthesized, followed by demethylation with BBr₃ to obtain hydroxy derivatives.^[2,3] The structures of newly prepared compounds were confirmed by means of ¹H and ¹³C NMR spectroscopy and MS spectrometry. All prepared compounds will be screened for their antioxidant capacity by several spectroscopic methods and antiproliferative activity in vitro on several human cancer cells.

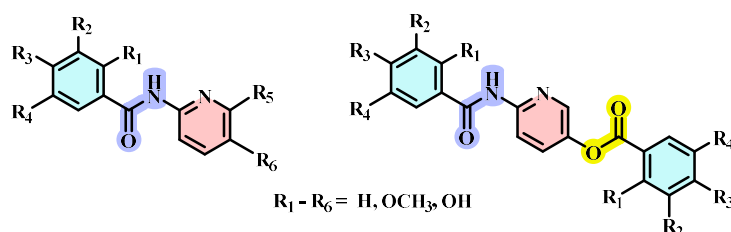


Figure 1. Structures of prepared 2-pyridyl benzamides

Acknowledgements. This work has been supported by the Croatian Science Foundation under the project BenzHetPot IP-2024-05-7208.

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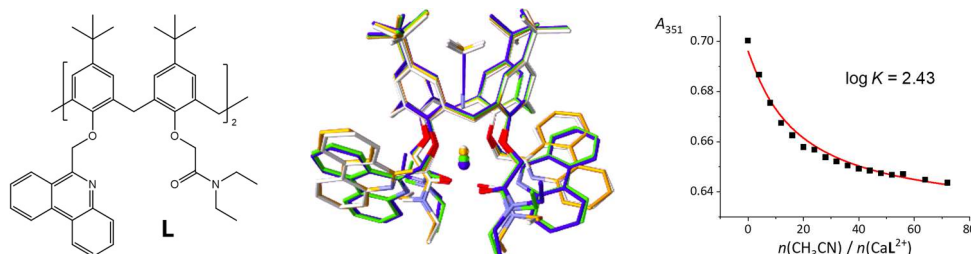
CALORIMETRIC, SPECTROSCOPIC, AND COMPUTATIONAL STUDIES OF CALIXARENE-SOLVENT ADDUCTS FORMATION

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

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



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

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QUANTUM-CHEMICAL STUDY OF THERMAL TRANSFORMATIONS OF O-DIVINYLBENZENE DERIVATIVES

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Computational methods enable the calculation and prediction of almost all chemical and physical properties of molecules and their interactions, therefore giving a deeper insight into the nature of the chemical process and the explanation of the obtained experimental data. The results of computer simulations are comparable to those of experiments and are widely used today as a supplement, guidance and very often as a complete replacement of experimental research, especially those that are time consuming, financially demanding and ecologically inappropriate. As a part of this study, quantum chemical DFT calculations were used to elucidate the reaction mechanism of the thermal transformations of *o*-divinylbenzene derivatives and to predict their outcomes.^[1]

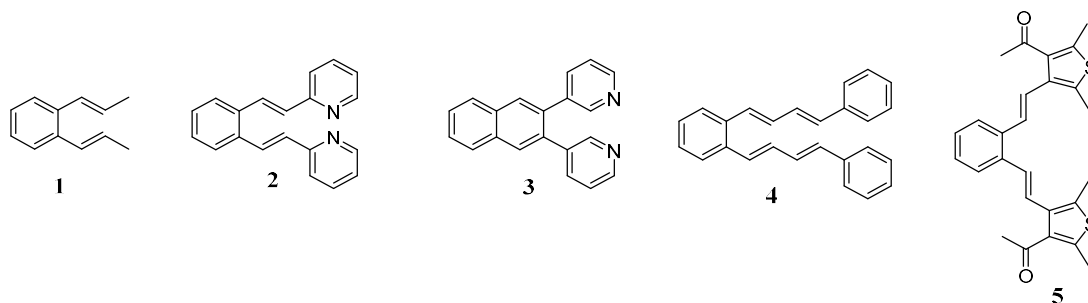


Figure 1. Investigated derivatives of *o*-divinylbenzene

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CRYSTALS ON THE EDGE: COFFEE-RING SYMMETRY, DIFFUSION, AND UNPREDICTABILITY IN A SINGLE DROP OF PANTOPRAZOLE

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When a droplet containing dissolved solids evaporates, the solute often migrates and deposits at the edge, forming a characteristic "coffee ring" pattern — a phenomenon that combines fundamental physical principles with complex self-assembly behavior. The crystallization of pharmaceuticals during solvent evaporation often results in complex patterns that reveal more than just phase transitions — they reflect hidden rules of self-organization, molecular dynamics, and physical instabilities. In this work, we investigate the coffee-ring effect in a single drying droplet of pantoprazole sodium, a proton pump inhibitor with known polymorphic behavior.

Using optical microscopy and quantitative image analysis, we demonstrate that the resulting crystalline deposit exhibits striking radial symmetry, dense peripheral accumulation, and structured anisotropy, despite the absence of any templating forces. In pattern present on figure 1 over 450 discrete object were identified, predominantly clustered along the drop edge, with size distributions suggesting a strong interplay between diffusion, capillary flow, and nucleation kinetics. The apparent order emerging from a stochastic process invites discussion on the boundary between symmetry and randomness in crystal growth.

We propose that such evaporative self-patterning may serve as a sensitive diagnostic tool for preformulation studies, particularly for compounds prone to morphological and polymorphic variability. Our findings highlight the potential of droplet-based crystallization models to uncover fundamental physico-chemical principles through seemingly simple experiments.

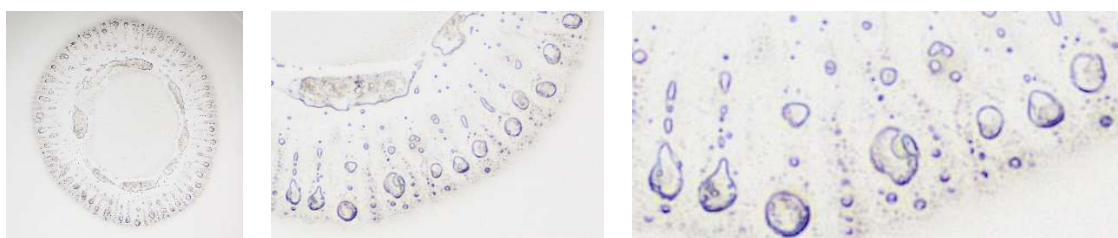


Figure 1. Selected Pattern of the Coffee-Ring Effect of Pantoprazole Sodium

Acknowledgements. This work has been fully supported by the Croatian Science Foundation, project IP-2024-05-4339 entitled " 'Coffee ring' effect in 'Lab on a Chip' environments in the development of new drug formulations." leader prof. Ernest Meštrović.

PHASE TRANSFORMATION AND SELF-HEALING OF A CHARGE-TRANSFER CRYSTAL

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Charge-transfer compounds comprising electron donor tetramethylphenylenediamine with electron acceptors tetrachloro- and tetrabromoquinone comprises stacks of alternating donor and acceptor moieties^[1] (Figure 1). Both compounds have two phases, with minor differences in stacking geometry: in the high-temperature (HT) phase the rings are parallel (Figure 1b), while in the low-temperature (LT) phase their mean planes are inclined by about 2.5° (Figure 1a).^[1]

The phase change proceeds via a single crystal-to-single crystal mechanism, similar to those observed in salts of pancake-bonded semiquinone radicals.^[2] Very small enthalpy and poor ordering of the crystals near temperature of the phase transition indicate a gradual, second-order mechanism consistent with small re-alignment of positions of the stacked moieties. These crystals represent a rare case of 'self-healing' crystals: upon cooling single crystals of the HT phase split into twins of the LT phase. Two domains in the LT phase are rotated by 180° about crystallographic axis *c*.

Details of electron density in partially charged TMPD and Cl₄Q moieties in HT phase of TMPD·Cl₄Q are studied by X-ray charge density. Maximum electron density between the rings exceeding 0.57 e Å⁻³ and presence of local electron density minima indicate existence of strong partially covalent interactions (pancake-bonds) between the rings (Figure 1c).

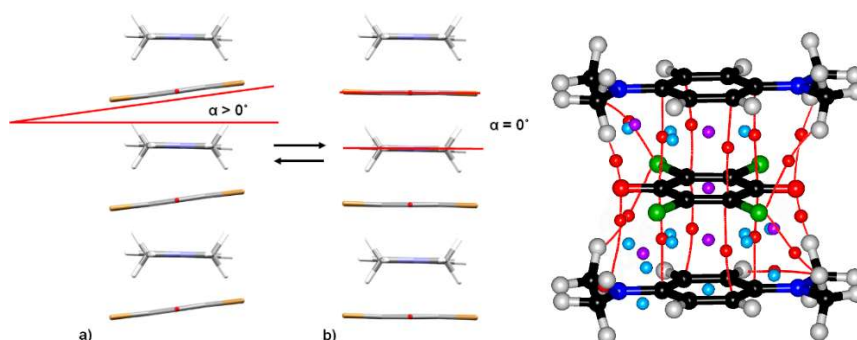


Figure 1. Stacks of alternating donor and acceptor moieties in TMPD·Br₄Q: a) LT phase and b) HT phase. c) Critical points in a pancake-bonded contact between TMPD and Cl₄Q moieties.

Acknowledgements. This work has been supported by the Croatian Science Foundation, grant IP-2024-05-8711.

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STRUCTURAL AND MAGNETIC PROPERTIES OF THE OXALATE-BASED [Cu^{II}Cr^{III}] COMPLEXES: THE INFLUENCE OF SOLUTION ON DIMENSIONALITY

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The design and synthesis of new materials with targeted physical properties represents an operative area of research for materials scientists. The combination of magnetic oxalate-based coordination polymers with organic/inorganic functional cations provides a suitable approach for designing hybrid magnetic materials exhibiting multifunctional properties. The oxalate moiety, C₂O₄²⁻, acts as a linker between metal centers, with various possibilities of coordination to metal centers yielding open structures with dimensionalities ranging from 0 to 3. A property of oxalate ions that has been of specific interest is their ability to mediate electronic effects between paramagnetic metal ions. The synthetic strategy for the preparation of (hetero)polynuclear species is "building block chemistry", in which a molecular anionic ligand, very often the tris(oxalato)metallate anion [M^{III}(C₂O₄)₃]³⁻ (M^{III} = Cr, Fe, Ru, Rh, Mn or V), is used as a ligand towards other metal cations.^[1,2]

Four novel oxalate-based [Cu^{II}Cr^{III}] compounds: {[Cu(phen)₂Cl][CrCu(phen)₂(C₂O₄)₃]}₂·8H₂O·6CH₃OH (**1**; phen = 1,10-phenanthroline), [CrCu₂(phen)₄(C₂O₄)₃][CrCu(phen)₂·(C₂O₄)₃]·11H₂O (**2**), {[CrCu(phen)(C₂O₄)₃][CrCu₃(H₂O)(phen)₃(C₂O₄)₄]·2CH₃CN·3H₂O}_n (**3**) and [Cu(H₂O)(phen)₂][Cu(phen)₂Cl][Cr(C₂O₄)₃]·7H₂O·CH₃CN (**4**) were obtained from the reaction of an aqueous solution of the building block [Cr(C₂O₄)₃]³⁻ and a methanol or acetonitrile solution containing Cu²⁺ ions and the phen ligand by the layering technique. Interestingly, changing only the solvent in synthesis (methanol vs. acetonitrile), structurally very different oxalate-bridged compounds were obtained (dinuclear vs. one-dimensional). These systems are the first representatives of compounds that simultaneously contain phenanthroline ligand and chromium(III) and copper(II) atoms bridged by oxalate group. Also, an interesting process of crystal disassembly/reassembly was observed for two new crystal forms. Compounds were characterized by single-crystal and powder X-ray diffraction, IR spectroscopy and by measurements on a SQUID magnetometer and TG analyzer.

Acknowledgements. This work has been supported by the Croatian Science Foundation under the project IP-2019-04-5742.

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MECHANOCHEMICAL SYNTHESIS OF COUMARIN BASED THIOSEMICARBAZIDES

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Mechanochemical synthesis, as one of the prominent green chemistry methods, finds its application in different chemical processes. When applied to synthetic processes, it is usually applied for *solvent-free* synthesis, which is accomplished through generation of mechanical force thus enhancing the overall reaction efficiency.^[1] In this research, mechanochemistry was applied in the synthesis of coumarin derivatives bearing thiosemicarbazide moiety. Umbeliferone was first converted to corresponding ethyl ester (**a**) in reaction with methyl bromoacetate, which in reaction with hydrazine hydrate yielded corresponding hydrazide (**b**). A mechanochemical approach was applied to the synthesis of thiosemicarbazides (**1-14**) from hydrazide and different isothiocyanates. Those compounds were obtained in high yields and purity in short time of 10 min. Mechanochemical approach was found to be very efficient and proved to enhance the overall reaction.

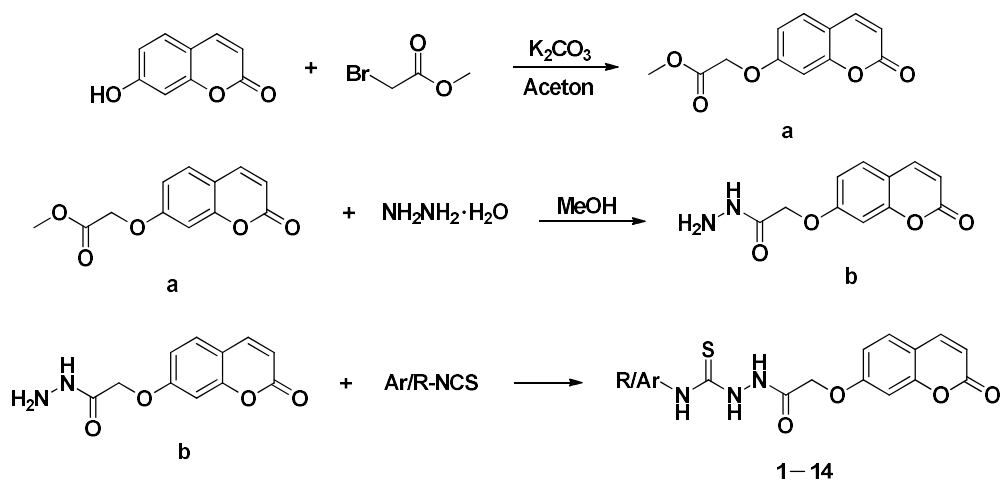



Figure 1. Synthesis of coumarinyl thiosemicarbazides.

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VANADIUM(V) AROYLHYDRAZONE COMPLEXES: SYNTHESIS, CHARACTERIZATION, CYTOTOXIC AND ANTIBACTERIAL ACTIVITY

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The coordination chemistry of vanadium continues to attract significant interest, particularly following the discovery of vanadium-dependent haloperoxidases and nitrogenases. Vanadium complexes participate in various physiological processes, including catalytic oxidative bromination, and show promise as experimental agents in diabetes and cancer research, as well as in the development of advanced functional materials.^[1,2] Their reactivity and stability are strongly influenced by the nature of the coordinating ligands. Hydrazones are versatile chelating ligands with distinctive physical and chemical properties and broad biological activity. Their modular synthesis, multidentate coordination modes, and structural tunability make them excellent ligands for stabilizing vanadium in its highest oxidation state.^[3]

Here, we report the synthesis and characterization of vanadium(V) complexes with selected aroylhydrazones ($R^1R^2C=N-NH-(C=O)R^3$), and their *in vitro* cytotoxic and antibacterial activity. The reactions of NH_4VO_3 with these ligands in methanol were monitored by UV-Vis spectroscopy, and time-dependent spectral changes were analyzed using principal component analysis (PCA). Cytotoxicity was assessed against THP-1 and HepG2 cell lines using the MTS assay, and half maximal inhibitory concentration (IC_{50}) values were derived from dose-response curves. Antibacterial activity was evaluated against *Escherichia coli* and *Moraxella catarrhalis* by the broth microdilution method, with results reported as minimum inhibitory concentration (MIC) values.

Acknowledgements. This work has been supported by the Croatian Science Foundation (HRZZ) under the project IP-2022-10-7368 (MOCASS).

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GREEN MICROWAVE-HYDROTHERMAL SYNTHESIS OF MIXED-PHASE COPPER/COPPER OXIDES: CHAMOMILE EXTRACT'S EFFECT ON RELATIVE PHASE ABUNDANCE AND ANTIBACTERIAL POTENTIAL

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Elemental copper and its oxides (Cu, Cu₂O, CuO) exhibit potent catalytic and antimicrobial properties that, combined with tunable particle size, morphology, and surface area, enable applications across environmental, agricultural, and biomedical sectors.^[1] Green synthesis using plant extracts offers a simpler, safer, and more cost-effective alternative to conventional routes, with phytochemicals acting as both reducing and stabilizing agents to yield eco-friendly Cu/Cu₂O/CuO particles with potent antimicrobial properties.^[2] Building on our prior study of microwave-hydrothermal syntheses,^[3] we prepared mixed-phase Cu/Cu₂O/CuO particles at 200 °C in 20 min using *Matricaria chamomilla* extract. Fourier transform infrared spectroscopy confirmed the presence of organic material within the inorganic product, while X-ray diffraction (Fig. 1) revealed that extract concentration tunes the phase composition of Cu, Cu₂O and CuO. Scanning electron microscopy provided preliminary insight into particle morphology and size distribution. Antibacterial efficacy against *E. coli* and *S. aureus* was assessed. This rapid, tunable, green microwave-hydrothermal method underscores the potential of chamomile-mediated Cu/Cu-oxide materials for sustainable biomedical and environmental applications.

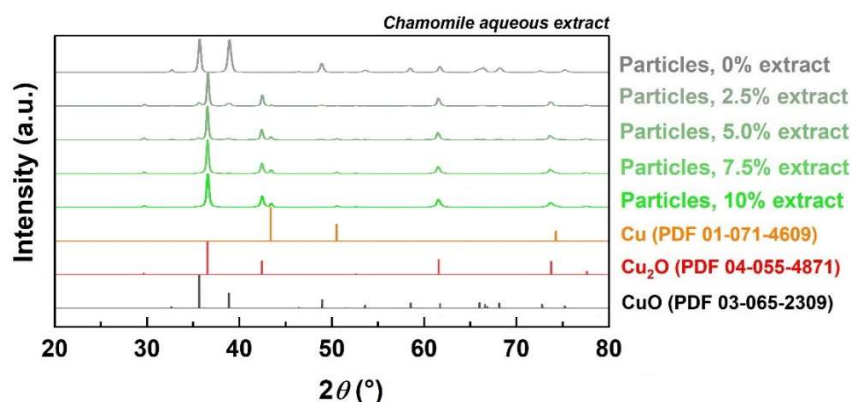


Figure 1. X-ray diffraction patterns of prepared mixed-phase Cu/Cu₂O/CuO particles.

Acknowledgements. This work has been supported by the Croatian Science Foundation (HrZZ), project title: *Outbound Mobility of Research Assistant*, project code: MOBDOK-2023-6241.

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QUINUCLIDINE BISQACS: STRUCTURE–ACTIVITY RELATIONSHIP ANALYSIS WITH FOCUS ON ANTIMICROBIAL RESISTANCE

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The growing prevalence of resistant bacterial strains has driven the search for novel membrane-targeting antimicrobial agents. Bisquaternary ammonium compounds (bisQACs) exhibit superior activity compared to monoquaternary analogs due to dual cationic centers that enhance interactions with negatively charged bacterial membranes.^[1] We synthesized and evaluated twelve quinuclidine-based bisQACs, systematically varying in alkyl chain length (C_{12} , C_{14} and C_{16}), linker length, i.e., molecular flexibility (3C, 4C and 6C atoms), to determine structure–activity relationships. Compounds showed potent activity against *Staphylococcus aureus*, *Listeria monocytogenes*, and *Escherichia coli*. Biological assays included MICs, time-kill kinetics, biofilm inhibition, membrane permeabilization (PI uptake), cytotoxicity on human cells, and resistance development. Physicochemical parameters such as cLogP were calculated. Molecular docking showed weak binding of $2(QC_{16})_6$ to the QacR efflux pump repressor, suggesting reduced efflux-mediated resistance. This dual-action mechanism—membrane disruption combined with efflux evasion—supports its potential against multidrug-resistant pathogens.

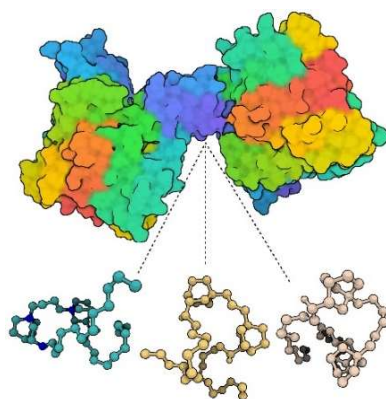


Figure 1. Schematic representation of molecular docking of a bisQAC derivative of 3-substituted quinuclidine into the QacR protein binding site.

Acknowledgements. This work was supported by the Croatian Science Foundation under grant no. UIP-2020-02-2356 awarded to M. Š.

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IDENTIFICATION AND CHARACTERIZATION OF NOVEL PLA-DEGRADING ESTERASES FROM METAGENOMIC DATABASES

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Poly(lactic acid) (PLA) is a biopolymer that represents a substantial portion of global bioplastic production—approximately 37.1 %. PLA offers several environmental advantages, including biodegradability, use of renewable raw materials, and a reduced carbon footprint compared to conventional fossil-based plastics. However, despite being a biopolymer, PLA does not naturally occur in the environment, which means that efficient enzymes for its degradation have not evolved through natural selection. Currently, only a limited number of hydrolytic enzymes are known to act on PLA. To improve their efficiency and substrate specificity, new enzyme variants must be designed using computational and experimental tools.^[1]

In this study, we identified novel esterases with activity toward PLA by screening the MGnify metagenomic database.^[2] The selected esterases were heterologously expressed and purified from *Escherichia coli* BL21 (DE3). Their thermal stability was analyzed using differential scanning calorimetry (DSC), while enzymatic activity toward PLA was evaluated via a solid-phase agarose emulsion assay. The release of lactic acid over time was quantified using high-performance liquid chromatography (HPLC) to provide insights into the enzymatic degradation kinetics of PLA.

This research supports the development of engineered enzymes with improved activity towards PLA biodegradation, offering a sustainable solution for its recycling. Enhancing enzymatic degradation of PLA could play a crucial role in reducing bioplastic accumulation and its environmental impact.

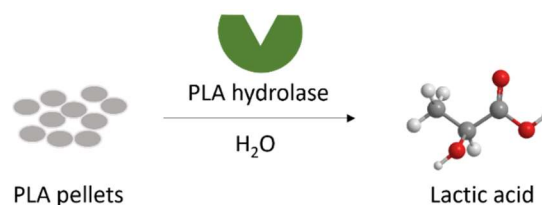


Figure 1. Enzymatic breakdown of PLA pellets into lactic acid shown schematically.

Acknowledgements. This research was funded through National Recovery and Resilience Programme, The Development Research Support (NextGenerationEU), project Enzyme engineering for sustainable recycling of bioplastics (NPOO.C3.2.R2-I1.06.0041).

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PREPARATION OF A POTENTIAL UREA-BASED ORGANOCATALYST FROM D-(-)-QUINIC ACID

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Jacobsen urea organocatalysts represent a significant class of bifunctional hydrogen-bonding catalysts that have advanced asymmetric synthesis considerably. These catalysts generally feature a urea or thiourea group, which forms strong, directional hydrogen bonds with electrophilic substrates such as carbonyl compounds and imines.^[1] Their catalytic action relies on dual activation: the urea moiety forms hydrogen bonds with the electrophilic substrate to increase its reactivity, while a nearby basic site, commonly a tertiary amine, activates the nucleophile to promote its nucleophilic attack.^[2] Jacobsen-type urea catalysts have been effectively utilized in enantioselective Mannich reactions, allowing for the preparation of

β -amino acid derivatives with excellent stereocontrol. They have also demonstrated outstanding results in Strecker reactions, enabling the synthesis of α -amino nitriles under mild conditions. Additionally, these catalysts perform well in Diels–Alder reactions, facilitating the formation of six-membered rings with high enantioselectivity, highlighting their versatile applications in pharmaceutical and natural product synthesis.^[3]

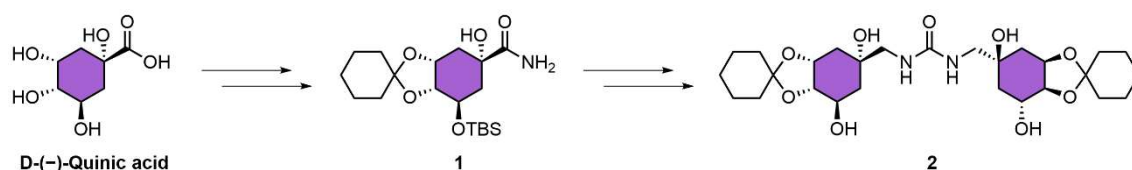


Figure 1. Construction of a urea derivative from D-(-)-quinic acid.

In this study, we describe the synthesis of urea starting from D-(-)-quinic acid, an inexpensive chiral precursor. The process begins by protecting the cis-diol group as a cyclohexylidene acetal, which also promotes the formation of a lactone ring. This is followed by transesterification, protection of the secondary alcohol as a silyl ether, and amidation to produce the amide intermediate **1**. Reduction of the primary amide then yields the corresponding amine, which is transformed into a symmetrically substituted urea through reaction with triphosgene. Finally, removal of the silyl protecting groups affords the desired target compound **2**.

Acknowledgements. This work has been supported by the Croatian Science Foundation, Grant Number 9617.

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AZO-BRIDGED POROUS ORGANIC POLYMERS FOR CO₂ CAPTURE AND CONVERSION

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Porous organic polymers bridged by azo bonds (azo polymers) are highly promising materials for the selective separation and capture of carbon dioxide (CO₂), one of the major greenhouse gases. Their nitrogen-rich structure, large surface area, strong CO₂ adsorption capacity, and high physicochemical stability make azo polymers excellent candidates for the development of new, more efficient CO₂ adsorbents.^[1] Azo polymers can also serve as catalysts for incorporating CO₂ into other organic compounds, such as styrene oxide or phenyl glycidyl ether, thus producing high-value products such as cyclic carbonates.^[2]

Our recent studies have demonstrated that different synthesis methods and central units significantly influence the porosity and CO₂ adsorption performance of azo polymers.^[3–5] In this work, we investigated the catalytic ability of selected azo polymers for the fixation of CO₂ into phenyl glycidyl ether. Several azo polymers with various central units (adamantane, porphyrin, pyridine, and triazine) were synthesized and characterized using multiple techniques. The results showed that all polymers are amorphous solids with good thermal stability and are insoluble in common organic solvents. The obtained azo polymers exhibit Brunauer–Emmett–Teller (BET) surface areas of up to 608 m² g^{−1}, CO₂ uptake capacities of up to 41 mg g^{−1} at 306 K, and CO₂ conversion efficiencies of up to 70 %, making them promising candidates for the development of new materials for efficient CO₂ capture and conversion.

Acknowledgements. This work has been fully supported by Croatian Science Foundation under the project IP-2020-02-4467.

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SMART BIOSENSOR DESIGN: HARNESSING G-QUADRUPLEX AND ANTIMICROBIAL PEPTIDES FOR SELECTIVE PATHOGEN DETECTION

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Bacterial infections cause over 7 million deaths annually, highlighting the need for rapid, cost-effective diagnostics. Current methods, such as culture-based assays and PCR, are either slow or expensive and require specialized equipment. To overcome these challenges, we developed a low-cost biosensor using antimicrobial peptides (AMPs) conjugated to G-quadruplex (G4) DNazymes. AMPs selectively bind to bacterial membranes, while G4 DNazymes—guanine-rich sequences complexed with hemin—mimic HRP activity to catalyze a colorimetric reaction. This system combines high bacterial affinity with stable, enzyme-free signal generation for efficient pathogen detection. We studied two G-rich sequences (AGRO100, PS5.M) with strong peroxidase activity and developed chemical methods to conjugate them to AMPs. Initial SPAAC coupling gave heterogeneous products due to multiple amines in AMPs, so we used SMCC for site-specific linking via a single cysteine, producing uniform conjugates.

These AMP–G4 conjugates were tested in two assays: a rapid filter-based method detecting high bacterial loads in 30 minutes, and a sensitive ELISA-like assay for low concentrations and binding analysis. These results highlight the potential of AMP–DNAzyme hybrids for fast, reliable bacterial diagnostics. Finally, molecular dynamics simulations helped clarify how structural properties affect detection efficiency.

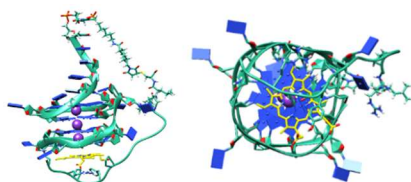


Figure 1. Conformation of AMP (Apidecin C) conjugated to G-rich sequences (AGRO100 G-quadruplex), during MD simulations obtained by the cluster analysis.

Acknowledgements. This work has been supported by the Croatian Science Foundation under the project number HRZZ IP-2022-10-9829 and by the European Union's Horizon 2020 research and innovation programme under grant agreement No. 952110.

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TOXICITY OF CARBAMATE HERBICIDES – IMPACT ON HUMAN

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Herbicides are a type of pesticide mostly considered as compounds with low- or non-toxicity. In general, research about the herbicide toxicity mechanisms has been underestimated because most herbicides act on weeds by mechanisms not found in humans and other mammals.^[1] Carbamates are compounds that have found applications in various fields such as medicine, agriculture, and chemical warfare agents.^[2] Derivates of carbamic acid, thiocarbamic acid and dithiocarbamic acid are used as carbamate herbicides to kill the weeds. Also, when used properly, they preserve and increase agricultural production.^[3] Unfortunately, in developing countries the lack of control of pesticides and its improper use by local agricultural practices induces highly toxic effects leading to the risk of severe toxicity and very often fatal consequences.^[4] Carbamates have low to moderate toxicity in rats and do not pose acute toxicity.^[5]

However, studies by Vidal et al. showed that carbamates cause reproductive and developmental toxicity in aquatic organisms *Daphnia spp.*^[6] Also, Pehar et al. have shown that herbicides can be effective cholinesterase inhibitors, and *in silico* prediction of physicochemical properties indicate their passage through the blood-brain barrier (BBB) and potential neurotoxic action in the brain.^[7] Hence, insufficient research on the toxicity of carbamate compounds raises questions about their harmful effects on the environment and human health.^[2]

A set of commercial carbamate herbicides collected from available *online* databases and literature sources was subjected to *in silico* analysis in order to evaluate their potential for causing different types of toxicity, calculate the physicochemical characteristic for their potential passage through the blood-brain barrier (BBB) and the potential for causing neurotoxicity.

In silico analysis will be used to screen potentially toxic carbamate herbicides for *in vitro* analysis. Furthermore, the results of the conducted study will bring new knowledge about the potential toxicity of carbamate herbicides and possible application in the design of a new and safe carbamate herbicides for human health and the environment.

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SHAPE MATTERS: THE ROLE OF GOLD NANOPARTICLE MORPHOLOGY IN SERS DETECTION OF G-QUADRUPLEX

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Surface-Enhanced Raman Scattering (SERS) spectroscopy is a sensitive technique that enhances Raman signal of molecules adsorbed on nanostructured metal surfaces, enabling the detection of low-concentration biomolecules.^[1] SERS is useful for investigating G-quadruplexes, non-canonical DNA structures formed by guanine-rich sequences, which are involved in crucial biological processes like telomere maintenance and gene regulation. Understanding their formation is important for studying diseases such as cancer.^[2] The enhancement of Raman signal depends on the size, shape, and arrangement of the metal substrate, with nanostars providing stronger field localization compared to nanospheres.^[3] However, choosing the optimal substrate for each analyte is essential for accurate detection.

In this study, gold nanospheres and nanostars were prepared, characterized and used to analyze the structural forms of the human telomeric sequence d[TTAGGG]₄ (Tel24), which forms a G-quadruplex in the presence of sodium ions. Near-infrared excitation at 785 nm enabled detection of structural transitions from the unfolded oligonucleotide to the G4 form, with distinct SERS signatures, particularly the bands associated with the breathing vibrations of adenine and guanine aromatic rings.^[4] The SERS efficiency of both gold substrates was compared.

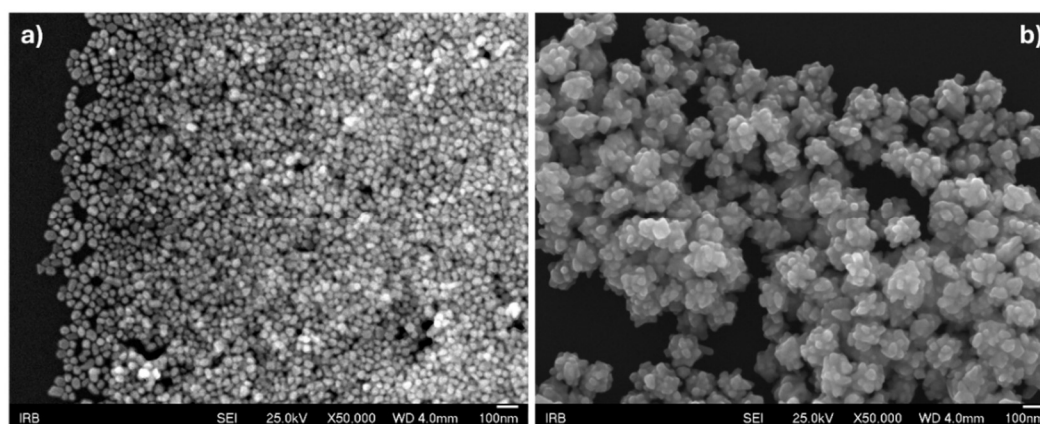


Figure 1. SEM pictures of a) gold nanospheres and b) branched gold nanostars.

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SYNTHESIS OF CHOLESTEROL DERIVATIVES OF MANNOSYLATED DESMURAMYL PEPTIDE

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Muramyl dipeptide (MDP, MurNAc-L-Ala-D-isoGln), desmuramyl peptide (DMP, L-Ala-D-isoGln) and their derivatives are well-known adjuvants.^[1] Our previous studies of DMP derivatives have shown that the introduction of lipophilic subunits, such as adamantan-1-yl, adamantan-1-ylethyl and C₁₂ alkyl chain, as well as mannosylation can significantly increase their *in vivo* adjuvant activity.^[2,3] The best site for the binding of the lipophilic subunits was the α -position of D-isoGln, to which the subunits were introduced via an amide bond. In addition, the introduction of a triazole ring between DMP and the lipophilic subunit increased the adjuvant activity of tested compounds.

In our recent work, we focused on the preparation of cholesterol derivatives of mannosylated DMPs linked to the α -position of D-isoGln directly or via a triazole subunit (Figure 1, subunits (a) and (b)). Herein we report the synthesis of novel mannosylated cholesterol derivatives of DMP linked to the same position of D-isoGln via a triethylene glycol linker or a triazole-triethylene glycol linker (Figure 1, subunits (c) and (d)). Design of these target molecules will determine the influence of the flexible linker and the triazole ring on the adjuvant activity. Prepared compounds will be tested *in vivo* in mouse model.

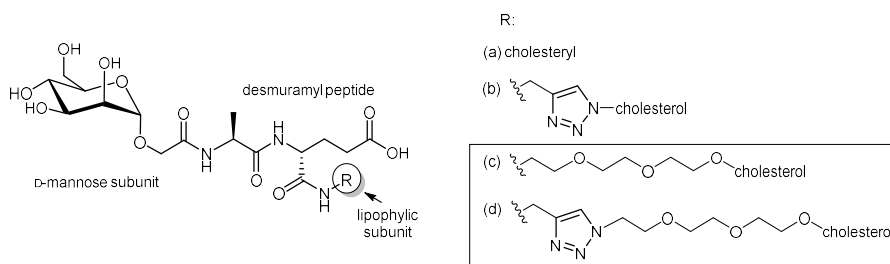


Figure 1. Novel cholesterol derivatives of mannosylated DMPs

Acknowledgements. This work has been supported by University of Zagreb Faculty of Science (institutional support 20286719) and UNIN-BIOMED-24-1-2.

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SUPRAMOLECULAR SELF-ASSEMBLED HEXACYANO-FERRATE(II)-BASED CHARGE-TRANSFER COMPLEXES

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Hexacyanoferrate(II) (HCF^{4-}) and related polycyanometallates have long been recognized as multiple electron donors. Their rigid octahedral geometry and ability to participate in extensive hydrogen bonding make them excellent platforms for assembling supramolecular multidimensional charge-transfer complexes (CTCs) with various organic electron acceptors. Among these, pyridinium oximes are intriguing due to their dual role as electron acceptors and hydrogen bond donors/acceptors. Recent studies showed that supramolecular association of pyridinium oximes and HCF^{4-} resulted in formation of CTCs with intricate stimuli-responsive optical properties revealed as reversible redox-active^[1] or redox-inert^[2] hydrochromic behavior. Despite their promising role in building functionalized materials, an understanding of how structural modifications within pyridinium oxime moiety affect the properties of self-assembled CTCs is still limited.

The present study addresses this gap by a comparative solid-state structural and spectroscopic study of novel HCF^{4-} -based pyridinium-oxime CTCs. Variations in the number and position of an oxime group on the pyridinium ring allowed us to elucidate the intricate relationship between their structural features and structural and optical properties of their HCF^{4-} -based charge-transfer complexes.

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PORPHYRIN-BASED AZO-BRIDGED POROUS ORGANIC POLYMERS: CO₂ CAPTURE AND CONVERSION TOWARDS SUSTAINABLE SOLUTIONS

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Porous organic polymers (POPs) are solids with crystalline or amorphous structure formed by covalently linked organic monomers. POPs show promise in gas storage, separation, and conversion, particularly in capturing and transforming carbon dioxide (CO₂).^[1] Using diverse building blocks allows the synthesis of POPs with specific characteristics. Incorporation of polar functional groups can increase the affinity of POPs for CO₂, while sterically hindering groups can generate more accessible adsorption sites. These modifications enhance POPs capacity to capture and convert CO₂ into high value molecules.^[2,3] Azo-bridged POPs have shown promise in CO₂ adsorption. It was found that incorporation of azo groups can improve interactions with CO₂ molecules, leading to enhanced CO₂ uptake and high CO₂/N₂ selectivity.^[4-6] In this study, we report the synthesis and characterization of a series of porphyrin-based azo-bridged POPs designed for enhanced CO₂ adsorption and catalytic conversion. The POPs were synthesized via condensation reaction of 5,10,15,20-tetrakis(4-nitrophenyl)-21*H*,23*H*-porphyrin (TNPP) and functionalized and sterically hindered aromatic diamines. The POPs were characterized using ¹³C CP/MAS NMR and IR spectroscopy, confirming their molecular structure. Powder X-ray diffraction (PXRD) analysis revealed that POPs exhibit amorphous characteristics. Additionally, the CO₂ adsorption capacity was evaluated, revealing a notable uptake of up to 49 mg g⁻¹ at 306 K. The POPs also demonstrated catalytic activity in the cycloaddition of CO₂ using phenyl glycidyl ether as model substrate, achieving conversion efficiencies of up to 69 %. This work underscores the potential of porphyrin-based azo-bridged POPs as platform for both CO₂ capture and catalytic transformation, contributing to sustainable carbon management strategies.

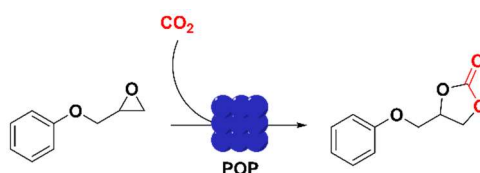


Figure 1. CO₂ conversion using POPs as catalysts.

Acknowledgements. This work has been fully supported by the Croatian Science Foundation under the project IP-2020-02-4467.

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THERMODYNAMIC INSIGHTS INTO THE CHELATE EFFECT; THE CALIX[4]ARENE CONFORMATION INFLUENCE ON CATION COMPLEXATION

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Calixarenes are probably the most widely used macrocyclic scaffolds for preparation of a range of ion receptors and binders of neutral species.^[1,2] These compounds can be relatively easily functionalized at both upper and lower rim, which allows the preparation of selective receptors in a range of media, including water.^[2–6] Among a variety of prepared calixarene derivatives functionalized at the lower rim those comprised of four subunits with carbonyl containing functionalities have been recognized as a particularly efficient hosts for alkali and alkaline-earth metal cations.^[2–6] Apart from the realization of multiple cation-ligand interactions, the complexes are often stabilized by the inclusion of a solvent molecule within the electron-rich ligand *basket*, whereby the solvent occasionally participates in cation coordination.^[2–6]

The presented work examines the calix[4]arene ketone derivative conformation influence on the binding of first and second group metal cations in acetonitrile and methanol. The carried-out thermodynamic, computational, and structural investigations, both in solution and in the solid state, offer a particularly rich account of the misplaced subunit influence on the calixarene hosting properties and the chelate effect in general.

Acknowledgments. This work has been supported by Croatian Science Foundation (IP-2024-05-3012) and the European Regional Development Fund (KK.01.1.1.02.0016).

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PHOTOACTIVE PHENYLBORONIC ACID DERIVATIVES: LIGHT-MODULATED ANTIPROLIFERATIVE ACTION OF AZOBENZENE BORONIC ACID ON BREAST CANCER CELLS

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Phenylboronic acid (PBA) and its derivatives have gained attention due to their unique chemical properties and biological potential, particularly in targeted cancer therapy. Their ability to selectively and reversibly bind to sialic acids on cell surfaces enables the development of novel therapeutic approaches.^[1] Among them, azobenzene-containing PBA derivatives offer a means of external control over biological activity through light activation. Previous studies have shown that PBA derivatives, particularly those incorporating azo moieties, demonstrate significant promise in biological activity, especially in combating antibiotic resistance and inhibiting HIV-1.^[2,3] The antiproliferative effects of two azobenzeneboronic acid derivatives and a control compound were assessed on triple-negative breast cancer (MDA-MB-231) cell lines using the MTT assay to determine cell viability in the dark and under light irradiation. We tested the influence of light activation on the antiproliferative potential of the tested compounds, which could support further exploration of photoactive PBA derivatives in light-controlled anticancer therapy.

Acknowledgements: This work is the result of the project “*Photoactive derivatives of phenylboronic acid: synthesis, interactions with sialic acids and biological activity*”, funded by the Adris Foundation, Croatia.

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TOTAL SYNTHESIS OF DISPYRROLOPYRIDINE A

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Since the 1950s, marine natural products have attracted considerable attention in the field of drug discovery because of their structural diversity and potent biological activities.^[1] Among them, nitrogen-containing heterocycles such as pyrrolopyridines, made up of fused pyridine and pyrrole rings, have been studied as bioisosteres of indole for their interesting chemical and biological properties and potential application in the fields of pharmacology and medicine.^[2] Recently, a newly discovered marine alkaloid dispyrrolopyridine A, from *Tenacibaculum discolor*, showed broad-spectrum activity against Gram-positive bacteria, fungi and nematodes.³

The main difficulty in the research of marine natural products for the development of new therapeutic agents has been the lack of material, which is most easily solved by total synthesis. Starting from the commercially available 6-bromo-1H-pyrrolo[3,2-b]pyridine, we have successfully prepared marine alkaloid dispyrrolopyridine A. Functionalisation of the starting compound was achieved by Suzuki coupling, lithiation and subsequent alkylation of the C2 carbon atom and on pyrrole and pyridine nitrogen atoms, Figure 1. Optimisation of these transformations enabled efficient synthesis of dispyrrolopyridine A, demonstrating a practical approach to accessing complex pyrrolopyridine structures.

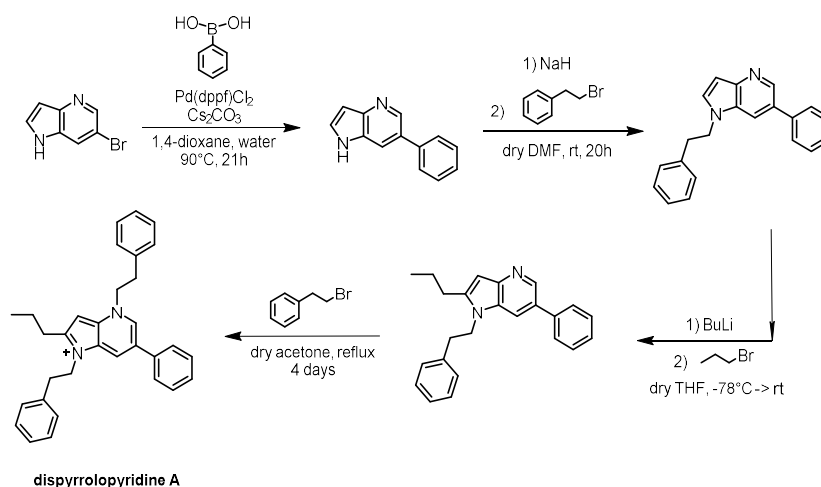


Figure 1. Synthesis of dispyrrolopyridine A from 6-bromo-1H-pyrrolo[3,2-b]pyridine.

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

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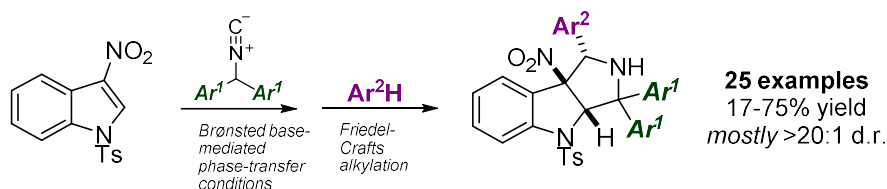
ONE-POT SYNTHESIS OF FUNCTIONALIZED PYRROLO[3,4-B]INDOLES VIA A TANDEM BARTON–ZARD AND FRIEDEL–CRAFTS APPROACH

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The Barton–Zard reaction provides a straightforward route to aromatic 2-carboxyl-3,4-disubstituted pyrroles via the reaction of electron-deficient alkenes, nitroarenes, or nitroindoles with α -isocyanoacetates under basic conditions.^[1] However, when α -substituted isocyanoacetates are employed, the typical rearomatization step is disrupted, leading instead to the formation of non-aromatic polycyclic structures – a transformation known as the interrupted Barton–Zard reaction.^[2] We hypothesized that α,α -diaryl-substituted methyleneisocyanides could participate in a similar interrupted process, enabling the *in situ* construction of densely functionalized hexahydropyrrolo[3,4-*b*]indole scaffolds. To date, only one example of such 3,3-diaryl-substituted polycyclic scaffolds has been documented, and solely as a postmodification.^[3] Herein, we report a novel telescoped sequence combining the interrupted Barton–Zard reaction with a Friedel–Crafts alkylation for the direct synthesis of aryl-substituted hexahydropyrrolo[3,4-*b*]indole scaffolds. Under Brønsted base-mediated phase-transfer conditions, 3-nitroindoles (**1a–p**) react with benzophenone-derived isocyanides (**2a–c**), forming pyrrolo[3,4-*b*]indole intermediates that undergo *in situ* alkylation with aromatic and heteroaromatic nucleophiles under acidic conditions (Scheme 1). This method delivers final products (**3–27**) in moderate to good yields, typically as single diastereomers.^[4]



Scheme 1. Developed telescoped reaction for the synthesis of polycyclic pyrrolo[3,4-*b*] indole scaffolds.

Acknowledgements. This work was supported by the Croatian Science Foundation under the project number IP-2022-10-5184.

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GREEN SYNTHESIS OF METAL NANOPARTICLES FOR INVESTIGATION OF THE COFFEE – RING EFFECT

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Green-synthesized nanoparticles demonstrate unique behaviors due to their functionalized surfaces, which affected inter-particle interactions and adhesion, altering the dynamics of the coffee-ring effect. The coffee-ring effect is a common phenomenon occurring during the evaporation of a liquid droplet containing suspended particles which leads to the accumulation of particles at the droplet's periphery. The coffee-ring effect was investigated in our preliminary studies utilizing several models that included the active substances pantoprazole and doxycycline, combined with excipients such as sodium chloride and 2-hydroxypropyl β -cyclodextrin, under various experimental conditions. Microscopic analysis was employed to identify characteristic patterns, with particular focus on the behavior of saline solutions. The collected data were systematically grouped into clusters. In the model incorporating pantoprazole and 2-hydroxypropyl β -cyclodextrin, interactions between the two components were detected and further examined through differential scanning calorimetry. This preliminary research supported the hypothesis that the coffee-ring effect can be effectively used to investigate the properties of soluble formulations. While traditionally viewed as a challenge for achieving uniform coatings, this effect has recently gained attention as a tool for innovative applications in materials science, offering new opportunities for controlled particle deposition and pattern formation. Therefore, the results of our study were collected with the aim to systematically analyze how green synthesized copper nanoparticles, solvate and solvent properties influence the distribution and deposition patterns during drop evaporation. Parameters of interest were firstly the size of nanoparticles, as smaller nanoparticles exhibit more uniform deposition patterns due to enhanced Brownian motion counteracting edge accumulation. Secondly, it was the possibility of surface modifications that can reduce particle aggregation, leading to more controlled ring formations, and thirdly the focus was on variations in solvent viscosity and evaporation rates that significantly influence the ring morphology, providing insights for optimizing coatings and printing technologies.

Acknowledgements. This work has been fully supported by the Croatian Science Foundation, project IP-2024-05-4339 entitled "Coffee ring' effect in 'Lab on a Chip' environments in the development of new drug formulations" leader prof. Ernest Meštrović.

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TUNING THE MAGNETISM IN COPPER(II) SYSTEMS: FROM DISCRETE COMPLEXES TO LOW-DIMENSIONAL HYBRID ORGANIC-INORGANIC MATERIALS

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Copper(II) coordination compounds are among the most extensively studied systems due to their diverse structural features and a rich assortment of inherent properties. These characteristics open avenues for potential applications in magnetism, optics, catalysis, and biomedicine.^[1,2] In recent years, significant advances have been made in the development of copper-based hybrid organic-inorganic materials, which are emerging as greener and more versatile alternatives to their lead-based counterparts,^[3] with magnetism as additional functionality.

To bridge the gap between discrete molecular systems and extended hybrid materials, we have synthesized a series of copper compounds based on 2-methoxyethylamine. Depending on the reaction conditions, we obtained discrete mononuclear complexes, as well as one- and two-dimensional hybrid structures. The structural features of all synthesized compounds were determined by single-crystal X-ray diffraction, and their magnetic behavior was studied over a wide temperature range. Each structural type exhibits distinct magnetic properties. For instance, both mononuclear copper(II) complexes exhibit antiferromagnetic chain behavior due to weak magnetic interaction along one crystallographic direction, while the one-dimensional hybrids display either ferromagnetic or antiferromagnetic spin-chain characteristics, depending on the choice of halide anion, with superexchange interaction between magnetic ions being stronger than in mononuclear complexes. The two-dimensional hybrid material shows a ferromagnetically ordered state below $T = 6.4$ K, with stronger ferromagnetic interactions within the layers and much weaker antiferromagnetic interactions occurring between the layers.

Acknowledgements. This work has been fully supported by the Croatian Science Foundation under the project number IP-2022-10-6321.

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SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF NEW NITRO(TRIAZOLE/IMIDAZOLE)-APPENDED QUINOLINES WITH POTENTIAL ANTITRYPANOSOMAL ACTIVITY

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Human African trypanosomiasis (HAT), commonly known as sleeping sickness, is a neglected tropical disease caused by the protozoan parasite, *Trypanosoma brucei*. Current treatment options are limited in their efficacy across different stages and subspecies of the parasite, drawing attention to develop more effective antitrypanosomal therapy.^[1–3] In this work, novel quinoline derivatives containing 3-nitrotriazole or 4-nitroimidazole connected by different 1,2,3-triazoline linkers are designed, synthesized and structurally characterized. The design of novel quinoline derivatives was focused on exploring diverse linker types, alongside modifications to nitro-substituted heterocycles, with the aim of identifying compounds exhibiting optimal biological activity. The synthesis of new derivatives was carried out by Huisgen 1,3-dipolar cycloaddition from previously synthesized alkynes and azides. Structurally suitable compounds were used as ligands in the subsequent synthesis of rhenium(I) tricarbonyl complexes to improve the physicochemical properties of compounds and increase their potency.

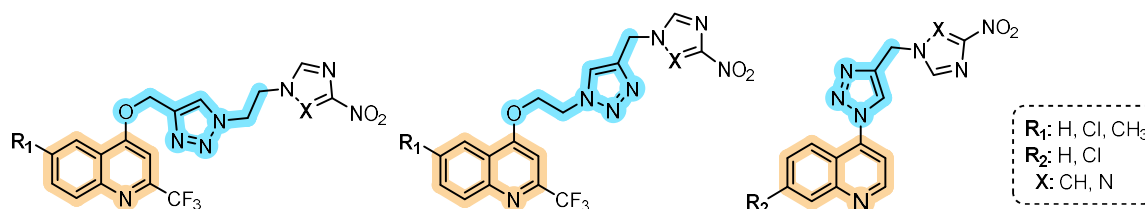


Figure 1. Structures of synthesized quinoline derivatives.

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

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NEW POTENTIOMETRIC SENSOR FOR ANIONIC SURFACTANTS

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Surfactants are organic molecules that lower surface tension. Nearly 60 % of the global surfactant market consists of anionic surfactants, which are widely used in cleaning and washing applications both at home and in industry.^[1] This widespread use contributes to the environmental release of surfactants. Classical methods for quantifying anionic surfactants are time-consuming, complicated, and require the use of toxic solvents. The newly developed potentiometric surfactant sensor for anionic surfactants is based on the innovative active molecule (Figure 1) 1,3-didecyl-2-methyl-1*H*-imidazol-3-ium tetrakis(perfluorophenyl)borate (DMI-TPFPB). DMI-TPFPB is incorporated into an organic matrix (PVC and plasticizer) to create the sensing membrane. To produce a fully functional sensor, the sensing membrane is integrated into the electrode body, which is filled with NaCl as the inner electrolyte. The performance of the DMI-TPFPB surfactant sensor was evaluated in terms of sensitivity, selectivity, response time, and stability. The sensor demonstrated high sensitivity to commonly used anionic surfactants. It showed a low limit of detections (up to 7×10^{-8} M) for selected anionic surfactants and exhibited excellent stability against common interfering anions, with a stable signal response across a broad pH range (2–9). The sensor was successfully applied in potentiometric titrations of anionic surfactants in both model and real environmental samples, achieving high recoveries (98 % to 99.5 %). These results demonstrate the potential of this potentiometric sensor for applications in environmental monitoring, water quality assessment, and industrial effluent analysis, offering a low-cost, simple, and practical solution for anionic surfactant monitoring.

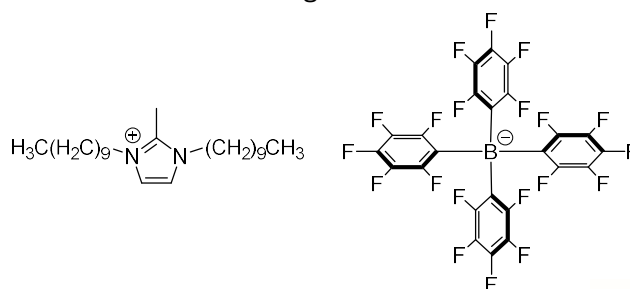


Figure 1. 1,3-didecyl-2-methyl-1*H*-imidazol-3-ium tetrakis(perfluorophenyl)borate.

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INFLUENCE OF ALKYL CHAIN LENGTH ON ANTIBACTERIAL AND ANTIFUNGAL ACTIVITIES OF VINYLIMIDAZOLIUM QUATERNARY AMMONIUM COMPOUNDS

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Modern society urgently needs new antimicrobials that provide broad antimicrobial protection. Due to their amphipathic structure, quaternary ammonium salts (QACs) have a mechanism of action similar to that of surfactants. They interact with microorganisms, reducing membrane permeability, interfering with cellular respiration and ATP synthesis, and leading to membrane rupture. Quaternization reactions of 1-vinylimidazole with alkyl halides were carried out with the alkyl chain length varying between 12 and 20 carbon atoms. The influence of the carbon chain length on antifungal and antibacterial activities was studied, and potent antimicrobial properties were demonstrated. The antibacterial efficacy of QACs generally increases with increasing alkyl chain length until a critical value.^[1] A cut-off effect is evident at chain lengths of 16 or 18 for the imidazolium cation, which is also confirmed by our studies. Among the tested compounds, 3-hexadecyl-1-vinyl-1*H*-imidazol-3-ium bromide exhibited the strongest antifungal effect against *Candida* species, while other compounds demonstrated notable activity against *Fusarium*, *Aspergillus*, and *Penicillium* species. Additionally, the investigated compounds showed potent antibacterial effects, particularly against *E. coli* and *S. aureus*, suggesting potential for broad-spectrum antimicrobial application. The bacteria used in testing imidazole surface active ionic liquid salts were Gram-positive bacteria (*S. aureus* and *B. subtilis*) and Gram-negative bacteria (*E. coli*, *K. pneumoniae*, and *P. aeruginosa*). 1-vinylimidazole compounds alkylated with an alkyl chain varying between 12 – 18 carbon atoms showed complete inhibition (MIC) against all tested Gram-negative bacteria. The findings highlight the need for further research on these surface-active chemicals, which possess antibacterial activity and also act as efficient antifungicides.

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DEVELOPMENT OF THE NEW MIP-BASED THIABENDAZOLE-SELECTIVE SENSOR

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Thiabendazole (TBZ) or 4-(1H-benzimidazol-2-yl)-1,3-thiazole is a widely used pesticide for preharvest and post-harvest protection of fruit and vegetables from fungal diseases and to minimize spoilage during storage and transport. The US Environmental Protection Agency (EPA) has classified TBZ as likely to be carcinogenic at doses high enough to disrupt the thyroid hormone balance.^[1] Also, it has been associated with nephrotoxic and hepatotoxic adverse effects.^[2] Considering its resistance to removal by washing and stability during food processing, its presence on food products is a matter of concern.^[3,4] Various analytical methods have been used to determine its concentration in different samples, but most of them are time-consuming, require costly instrumentation, and involve complex analytical procedures. Therefore, TBZ-selective potentiometric sensors present an excellent alternative due to their accuracy and simplicity.

The new potentiometric TBZ-selective sensor is an ion-selective electrode. Its membrane contains molecularly imprinted polymer (MIP) as sensor material. The content of the sensor material and the type of plasticizer were optimized to develop the sensor with the best response characteristics. The main aim of the sensor is to determine TBZ levels in fruit samples. All measurements were carried out using direct potentiometry. The new sensor showed excellent analytical performance.

Acknowledgements. This work has been supported by the internal project of the Department of Chemistry “Development of sensors for pesticide determination based on molecularly imprinted polymers”.

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VOLATILE AROMA COMPOUNDS OF TRADITIONAL CROATIAN CHEESE “PRGICA”

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Traditional products have specific characteristics that distinguish them from other similar products in the same category, due to the use of traditional ingredients, traditional production methods and/or processing methods. In recent years, interest in the consumption of traditional cheeses has increased, mainly because no additives are used in their production and they can have a beneficial impact on human health.^[1]

Prgica is a traditional cheese from the Bilogora-Podravina and Međimurje regions. It is made from fresh cow's milk, which is fermented for a few days and then strained through a thick cloth to remove the whey. Salt and ground sweet red paprika are added to the strained cheese. Once the ingredients are mixed, the cheese is shaped into a cone. The cheese is dried in the sun, at room temperature or by smoking, which gives the final product a different flavour.

The flavour of cheese, *i.e.* the combination of taste and odour, is one of the decisive criteria for consumer choice and acceptance. The concentration and composition of volatile compounds, often designated as aroma compounds, directly affect the flavour of the cheese.^[2] The objective of this research was to determine volatile compounds of „Prgica“ and relate them with aroma of this traditional cheese.

The volatile compounds were isolated by solid-phase microextraction (HS-SPME) using two fibers of different compositions (divinylbenzene/ carboxen/ polydimethylsiloxane (DVB/ CAR/ PDMS) fiber and polydimethylsiloxane/ divinylbenzene (PDMS/ DVB) fiber). Adsorption of the volatile compounds on the fibers was carried out for 40, 60 and 80 minutes. All samples were analysed by coupled gas chromatography-mass spectrometry system on a HP-5MS column, and the results were compared. A total of 33 volatiles were identified in the cheese samples. Alcohols and esters were the predominant groups of volatile compounds, with ethanol (29.84–35.64 %) and ethyl acetate (18.74–32.88 %) being the most abundant in all samples. The results showed that a longer adsorption time increases the number of identified compounds.

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DEGRADATION PROFILING AND *IN SILICO* TOXICITY ASSESSMENT OF LIFITEGRAST

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Lifitegrast (**LIF**) is a relatively new LFA-1 antagonist approved for the treatment of dry eye disease, known for its targeted mechanism of action and favourable safety profile.^[1] In this study, we aimed to investigate the oxidative stability of lifitegrast in solution and to elucidate its degradation behaviour under stress conditions. Three structural weak points were identified (Figure 1), leading to the formation of three degradation products (**DP1**, **DP2**, and **DP3**). These degradation products were structurally characterized using high-resolution mass spectrometry (HRMS), tandem mass spectrometry (MSⁿ), and nuclear magnetic resonance (NMR) spectroscopy. Structural elucidation of **DP3** proved particularly challenging due to its complex fragmentation and spectral patterns. Furthermore, **DP2** and **DP3** identified consistently across degradation studies were selected for *in silico* toxicity assessment. The predicted toxicity profiles of both impurities were comparable to or lower than that of the parent compound. These findings contribute to a better understanding of Lifitegrast's oxidative degradation pathway and support the qualification and risk assessment of active substance degradation in pharmaceutical formulations.

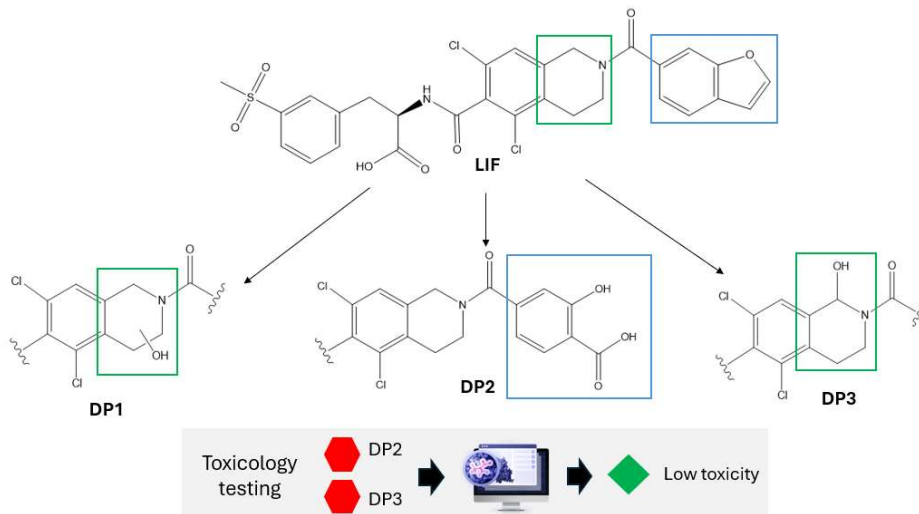


Figure 1. Analysis of degradation products **DP1**, **DP2**, and **DP3**, within this work.

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SELF-HEALING OIL ORGANOGELETS AS FAT SUBSTITUTES IN FOOD SPREADS

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Patent protected Low molecular weight organic gelators are molecules capable of forming unidirectional self-assembled aggregates, specifically through no-covalent interactions and they show remarkable gelation efficiency in vegetable oils, self-healing properties, and a long period of stability. The applicability of oil gelators is envisaged in food, cosmetics, and the pharmaceutical industry. Special emphasis was given to the potential applications of the examined oil gels as fat substitutes in food products. The regulations requiring the elimination of saturated fats and rising concerns among consumers health motivated us to investigate small organic molecules capable of efficiently transforming from liquid oil to a gel state.^[1,2]

The physical properties of the gels, in this study gelator 1, were analysed by oscillatory rheology. The gelators showed thixotropic properties in vegetable oils with a minimum gelation concentration of just 0.06 wt%. Further research was focused on the substitution of palm fats with gelled sunflower oil applied in cocoa spread at gelator concentrations of 0.06-1.0 wt%. The gelled cocoa spread with 0.06 wt% of gelator 1 showed storage modulus of 2859 Pa and a loss factor 0.32 while the gelled cocoa spread with 0.2 wt% of gelator 1 showed a storage modulus of 11245 and a loss factor 0.25. By changing the concentration of the gelator, it is possible to achieve the viscoelastic properties of gelled spreads comparable to those of spreads containing palm fat.

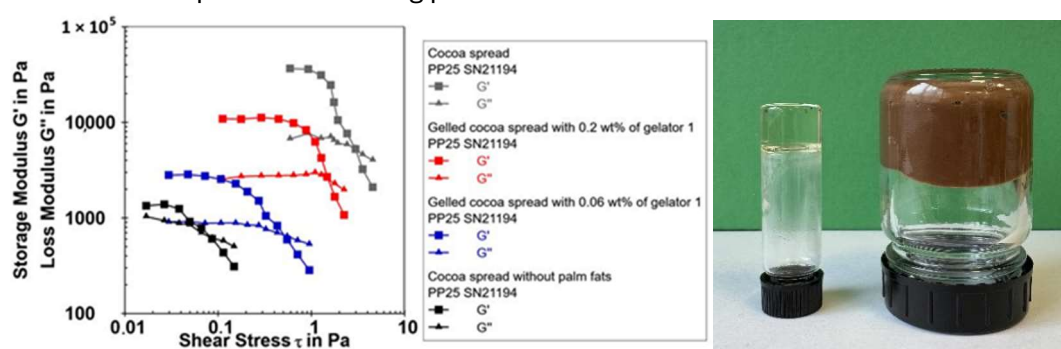


Figure 1. a) Amplitude sweep test of cocoa spread, gelled cocoa spread with 0.06 and 0.2 wt% of gelator 1, b) Gelled sunflower oil with gelator 1 and standard cocoa spread.

Acknowledgements. This work has been supported by the project *Support for technology transfer* under NPOO.C3.2.R3-I1.02.0018, PTT Project, “*Technology transfer of patented gelators in the food industry*” (TTG-FOOD)

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CONFORMATIONAL CONTROL AND FUNCTIONAL MODULATION OF PEPTIDES USING AMINOSHIKIMIC ACID

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Aminoshikimic acid, a stereochemically rich analogue of shikimic acid, is involved in the biosynthesis of aromatic amino acids in plants, bacteria and fungi.^[1] Due to its multiple stereogenic centres and diverse functional groups, it serves as a promising synthetic intermediate and alternative to shikimic acid for the production of oseltamivir phosphate (Tamiflu), a neuraminidase inhibitor used in the treatment of influenza.^[2] Despite its potential as a versatile γ -amino acid scaffold for the development of combinatorial libraries, its broader utility remains under-explored, primarily due to limited insight into the conformational and functional perturbations caused by its structural incorporation.

In this study, we report a high-yield, five-step synthesis of aminoshikimic acid and investigate its structural impact in peptide architectures. The hydroxyl-rich side chains of the compound allow easy derivatisation with biologically relevant components such as lipids, phosphates or fluorophores and thus fine-tuning of solubility, stability and bioavailability. Preliminary results indicate that the incorporation of amino acids gives rise to different secondary structures, which are probably determined by specific non-covalent interactions. Ongoing work is focussed on elucidating the structural determinants underlying these conformational effects.

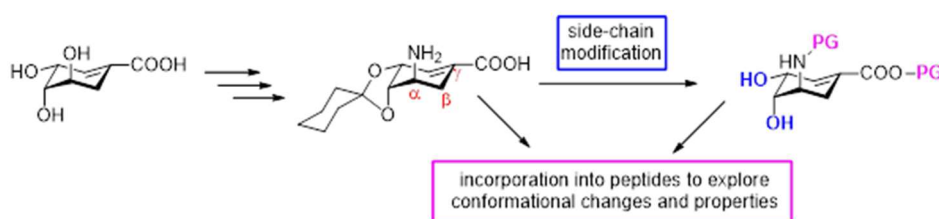


Figure 1. Aminoshikimic acid pathway

Incorporation of "3D structural diversity" into the design of peptidomimetics to cover the wide range of peptide secondary structures is of high interest, not only to medicinal chemistry, but also to other fields, such as materials science and catalyst design.

Acknowledgements. This work has been supported by the Croatian Science Foundation, Grant number 9617.

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BENZENE-1,3,5-TRICARBOXAMIDE SYSTEMS: HOST-GUEST INTERACTIONS, PHOTOSWITCHING, AND ION COORDINATION

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Benzene-1,3,5-tricarboxamide (BTA) derivatives are well-established and versatile building blocks in supramolecular chemistry, known for their capacity to form a range of non-covalent interactions, such as hydrogen bonds and π - π stacking.^[1] Acyl hydrazones, when introduced into such frameworks, bring additional functionalities. They are dynamic covalent units capable of reversible structural changes upon exposure to e.g. light,^[2] and may exhibit (non-)covalent binding of both cationic and anionic species^[3] with a potential to form discrete cage-like structures.

A series of chiral and achiral BTA derivatives were synthesized containing acyl-hydrazone groups (Figure 1). These compounds were studied to understand their supramolecular behavior and ion binding properties (e.g. transition and alkali metals, halide anions), both in solution and the solid state. A variety of analytical techniques—such as NMR, ATR-IR, MS, UV-Vis, CD, and SCXRD—were employed to fully characterize their structural and functional features. Titrations were performed to better understand the thermodynamics of the system and quantify interactions with ionic species. The ligands exhibited chemical exchange in 2D NOESY spectra, indicating the presence of different interchanging species, likely connected to supramolecular interactions within the system. Exposure to light of different wavelengths induced isomerization of the acyl-hydrazone units, affecting the ligands' ability to form supramolecular interactions as well ion coordination ability. These findings contribute to better understanding of stimuli-responsive coordination systems and supramolecular assemblies, with potential applications in ligand design and selective catalysis.

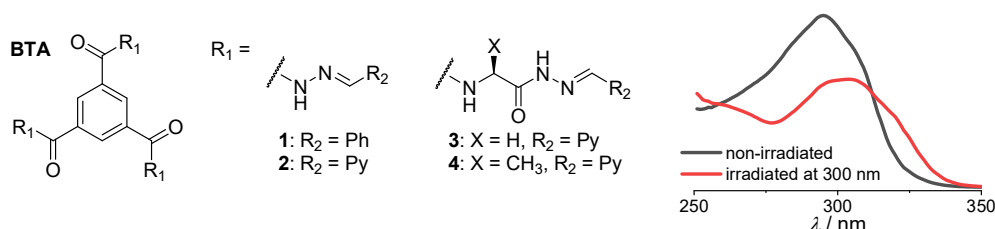


Figure 1. Prepared BTA derivatives and UV-Vis spectrum (DMSO) of compound **4**.

Acknowledgements. This work was supported by the Croatian Science Foundation under the project number IP-2022-10-8456, and by European Union under the NextGenerationEU Programme.

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SYNERGISTIC UV PHOTOCATALYSIS USING ZnO AND BIOMASS CARBON IN A HYDROGEL MATRIX

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Photocatalytic removal of organic pollutants from wastewater is recognized as a cost-efficient and environmentally friendly treatment approach. In this study, we developed ZnO-based hydrogels coated with a biomass-derived carbon nanocomposite, which demonstrated outstanding performance in degrading methylene blue (MB) dye under UV light exposure. The synthesized photocatalysts were thoroughly characterized using techniques such as Bragg–Brentano X-ray diffraction (BT-XRD), transmission electron microscopy (TEM), field emission scanning electron microscopy (FESEM), and UV–visible diffuse reflectance spectroscopy (UV-DRS).

Photocatalytic activity tests showed that the nanocomposite achieved approximately 97 % degradation of MB within 120 minutes—significantly surpassing the performance of pure ZnO. This enhanced efficiency is primarily attributed to the reduced electron–hole recombination rate and the narrowed bandgap, which are facilitated by the incorporation of conductive biomass carbon into the ZnO hydrogel matrix.

Acknowledgement- Special thanks to Central Instrumentation Facility (CIF), IIT BHU for providing instrumental facilities.

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STRUCTURAL FEATURES AND MAGNETIC PROPERTIES OF COPPER(II) HYDRAZONATO COMPLEXES

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A series of copper(II) nitrate complexes were synthesized using six structurally related hydrazone ligands bearing 2-pyridyl, 3-pyridyl and 2-pyrazyl functional groups. The isolated complexes were characterized in the solid state, and their thermal and magnetic properties investigated.

Depending on the selected ligand and reaction conditions, mononuclear complexes, 1D polynuclear chains and 3D polynuclear networks could be isolated, with the copper(II) metal center exhibiting four different coordination environments. Moreover, nitrate ion was observed as a monodentate terminal, bidentate terminal, bi- and tridentate bridging ligand, as well as a non-coordinated counterion. Lastly, the hydrazone ligand, usually found in enolato-imino tautomeric form, was in one case observed in keto-amido form and as a bridging pentadentate ligand, previously unreported of for hydrazone ligands (Figure 1).

Such rich structural landscape was complemented with a combination of relatively high thermal stability followed by explosive decomposition above 250–300 °C, as expected for nitrate salts/complexes. The measured magnetic properties of the compounds reflect the structural complexity and an interplay between short- and long range interactions. Prepared materials represent a „coordination playground“ with plentiful opportunities in material design and property fine-tuning.

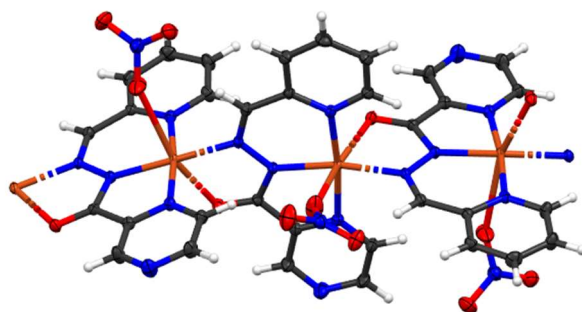


Figure 1. Cu(II) polymeric complex with pentadentate bridging hydrazone ligand

Acknowledgements. This work has been supported by Croatian Science Foundation, projects HRZZ-IP-2022-10-7368 and HRZZ-IP-2022-10-6321.

EFFICIENT CYCLIZATION OF FUNCTIONALIZED PEPTIDES via CHLORIDE TEMPLATING

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Cyclic peptides are an important class of bioactive compounds known for their enhanced metabolic stability, improved bioavailability, and superior selectivity toward biological targets compared to their linear counterparts. Despite these advantages, their synthesis remains a significant challenge due to low cyclization yields, conformational constraints, and side reactions. To address these issues, our group has developed a chloride-templated cyclization strategy in which chloride anions promote efficient head-to-tail cyclization through non-covalent interactions with backbone amides.^[1] In this study, we extend this methodology to tyrosine- and ornithine-based peptides, which feature bulky and polar side chains, respectively. Linear peptides were synthesized *via* solution-phase peptide synthesis using appropriate side-chain protecting groups and served as precursors for the preparation of cyclic tetra-, and pentapeptides using both solution-based and mechanochemical approaches. The mechanochemical method, previously established in our laboratory, overcomes limitations of classical solution-phase synthesis such as high dilution, long reaction times, and poor solubility.^[2] By applying both synthetic approaches to structurally diverse peptide sequences, we aim to demonstrate that chloride-assisted cyclization is a robust and versatile strategy suitable for a wide range of amino acid residues and side-chain protection patterns.

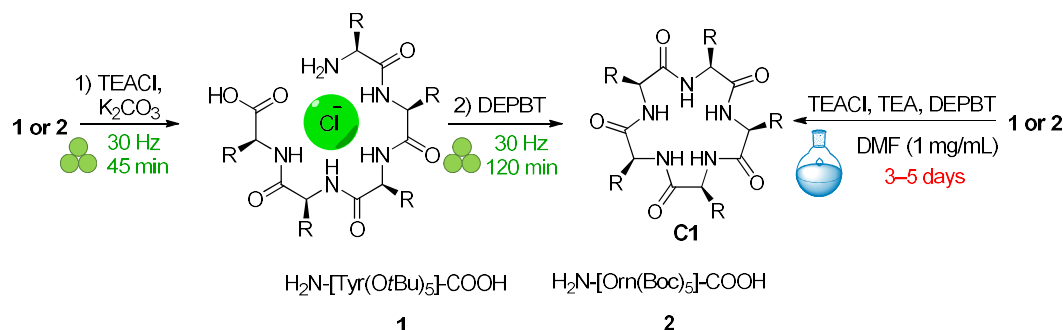


Figure 1. Synthesis of cyclic pentaornithine and pentatyrosine by solution-based and mechanochemical approach.

Acknowledgements. This work has been supported by the Croatian Science Foundation under the project IP-2024-05-5352

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ANTIOXIDANT CHARACTERIZATION OF SPICES AND AUTOCHTHONOUS DALMATIAN SPECIES BY ELECTROCHEMICAL AND SPECTROPHOTOMETRIC METHODS

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As part of a study on gallic acid oxidation, five carbon-based electrodes were developed to investigate their electrochemical performance. The dependence of the peak current on pH was investigated by cyclic voltammetry in phosphate buffer solutions with and without gallic acid on all electrodes. The single-walled carbon nanotube electrode (SWCNT/GCE) was selected as the simplest and most sensitive electrochemical sensor. A unique sensor was produced for the direct determination of total phenol content as gallic acid equivalent. The results show that the SWCNT/GCE sensor can significantly improve the oxidation signal and shift the peak potentials to less positive values. Under optimized conditions, the sensor showed an exceptionally linear response over the entire concentration range; $\Delta I = 0.280 \times c$, (sensitivity $0.280 \mu\text{A mol}^{-1} \text{dm}^3$), from 2×10^{-7} to $1 \times 10^{-4} \text{ mol dm}^{-3}$, with a detection limit of $1 \times 10^{-7} \text{ mol dm}^{-3}$. The constructed sensor exhibits good stability and repeatability. To validate the proposed method, aqueous extracts of lavender, immortelle, sage, nutmeg, cinnamon and cloves were prepared by microwave extraction. Total phenols were determined spectrophotometrically by the Folin–Ciocalte method and antioxidant capacity by the FRAP method. The FRAP/SWV ratio indicates that the proposed method is not suitable for the estimation of antioxidant capacity. The results obtained showed a very good agreement between the proposed and standard estimates of total phenols as SWV/FC ratio and indicate the possibility of using such a methodology for estimating total phenols in real samples as a standard method.

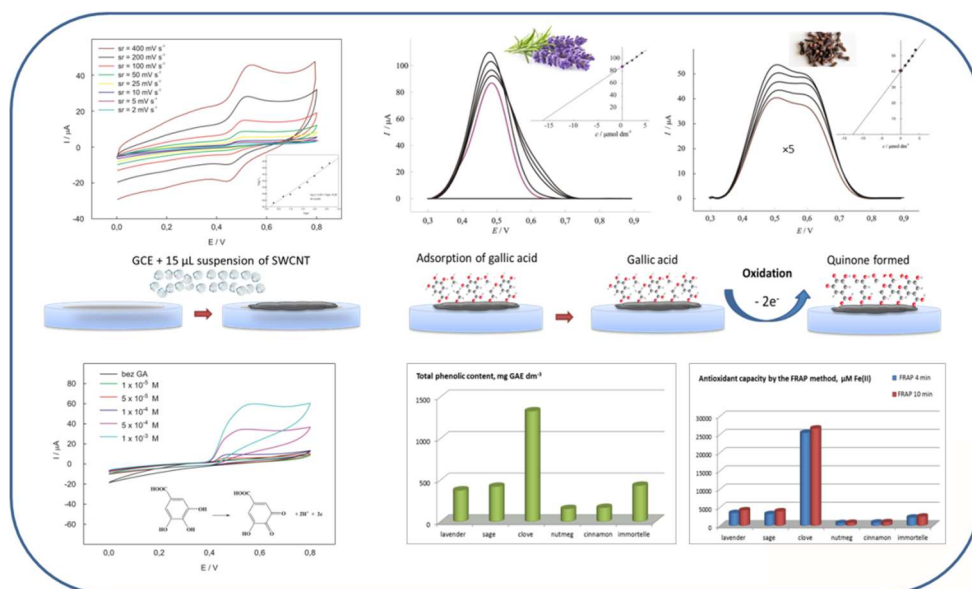


Figure 1. Electrochemical and spectrophotometric characterization of gallic acid (total phenolic) and antioxidant activity.

NOBLE METAL NANOSTRUCTURES AND CANNABINOIDS: A SYNERGISTIC APPROACH TO BIOACTIVITY

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Metal nanoclusters (NCs), such as Au, Ag, Pt, and Cu, have emerged as promising tools in biomedicine due to their ultra-small size, tunable fluorescence, and excellent biocompatibility. Alongside NCs, metal nanoparticles (NPs) are also widely explored for biomedical applications including bioimaging, sensing, drug delivery, and phototherapy. When stabilized with biomolecules like BSA, HSA, DNA, or HRP, these nanosystems offer enhanced functionality and specificity. In the NPOO DIK project, we investigated the synergistic interactions between noble metal nanoclusters, nanoparticles and cannabinoid compounds using UV/Vis and fluorescence spectroscopy. Techniques including fluorimetric titrations, time-resolved fluorescence, and UV/Vis spectroscopy are employed to study their physicochemical properties and interactions under physiological conditions.^[1–3]

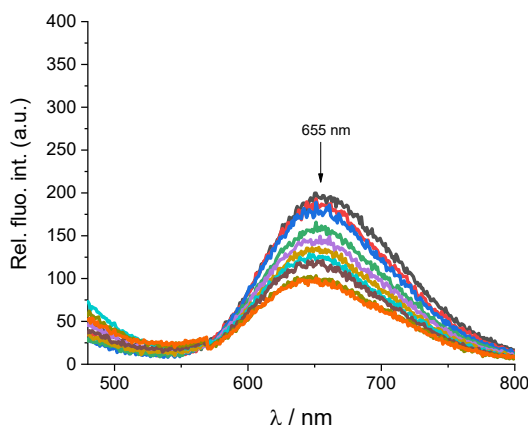


Figure 1. Changes in fluorescence spectrum of a **Noble metal nanocluster** upon titration with a **Cannabinoid** in aqueous media.

Acknowledgements. This work has been funded by the European Union – NextGenerationEU.

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EFFECT OF ADDITIVES ON THE STRUCTURAL PROPERTIES OF OLEOGELS

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Oleogels are composed of liquid oils—such as sunflower, soybean, or olive oil—and a gelator. Low molecular weight organic gelators are small molecules capable of forming unidirectional self-assembled aggregates through non-covalent interactions, which entangle into a three-dimensional fibrous network. Patent-protected LMOGs demonstrate high gelation efficiency in vegetable oils and emulsions, along with thermal and mechanical stability, self-healing ability, long-term stability, and controlled release of both hydrophilic and lipophilic compounds.^[1,2]

We report here a rheological study of three different additives: lecithin, vegetable fat, and crystallizing agent. The samples were prepared in different gelator to additive ratios for each added additive and the influence on the structural and viscoelastic properties of the gels was monitored. Storage modulus (G') values of the gels with the additives were in the range from 500 to 6800 Pa, and yield point values from 0.2 Pa to 3.6 Pa. An increase in the amount of vegetable fat leads to a decrease in storage modulus values while the addition of lecithin and crystallizing agent induces an increase of viscoelastic parameters. Considering the increase in yield point values and the decrease in $\tan\delta$, the gels containing the crystallizing agent exhibit the highest degree of structural organization. In 3ITT thixotropy test, 25 % of the original G' values were recovered in 1 to 8 minutes. On average, it takes approximately 30 minutes for the oleogels to recover their initial structure.

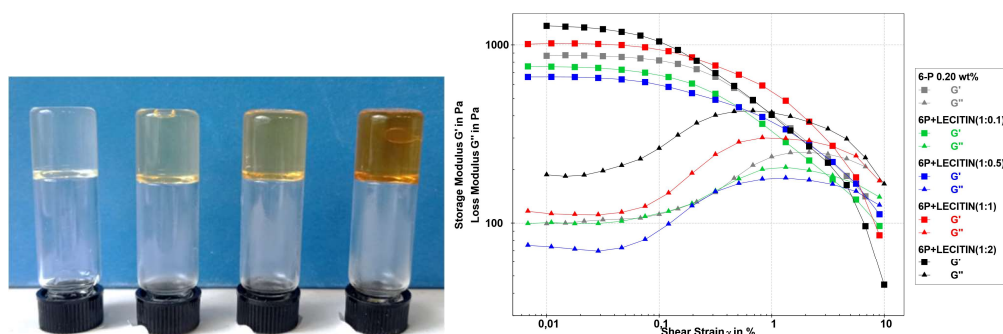


Figure 1. Visual observation and viscoelastic properties of 6P gels at different lecithin concentrations.

Acknowledgements. This work has been supported by the **Proof-of-Concept Project under NPOO.C3.2.R3-I1.05.0231: "Innovative Method for Replacing Palm Fat in Complex Food Matrices (INOFAFAT)"**

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AZITHROMYCIN SOLVATES: CORRELATING CRYSTAL STRUCTURE AND SURFACE PROPERTIES WITH TASTE PREDICTION

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Azithromycin is a clinically significant macrolide antibiotic, yet its intense bitterness—due to interactions between its crystal surfaces and taste receptors—poses a substantial barrier to the development of palatable oral formulations, particularly for pediatric patients. In this study, a series of crystalline solvates of azithromycin was examined, each incorporating water and one of four organic solvents: cyclohexane, 1,4-dioxane, tetrahydrofuran (THF), or methyl tert-butyl ether (MTBE).

To characterize these forms, single-crystal X-ray diffraction was utilized, revealing solvent-specific inclusion patterns, unique hydrogen-bonding arrangements, and distinct molecular packing motifs. To understand how these structural differences influence surface properties, we analyzed the identity and distribution of functional groups exposed on the crystal surfaces that may participate in receptor binding. Crystal growth habits were predicted using the Morphology module in Mercury, employing the Bravais–Friedel–Donnay–Harker (BFDH) model to identify the most prominent crystal faces. These predictions enabled us to infer the anisotropic display of surface chemical functionalities, as well as assess surface polarity and wettability.

The findings establish a clear link between crystal structure and surface characteristics, indicating that solvent incorporation and packing geometry can significantly influence taste perception. This work offers a foundation for the rational design of taste-masked azithromycin formulations through informed solid-form selection during early-stage drug development.^[1]

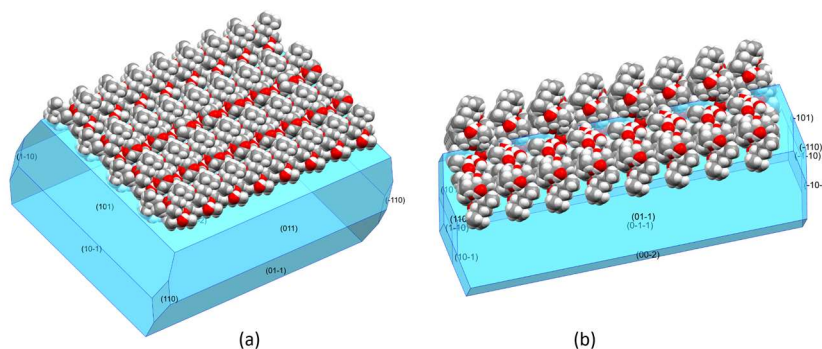


Figure 1. Predicted crystal morphology of azithromycin cyclohexane monohydrate, highlighting the dominant crystal faces (002) (a) and (011) (b) calculated by the BFDH method.

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

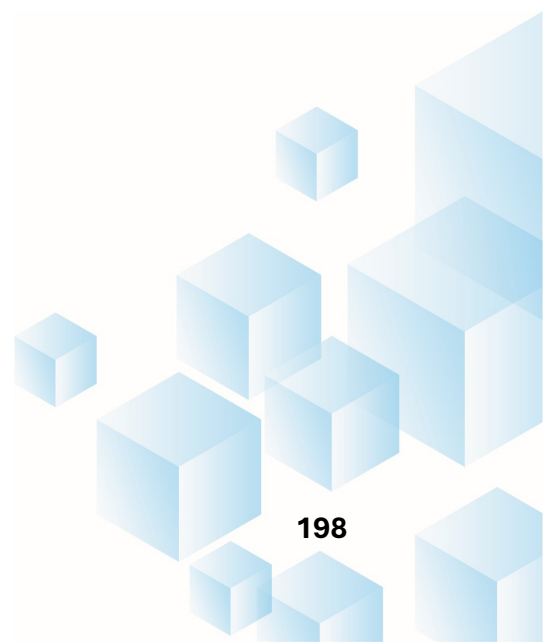
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POSTERS

CHEMICAL ENGINEERING AND BIOTECHNOLOGY





EVALUATION OF VARIOUS SCALE-UP CRITERIA FOR CERITINIB SPHERICAL CRYSTALLIZATION

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Spherical crystallization is a process that involves the simultaneous crystallization of an active pharmaceutical ingredient (API) and its agglomeration into spherical particles, resulting in particles with improved granulometric properties.^[1] Although spherical crystallization reduces the number of steps in the production of APIs and yields particles that are more favorable for tableting, the optimization and scale-up of this process are demanding and time-consuming. Namely, there are several scale-up criteria for mixing of suspensions, such as maintaining constant power per unit volume or Reynolds number, or using the Zwietering's equation for the minimum suspension mixing rate, but due to the complexity of the spherical crystallization process, a scale-up with a precisely defined criterion is difficult to implement.^[1,2] In this research, a combined method of spherical agglomeration and quasi-emulsion solvent diffusion was selected for the spherical crystallization of ceritinib, a drug used to treat non-small cell lung cancer. All experiments were conducted in a system consisting of tetrahydrofuran (solvent), water with 1 wt.% polyvinylpyrrolidone (antisolvent and additive), and heptane (bridging liquid) with solvent fractions of 14.0%, 77.5%, and 8.5%, respectively. For the scale-up of the process, double-jacketed batch crystallizers of 0.1 L and 1 L were used, along with two types of impellers which cause different flows in the crystallizer (a propeller and a turbine with six blades inclined at a 90° angle). Due to the complexity of the system, which evolves over time from a mixture of solvents into a suspension with varying particle size distributions, three different scale-up criteria were used, the visual just dispersed criterion, the visual just suspended criterion, and Zwietering's equation. The obtained particles were characterized by light and SEM microscopy, their particle size distributions were compared, and the roundness of the crystals was analyzed by image analysis in ImageJ software.

Acknowledgements. This research is funded by European Structural and Investment Funds, grant number KK.01.1.1.07.0017 (CrystAPC – Crystallization Advanced Process Control).

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DEVELOPMENT OF DEEP EUTECTIC SOLVENTS WITH ADJUSTABLE PROPERTIES FOR SUSTAINABLE ENZYMATIC PROCESSES

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The quest for sustainable and efficient biocatalytic processes has led to research into alternative solvents that can improve the stability and activity of enzymes. Deep eutectic solvents (DESs) formed by the combination of hydrogen bond acceptors (HBA) and hydrogen bond donors (HBD) have emerged as promising candidates due to their adjustable physicochemical properties, biodegradability and low toxicity. These solvents provide a versatile platform for customizing solvent environments to meet specific enzymatic requirements and overcome the limitations associated with traditional aqueous or organic systems. In the context of enzymatic reactions, factors such as the pH, viscosity, density and polarity of the solvent can significantly influence the performance of the enzymes. The aim of this study is to synthesize and characterize a series of DESs with different physicochemical properties to evaluate their suitability as media for enzymatic reactions (Figure 1). By understanding how different DES compositions affect key solvent properties, formulations that provide optimal environments for enzyme stability and activity can be identified. Such insights are essential for advancing the application of DES in biocatalysis and developing more sustainable and efficient bioprocesses.

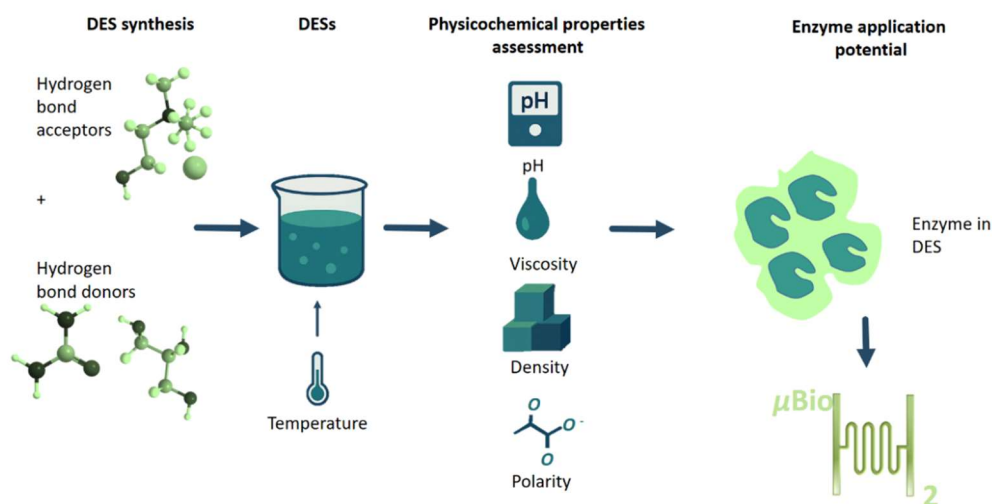


Figure 1. Strategic synthesis and comprehensive characterization of deep eutectic solvents for sustainable biocatalysis

Acknowledgements. This research was funded by Croatian Science Foundation (HrZZ), grant number IP-2022-10-2175 and DOK-NPOO-2023-10-3890.

INTEGRATION OF COMPUTATIONAL MODELLING AND EXPERIMENTAL VALIDATION TO IMPROVE THE STABILITY OF GDH AND HYDROGENASE IN DES-BASED SYSTEMS

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The stability and activity of enzymes are critical parameters in biocatalytic processes, especially for applications in sustainable energy production. This study investigates the use of deep eutectic solvents (DESs) to improve the stability and activity of glucose dehydrogenase (GDH) and hydrogenase enzymes (Figure 1). A comprehensive analysis of 37 DESs was performed, investigating their physicochemical properties such as pH, density, polarity and viscosity, as well as their effects on enzyme performance. Molecular descriptors, including σ -profiles obtained using COSMOtherm software, were used to characterize each DES. While there is limited specific data on the stability of GDH and hydrogenase in DESs, the favourable environment provided by certain DES formulations suggests potential benefits to their activity and stability. To predict and optimize enzyme performance, both linear regression and artificial neural network (ANN) models were developed to correlate DES properties with enzyme activity and stability. Validation of the optimized DES formulations in independent batch extractions showed improved enzyme stability and activity. This research highlights the potential of integrating computational modelling with experimental validation to optimize DES-based ATPS for enzyme stabilization and provides a sustainable and efficient approach for industrial biocatalytic applications.

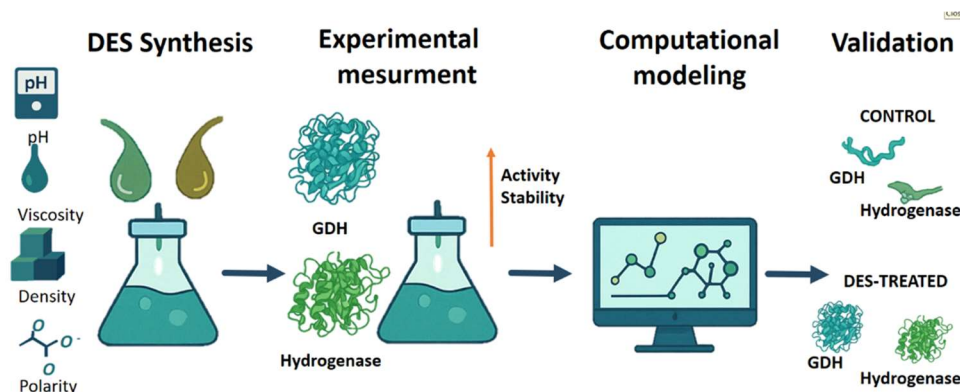


Figure 1. Integrated workflow to improve the stability of enzymes in DES-based systems by computational and experimental approaches

Acknowledgements. This research was funded by Croatian Science Foundation (HrZZ), grant number IP-2022-10-2175 and DOK-NPOO-2023-10-3890.

SALINITY-DEPENDENT CORROSION PROPERTIES OF COPPER IN SEAWATER

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Copper is widely used in industry and comes into contact with various aggressive media that can significantly impair its properties and durability. The corrosion behavior of copper depends strongly on the composition of the electrolyte that comes into contact with the metal surface.^[1,2] The corrosion properties of copper in different seawater, i.e. brackish water, natural seawater and seawater bittern, were studied using electrochemical techniques, and the specimens' surface was examined using an optical microscope and SEM/EDS. The study was conducted under the influence of seawater movement at 15, 25, and 35 °C to simulate the natural movement of seawater (Figure 1). All three seawater samples have different salinity and other parameters such as total dissolved solids, resistivity, conductivity, pH and corrosion rate. An increase temperature significantly increases the corrosion current density and decreases the polarization resistance, while its effect on the corrosion potential is almost negligible. The lowest polarization resistance value ($1.282 \text{ k}\Omega \text{ cm}^2$) was obtained at a temperature of 35 °C in seawater bittern, indicating a stronger corrosion of copper. The surface of the copper was analyzed by optical microscopy and SEM/EDS analysis after the electrochemical tests. The results showed that seawater bittern is the most aggressive medium for copper, which can cause significant corrosion damage to the material.

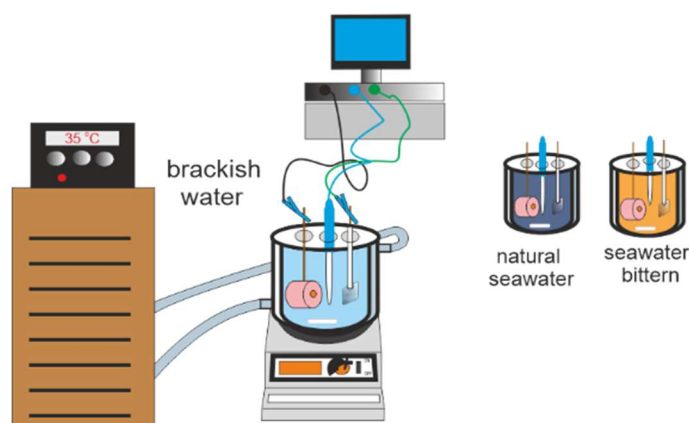


Figure 1. Schematic diagram of experiment.

Acknowledgements. This work has been supported by Croatian Academy of Sciences and Arts (CASA) under the project “Testing the corrosion behaviour of copper and steel and their alloys in seawater of different salinities”.

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OPTIMIZATION OF THE ACTIVATING AGENTS IN THE IMMOBILIZATION OF LACCASE ON MESOPOROUS SILICA AND MAGNETIC NANOPARTICLES

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Pharmaceutical residues in the aquatic environment are a growing problem worldwide, as conventional wastewater treatment processes are often unable to completely remove these persistent contaminants. Laccases – oxidative enzymes produced by fungi and bacteria – have shown promise in degrading a wide range of pharmaceutical compounds, including antibiotics, analgesics and hormones, through environmentally friendly catalytic processes.^[1]

However, the practical application of free laccase is limited by its low stability and sensitivity to wastewater constituents and lack of reusability, which hinders its use on a large scale. Immobilization of laccase on suitable supports has proven to be an effective strategy to overcome these problems. Immobilized laccases exhibit higher stability, a wider pH and temperature range, better reusability, and retain significant activity even after multiple cycles and prolonged storage.^[2]

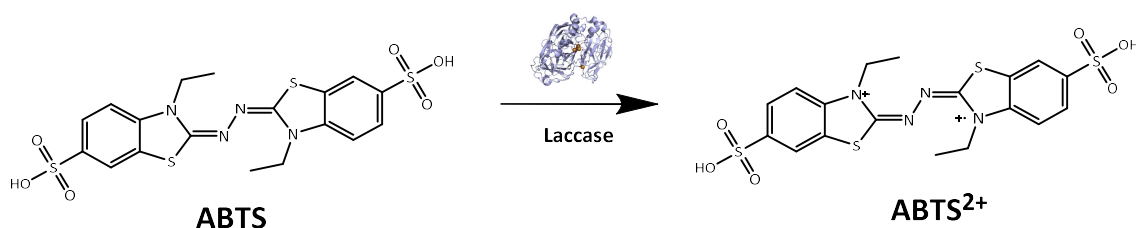


Figure 1. Oxidation of ABTS by laccase.

In this work, the covalent immobilization of laccase on mesoporous silica and magnetic nanoparticles was performed. Both supports were first functionalized with (3-aminopropyl) triethoxysilane (APTES) and then two different activating agents (benzoquinone and glutaraldehyde) in four different concentrations were tested for the covalent binding of the enzyme to the support. The immobilization yield was calculated using the Bradford assay, and the obtained activity of the immobilized laccase was compared with that of the free enzyme in the reaction of 2,2'-azino-bis (3-ethylbenzothiazoline-6-sulfonic acid) (ABTS) oxidation (Fig. 1).

Acknowledgements. This research was funded by Croatian Ministry of science and education in the frame of Croatian-Slovenian bilateral project “Enzyme immobilization and their application in chemical synthesis and wastewater treatment”.

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CHARACTERIZATION OF GINGER AND TURMERIC EXTRACTS

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Essential oils have long been valued for both practical and cultural reasons and are increasingly used in areas such as pharmaceuticals, food and cosmetics due to their complex composition and bioactivity. This work investigates the chemical composition and antimicrobial potential of essential oils extracted from the rhizomes of *Zingiber officinale* (ginger) and *Curcuma longa* (turmeric), focusing on how different extraction conditions affect yield and composition. Samples were extracted using different techniques, including hydrodistillation, Soxhlet extraction, maceration, ultrasound-assisted extraction and magnetic stirring, taking into account different drying and solvent conditions. Quantitative and qualitative analysis was carried out using thin-layer chromatography, gas chromatography–mass spectrometry, Fourier transform infrared spectroscopy and UV-Vis spectrophotometry. To assess the bioactivity, the antimicrobial effects of the extracts against *Bacillus subtilis*, *Pseudomonas aeruginosa*, *Staphylococcus aureus*, *Escherichia coli* and *Candida lipolytica* were evaluated by disk diffusion testing. Air drying resulted in the highest yields of essential oils for both plants, emphasizing the role of drying conditions. Ginger extracts were rich in α -zingiberene, while turmeric contained mainly turmerones. On the other hand, turmeric showed broad antimicrobial activity, while ginger was mainly effective against *B. subtilis* and *C. lipolytica*. The results suggest that extraction conditions significantly influence not only the chemical composition but also the functional potential of essential oils from plants. These findings contribute to a broader understanding of how natural products can be adapted for various practical applications, including but not limited to antimicrobial use.

THE INFLUENCE OF INTRAPHASE DIFFUSION ON THE OXIDATION OF TOLUENE OVER MANGANESE-BASED OXIDE – A COMPREHENSIVE THEORETICAL AND EXPERIMENTAL STUDY

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Mathematical models of varying complexity can be used for modelling of fixed-bed reactors, as described in the excellent textbooks and reviews on chemical reaction engineering.^[1,2] This is a consequence of the complex interactions of transport phenomena (heat and mass transfer and flow field) with the reaction kinetics. In addition to different industrial applications, fixed bed reactors also play a key role in environmental catalysis, e.g. in the catalytic oxidation of CO and volatile organic compounds (VOCs). The paper presents a detailed investigation of the influence of intraphase diffusion on the oxidation of the aromatic compound toluene on mixed manganese oxide, MnFeO_x, under isothermal operating conditions and with negligible resistance to interphase mass transfer. For this purpose, two mathematical models were developed, i.e. a one-dimensional (1D) pseudohomogeneous model and a one-dimensional (1D) heterogeneous model, and compared with experimental results. The procedure for numerically solving the equations of the proposed models is described in detail, with particular emphasis on the relevance of the 1D heterogeneous model. Detailed procedure of the MnFeO_x catalyst preparation has been described elsewhere.^[3] Catalytic tests were performed in an integral up-flow fixed-bed reactor operating at atmospheric pressure and under ideal flow conditions. Reaction was carried out at different total flow rates of the reaction mixture (23-138 cm³/min) over a constant amount of catalyst (0.05 g), constant inlet concentration of toluene (242 ppm of toluene/nitrogen), and in the temperature range of from 373 to 673 K using synthetic air as an oxidant. Two particle size fractions of the MnFeO_x catalyst were used: 0.315–0.400 mm and 0.500–0.650 mm. The catalytic activity was evaluated in terms of the recorded steady-state toluene conversion by measuring its concentration in the inlet and the outlet reaction stream using a Shimadzu GC-2014 gas chromatography system equipped with Carbowax 20M packed column (250/177 mm) and a flame ionization detector (FID). Although it was found that both models describe the studied experimental system quite well, the importance of the 1D heterogeneous model is especially emphasized, as it provides better insight into the behavior of the system by determining the relationship between the rate of the chemical reaction and the rate of intraphase diffusion.

Acknowledgements. This work has been supported by the Croatian Science Foundation under the project IN-PhotoCat (IP-2018-01-8669).

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AI-DRIVEN MODELING FOR QUALITY OPTIMISATION OF THE WASTEWATER TREATMENT PLANT'S OUTPUT STREAM

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The dynamics and complexity of wastewater treatment processes (WWTP) require advanced computational tools to optimise processes, ensure compliance and increase efficiency.

Numerous deterministic, stochastic and time series models have been developed to predict the efficient operation of WWTPs.

In this work, a data-driven approach was used that utilises the monitoring data of the physical, chemical and biological parameters of the wastewater treatment plant. The Automatic Network Designer tool in the Statistica software was implemented to automate the selection of optimal Artificial Neural Network (ANN) architectures and simplify the testing of different network configurations.

The results showed that the selected ANNs can estimate the quality of wastewater, expressed as COD values, with high accuracy. Their suitability for modelling non-linear processes and numerous parameter interactions in wastewater treatment processes was confirmed. This work underlines the potential of AI in environmental engineering and provides a reproducible template for the optimisation of wastewater treatment processes.

THE MOLD BATTLE: TRADITIONAL AND CONVENTIONAL APPLE CULTIVARS VS *Penicillium expansum*

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Approximately 50 % of global fruit losses are caused by mycotoxigenic foodborne fungi, mainly by *Penicillium expansum*. Apart from the fact that the contamination with *P. expansum* affects economic losses, it also leads to the production of the mycotoxin patulin which negatively affect food safety and human health.^[1] Accordingly, attention is drawn to traditional apple cultivars, which contain higher amounts of polyphenolic compounds and increased antioxidant activity. Polyphenols are the bearers of apple resistance to plant diseases and various abiotic stressors. Traditional apple cultivars have shown great potential for *P. expansum* infection resistance due to higher levels of polyphenols. Based on that, the resistance of traditional apple cultivars (‘Kanadska Reneta’, ‘Božićnica’, and ‘Winter Banane’) to infection by *P. expansum* was performed and compared with the resistance of conventional ones (‘Idared’, ‘Fuji’ and ‘Golden Delicious’) after harvesting. Furthermore, the total polyphenol and flavonoid content was compared as well as patulin content and antioxidant activity. Also, each apple cultivar was analysed by HPLC for the purpose of polyphenol profile determination. Results showed that traditional apple cultivars had higher content of total polyphenols, flavonoids and antioxidant activity than conventional ones. Moreover, patulin was detected only in ‘Winter Banane’ (16 µg/kg) and ‘Idared’ (327 µg/kg). These findings suggest that polyphenols play a crucial role in enhancing apple resistance to fungal infection and inhibiting patulin biosynthesis.

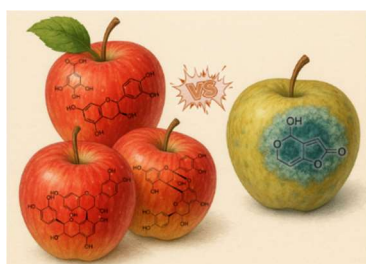


Figure 1. Natural defenders’ agents *Penicillium expansum*; polyphenols

Acknowledgements. This research has been supported by Croatian Science Foundation under the project ‘The possibility of exploiting traditional apple cultivars for the production of apples and apple juice with the reduced patulin content’ (UIP-2020-02-8461).

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IMPACT OF C-RATE ON BATTERY FORMATION AND SOLID ELECTROLYTE INTERPHASE LAYER DEVELOPMENT

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The formation process in lithium-ion batteries is a critical stage during which the solid electrolyte interphase (SEI) is established on the anode surface, having a major influence on electrochemical performance, cycle life and battery safety. Materials that are most commonly and commercially used are LiFePO₄ (LFP) as a cathode material, with a theoretical capacity of 170 mAh/g, and graphite as an anode material, with a somewhat higher theoretical capacity of 372 mAh/g. In reality, these materials don't always reach their full theoretical capacities. LFP typically gets close – around 95–99 %, while graphite might only go about 85–92 %, especially in early cycles, due to lithium consumption during the development and formation of the SEI layer. For that reason, the C-rate plays an important role in battery forming because it has an undeniable effect on irreversible capacity loss, voltage profile and cycle life, but also affects the quality of the SEI layer. Because it protects the anode, prevents lithium loss, and controls long-term stability while minimizing side reactions and ensuring battery safety, the SEI layer can reduce impedance growth if it forms properly during the first cycles. This study investigates the impact of various C-rates on overall cell behavior during the initial formation of LFP-graphite cells, as well as forming an anodic SEI layer. Cells were investigated at the following C rates: C/1, C/2, and C/10, to assess how the formation speed affects SEI stability and forming, as well as internal resistance. Electrochemical techniques like electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV), were employed both before and after the formation cycles to evaluate changes in charge transfer resistance and SEI stability.

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

OPTIMISATION OF THE IMIDACLOPRID PHOTODEGRADATION IN A ROTATING PHOTOREACTOR USING THE RESPONSE SURFACE METHODOLOGY

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In this work, an advanced design of a photoreactor is applied, which was invented considering the basic methodology of process intensification. An example of such a reactor is a rotating photoreactor in batch mode, which includes recirculation of the reaction mixture. Four identical 15 W UV-A lamps were used as an external source for photo-induced excitation of the photocatalyst, and titanium dioxide TiO_2 was used as a photocatalyst. In the work, special attention is paid to the application of the methodology of experimental design and analysis of the obtained process variables. The aim of this work is to study and optimise the process of photochemical degradation of imidacloprid in a rotating photoreactor using the response surface area method, thus contributing to the development of more efficient technologies for removing pesticides from aquatic systems and reducing their harmful effects on the environment.

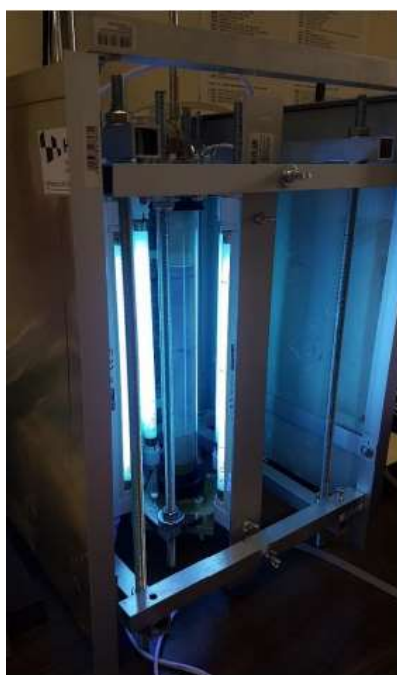


Figure 1. Rotating photoreactor.

Acknowledgements. This work has been supported by Croatian Science Foundation under the project IN-PhotoCat (IP-2018-01-8669).

PREDICTION AND CORRELATION OF WATER ACTIVITY USING THE COSMO-RS, WILSON AND REDLICH-KISTER MODELS IN DEEP EUTECTIC SYSTEMS (DES)

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The addition of water to nonaqueous deep eutectic solvents (DES) has developed into a common procedure for widening their application potential, in particular in terms of decreasing their viscosity. However, one must keep in mind that adding water may affect all the other properties and – in the high water concentration limit – even destroy the very nature of DES by turning it into dilute aqueous solution of DES components. Thereby the effect of water on all those properties of real solvents is dependent – just like for simple solvents – not on the amount or concentration of water but on the activity as the appropriate concentration variable. In this study, the activity of water was measured in aqueous solutions of six DES-forming components: betaine, urea, choline chloride, glucose, citric acid, and glycerol, as well as in eight DES systems prepared from those components. These data are presented for the first time for some systems. The experimental data were compared with the COSMO-RS model predictions. In addition, they were correlated by the Wilson and Redlich-Kister activity coefficient models. The advantages and drawbacks of various models are presented in light of the limited experimental dataset and the possibilities for further improvements are discussed.

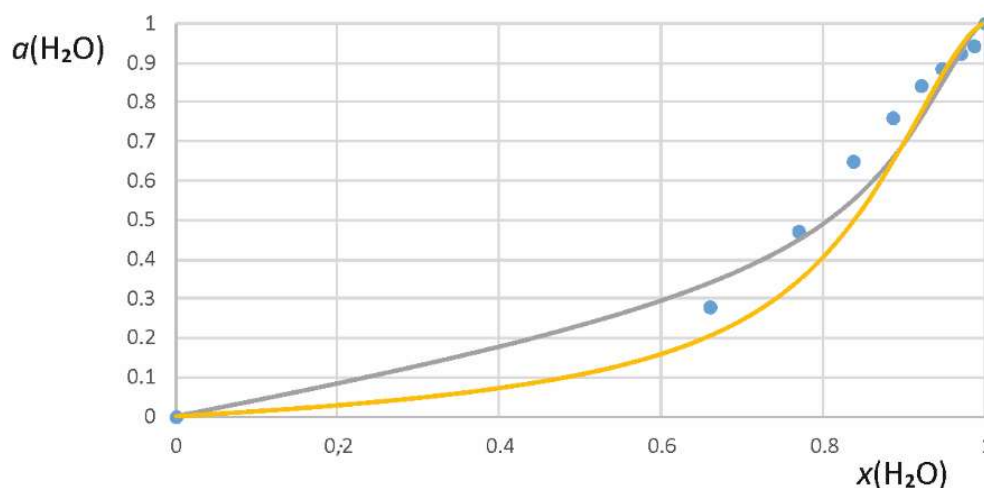



Figure 1. Activity of water as a function of its molar fraction in choline chloride solutions: symbols – experimental data, lines – COSMO-RS model predictions (gray and yellow line for the solute as a “molecular” moiety and as two distinct ions, respectively)

Acknowledgements. This work was supported by the Croatian Science Foundation (IPS-2022-02-3938 and IP-2024-05-9948).

INVESTIGATION OF REACTION KINETICS OF TWO PIPERAZATE SYNTHASES



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Non-proteinogenic amino acids are important building blocks of both microbial natural products and pharmaceuticals. The number of non-proteinogenic amino acids greatly exceed the number of proteinogenic amino acids^[1]. An example of a non-proteinogenic amino that is found in a large number of bacterial natural products with useful properties is piperazic acid, a six-membered cyclic hydrazino acid^[2]. The first enzyme that was discovered to synthesize this amino acid is the piperazate synthase KtzT, from the soil-dwelling actinomycete *Kutzneria* sp. 744^[3,4]. After the discovery of KtzT, several enzymes that catalyze the same reaction have been discovered in various microorganisms, but their kinetics have not yet been investigated in detail^[4].

In this work, the kinetics of the natural reaction of two piperazate synthases, namely KtzT from *Kutzneria* sp. 744 and *Streptomyces* sp. B93 were investigated. For this purpose, the initial reaction rate method was utilized. The investigated enzymes catalyze the conversion of N5-hydroxy-L-ornithine to piperazic acid. The activity of both enzymes was measured at varying concentrations of substrate, product and substrate precursor and the data obtained in such experiments as used to estimate the values of kinetic parameters such as V_m , K_M , and K_i . It was found that in the cases of both enzymes, the reaction follows Michaelis-Menten kinetics. In the case of KtzT, competitive product inhibition was observed, whereas that was not the case with SbPZS. Both enzyme showed significant activity loss over time at similar rates.

Acknowledgements. This work has been supported by the European Union's Horizon Europe research and innovation programme under the Marie Skłodowska-Curie grant agreement 101073065.

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POLYMER-SOLVENT MOLECULAR INTERACTIONS IN PDLLA/PLGA-DMSO SYSTEMS

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Molecular interactions, such as solvent-polymer and polymer-polymer interactions, play a key role in determining the properties of polymer solutions. These interactions affect the size of the polymer's hydrodynamic coil and directly influence the viscosity of the solution.^[1] Among polymers which gained widespread scientific and pharmaceutical attention in recent years are poly(D,L-lactide) (PDLLA) and poly(lactide-co-glycolide) (PLGA) whose rheological behaviour was investigated on a wide range of concentrations in dimethyl carbonate (DMC) using concentric cylinder geometry^[2] and dimethyl sulfoxide (DMSO) using cone-and-plate geometry,^[3] respectively. Moreover, viscosity of 10% polylactide (polymer consisting of 88% L-lactide by weight) solution as a function of the solvent ratio acetone-dimethylformamide (AC-DMF) was also studied.^[4] However, to the best of our knowledge, there is no literature for the determination of viscosity of PDLLA and PLGA solutions in DMSO using capillary viscometry, as well as the calculations of molecular interactions for these polymer solutions.

In this study, viscosities of PDLLA and PLGA polymer solutions in DMSO in the concentration range between 2 and 20 mg mL⁻¹ were determined at 30 °C using capillary viscometry, as well as rotational rheometry, where double gap geometry was used. Among studied polymers, strongest polymer-solvent molecular interactions are present in solution of PLGA copolymer with equal molar fractions of D,L-lactide and glycolide (50:50).

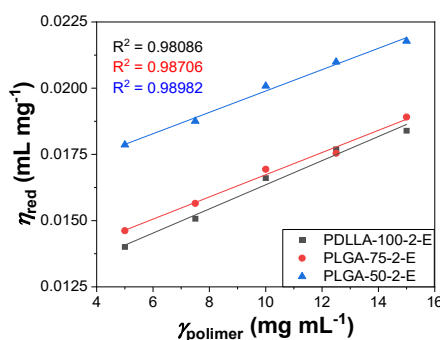


Figure 1. Reduced viscosities of different PDLLA and PLGA polymer solutions in DMSO.

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INSIGHTS INTO COPOLYMER SOLUTION VISCOSITY BEHAVIOUR – POTENTIAL SYSTEMS FOR DRUG DELIVERY

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Concentrated copolymer solutions play a crucial role in drug delivery systems where they serve as a vehicle for drug molecules enabling their controlled and extended release while enhancing their biocompatibility and chemical stability. Molecular weight and dispersity (\bar{D}) of copolymers significantly influence their solubility, degradation rate and drug release kinetics. Molecular weight and polymer concentration are key factors affecting solution viscosity. Molar mass is important for understanding polymer degradation behaviour and consequently drug release from drug delivery system^[1]. Higher molecular weight copolymers could form denser matrices that entrap drug molecules more effectively and slow their release^[2].

In this study, copolymers intended for drug delivery applications were characterized using gel permeation chromatography (GPC) and rheological measurements. GPC provided insights into molecular weight distribution and polymer uniformity. Rheological characterization, including shear tests, was conducted to evaluate viscosity of the copolymer solutions. To investigate formulations effects, viscosity was measured in two different biocompatible solvents for two copolymers having different molecular weight and/or monomer composition. Given that the optimal viscosity for pharmaceutical applications is between 5 and 50 mPa·s^[3], it can be tuned by adjusting polymer concentration, solvent, composition or by modifying molecular weight.

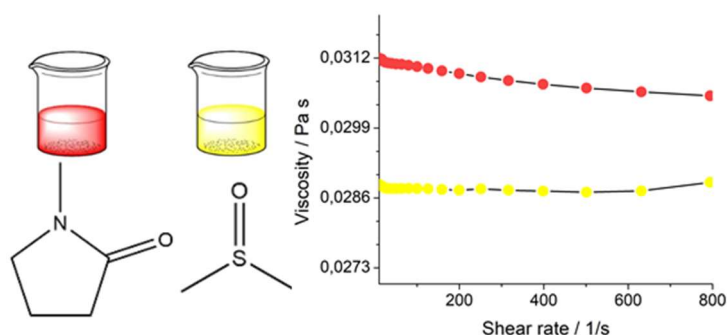


Figure 1. Viscosity vs. shear rate curves of the different copolymer solutions.

Acknowledgements. This work is part of the project “Development and characterization of complex prolonged release drug delivery systems based on biodegradable polymers” (NPOO.C3.2.R3-I1.04.0126) funded by NextGenerationEU.

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THERMAL DEGRADATION KINETICS OF THE PLGA COPOLYMERS OF DIFFERENT MOLAR MASS AND COMPOSITION (LACTIDE TO GLYCOLIDE MOLAR RATIO)

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Poly (lactic-co-glycolic acid) (PLGA) is a linear, biodegradable copolymer composed of lactic and glycolic acid units randomly distributed throughout the polymer chain. Due to its biodegradability, biocompatibility, and capacity for sustained drug release, PLGA has found widespread use as a drug delivery carrier.^[1] Since raw polymer materials often undergo thermal processing, factors such as processing temperature, atmosphere, and humidity are critical for characterizing PLGA and ensuring its suitability for drug delivery applications.^[2] For example, during melt extrusion, the copolymer undergoes different types of mechanical and thermal stress, so it is important to determine thermal degradation kinetics.^[3]

In this study, PLGA copolymers of varying composition and molar mass were thermally characterized using thermogravimetric analysis (TGA). Thermal degradation kinetics were evaluated using TG. The samples had varying molar fractions of PLA (ranging from 50 to 85 %), different inherent viscosities (0.2 to 0.5 dL g⁻¹) and two types of end-chain groups (acid and ester). Onset temperatures of thermal degradation were studied with values being higher with increased heating rate. Activation energies were calculated according to the ASTM E1641 standard method for decomposition kinetics by thermogravimetry using the Ozawa/Flynn/Wall method. It was concluded that with the increase of lactide content in the samples, as well as a decrease in molar mass, the thermal stability of the copolymer improves.

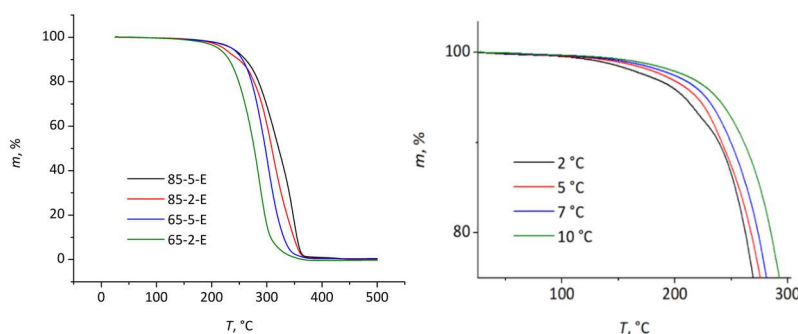


Figure 1. TG curves of PLGA samples with different composition and inherent viscosities (left) and TG curve of one sample heated by different heating rates.

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IMPACT OF MASS LOADING AND ACTIVE MATERIAL MICROSTRUCTURE ON CAPACITY OF LITHIUM IRON PHOSPHATE ELECTRODES

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Li-ion batteries are currently the most widely used type of batteries. High energy density, low self-discharge rate, and fast charging capabilities are some of the advantages of Li-ion batteries over conventional battery cells. Still, there are many challenges regarding Li-ion battery performance and longevity. Therefore, intensive efforts are being made to improve and develop them further.

In this work, mass loading and active material layer thickness were correlated with changes in the capacity and impedance before and after several charge-discharge cycles. A series of electrodes with a variety of mass loadings were prepared. Commercial battery grade LiFePO_4 (LFP) was used as active material, while PVDF and carbon black were used as a binder and conductive additive, respectively. LFP, along with additives, were dispersed in NMP to form a slurry. Prepared slurry was applied to the aluminium current collector via the doctor blade method. Differing mass loadings were achieved by varying the weight ratio of dry ingredients to NMP as well as the blade gap. Wet electrodes were dried in a vacuum oven for 24 hours. After drying, mass loading and thickness of the resulting layers were measured. Rheological properties of prepared slurries were examined using a rheometer. Electrochemical characterisation was performed on LFP-Li half-cells by potentiostatic electrochemical impedance spectroscopy (PEIS) and galvanostatic cycling with potential limitation (GCPL) techniques. Further analysis was performed by modelling equivalent circuits. Microstructural differences between electrodes were determined using scanning electron microscopy (SEM).

Significant differences in microstructure and particle packing caused by different slurry viscosities are observed. Findings demonstrate notable influence of mass loading and active material layer thickness on capacity and cycling stability, as well as impedance of the system represented by equivalent circuits. Electrochemical performance can be attributed to microstructural and packing differences between electrodes.

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

SIMULATION OF LUNG TISSUE IN A “LUNG-ON-A-CHIP” MODEL

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The development of physiologically relevant *in vitro* models remains a central challenge in respiratory research, particularly for evaluating the safety and efficacy of inhaled drug formulations. Conventional preclinical models often fall short in replicating the complexity of the lung, leading to discrepancies between experimental data and clinical outcomes.^[1] Organ-on-a-chip technologies have emerged as innovative platforms that address these limitations by recreating key structural and functional features of human tissues within a microengineered environment.^[2] This study focuses on the fabrication of a lung-on-a-chip system designed to replicate the alveolar–capillary barrier, with an emphasis on the production and characterization of the biocompatible membranes. These membranes were generated via electrospinning, and their fabrication parameters were optimized to reproduce the mechanical and morphological properties of lung tissue. Special attention was given to achieving a structure that supports cyclical deformation, mimicking the breathing motions of the alveoli. Mechanical behavior under simulated respiratory forces was assessed to evaluate the functional performance of the membrane within a dynamic setting. By enabling a realistic representation of the pulmonary interface, this platform offers new opportunities for the *in vitro* testing of inhalation therapies, and respiratory drug delivery. Ultimately, this membrane-based lung-on-a-chip system contributes to the development of more predictive, reproducible, and ethically sound alternatives to animal models in pharmaceutical and biomedical research.

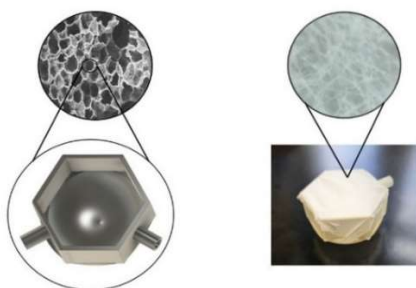


Figure 1. A lung-on-a-chip model.^[3]

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

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CARBOXYLIC ACID REDUCTASE: A KEY FOR ENZYMATIC ALDEHYDE SYNTHESIS

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Biocatalysis is an important scientific field for chemical production. Biocatalytic processes are utilised due to numerous advantages, such as mild reaction conditions and high catalytic power of enzymes.^[1] An example of enzymes studied for biocatalytic transformations are carboxylic acid reductases, also known as CARs. These enzymes are recognised for their potential in aldehyde preparation from carboxylic acids, as aldehydes are important building blocks for many industrial chemicals and play a role in fragrance and flavour industry. CARs are a part of the oxidoreductase family with a broad range of substrates.^[2,3] One prerequisite for employing CARs in large-scale applications is the regeneration of NADPH cofactor, as these enzymes are cofactor-dependent.^[2,4] The development of a successful CAR-driven biocatalytic process relies on the determination of kinetic parameters from the experimental data using mathematical modelling and enzyme activity assays. The work done so far focuses on finding the optimal reaction conditions for the targeted biotransformation (Figure 1).

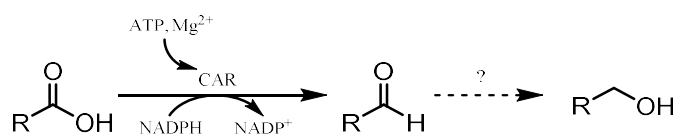


Figure 1. Reaction scheme.

Acknowledgements. This work has been supported by European Union's Horizon Europe Programme under the grant agreement No 101135542 (CirculH2).

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BIOCATALYTIC SYNTHESIS OF (R)-3-HYDROXY-γ-BUTYROLACTONE

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3-Hydroxy-γ-butyrolactone (HBL) is as a chiral building block for the synthesis of variety of pharmaceuticals, including statins, antibiotics, and HIV inhibitors.^[1] (R)-HBL can be synthesised from inexpensive achiral building block, *rac*-1,3-dichloro-2-propanol (*rac*-DCP), in three-step biocatalytic cascade involving two enzymes, halohydrin dehalogenase (HHDH) and nitrilase (Figure 1). This study focuses on the final step of the cascade, which is the nitrilase-catalyzed conversion of (R)-4-chloro-3-hydroxybutyronitrile ((R)-CHBN) to (R)-HBL. A panel of 24 nitrilases was screened under uniform conditions, and NITR-20 was identified as the most effective based on product yield after 24 hours. Detailed kinetic analysis showed that the reaction follows Michaelis-Menten kinetics with substrate inhibition, competitive inhibition by the product (R)-HBL, and non-competitive inhibition by NaCN and *rac*-DCP. Based on kinetic investigation, kinetic parameters were estimated and mathematical model was developed, followed by validation in both batch and fed-batch reactors. Model-based simulations guided the design and optimization of a fed-batch process, resulting in 96.7 % substrate conversion and a final isolated product yield of 53.1 % after 100 hours. This work demonstrates a promising enzymatic route to (R)-HBL production and highlights the usefulness of kinetic modelling for process optimization.^[2]

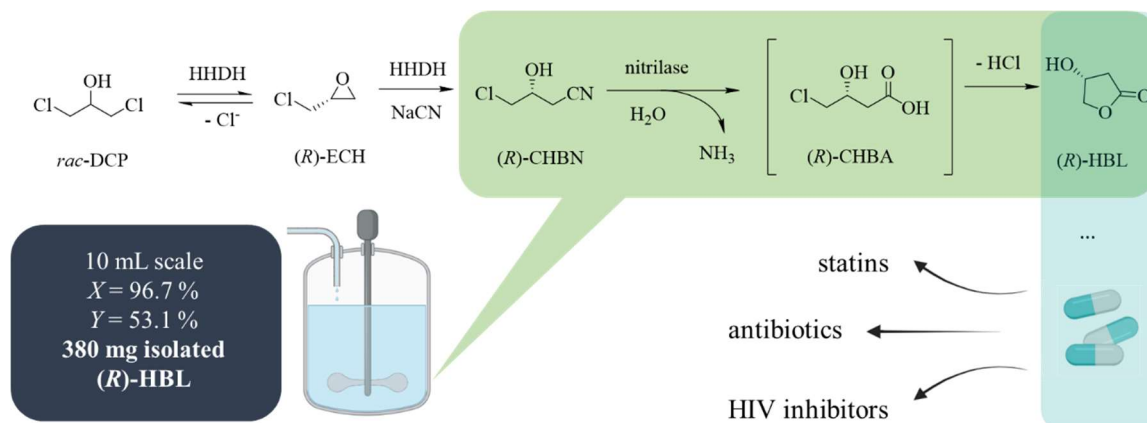


Figure 1. Cascade enzymatic synthesis of (R)-3-hydroxy-γ-butyrolactone ((R)-HBL).

Acknowledgements. This work has been supported by CATPHARMA (KK.01.1.1.04.0013).

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SIMULATION OF PULMONARY SOFT TISSUE USING A LUNG-ON-A-CHIP PLATFORM WITH INTEGRATED RESPIRATORY MONITORING SENSORS

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The pharmaceutical industry faces ongoing challenges in developing predictive, reproducible preclinical models for drug discovery, particularly for assessing the efficacy and toxicity of novel compounds prior to the onset of expensive clinical trials. Traditional in vivo models, including animal testing, often yield poor correlation with human physiological responses, while conventional in vitro systems fail to replicate the complex architecture and dynamic microenvironment of human tissues.^[1] Organ-on-a-chip platforms, particularly lung-on-a-chip models, offer a promising solution by replicating the structure and function of the alveolar microenvironment for studying inhaled drugs.^[2]

This study focuses on the development of a lung-on-a-chip system with a particular emphasis on the selection and optimization of hydrogels intended to simulate the soft tissue of pulmonary alveoli. Several hydrogel formulations were prepared and evaluated for biocompatibility, permeability, swelling, and mechanical properties. Hydrogels viscoelastic behavior, crucial for mimicking the elasticity of lung mucosa, was determined using a high sensitivity rheometer. The most suitable hydrogel will be integrated into the chip, along with a sensor designed to monitor drug diffusion through the gel matrix. The goal is to identify a hydrogel that most closely mimics the mechanical and functional characteristics of native lung tissue. The most suitable hydrogel will be integrated with a sensor and the diffusion of an active pharmaceutical ingredient through the gel matrix will be monitored. This sensor simulates the vascular interface, enabling real-time tracking of drug transport from the inhaled dose through the alveolar model to the systemic circulation.

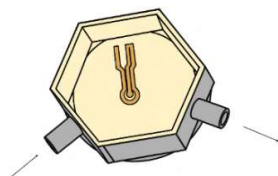


Figure 1. Hydrogel with an integrated respiratory monitoring sensor on a lung-on-a-chip platform.

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

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DEVELOPMENT AND CHARACTERIZATION OF SUSTAINED-RELEASE INDOMETHACIN DELIVERY SYSTEMS VIA ELECTROSPINNING

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Indomethacin is a widely used nonsteroidal anti-inflammatory drug (NSAID) known for its efficacy in managing pain and inflammation. However, its clinical utility is often limited by poor aqueous solubility and short biological half-life, necessitating frequent dosing and raising the risk of gastrointestinal side effects^[1]. To overcome these limitations, controlled drug delivery systems are being developed to enhance solubility, prolong release, and improve therapeutic outcomes. One promising approach involves embedding indomethacin within biodegradable polymeric matrices to enable localized and sustained release.

In this study, poly(lactic-co-glycolic acid) (PLGA) was used as the carrier polymer to fabricate electrospun nanofibrous membranes incorporating different concentrations of indomethacin. The resulting membranes were characterized using scanning electron microscopy (SEM) and optical microscopy, confirming uniform fiber morphology and successful integration of the drug without compromising structural integrity. Thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) validated drug encapsulation and provided insights into the thermal behavior and stability of the composite systems.

Drug release studies demonstrated a concentration-dependent release profile, with sustained release of indomethacin over extended time periods. These findings confirm that electrospun PLGA membranes offer a promising platform for the controlled delivery of poorly soluble drugs like indomethacin. The study supports the potential of such systems in biomedical applications requiring localized and prolonged therapeutic effects, such as in chronic inflammation and wound healing.

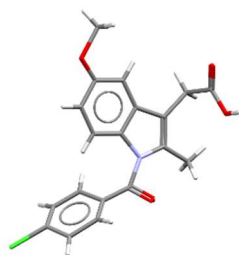


Figure 1. Molecular structure of indomethacine

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

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PHYTOCHEMICAL CHARACTERIZATION AND SKIN CELL MODULATORY POTENTIAL OF SUPERCRITICAL CO₂ EXTRACTS FROM *Foeniculum Vulgare* AND *Juniperus Communis*

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Plant-derived lipophilic extracts offer promising potential for dermocosmetic applications, particularly when obtained through green extraction methods such as supercritical CO₂ extraction. This study investigates the chemical composition and biological effects of supercritical extracts from fennel (*Foeniculum vulgare*) and juniper (*Juniperus communis*), focusing on their potential to modulate skin cell behavior.

Volatile and fatty acid profiles were determined using GC-MS and GC-FID, respectively. In *F. vulgare*, the major volatile components were *trans*-anethole (75.03 %) and fenchone (11.75 %). Fatty acid composition revealed a predominance of saturated fatty acids (SFA, 53.9 %), with lauric acid (C12:0) accounting for 40.3 ± 1.2 %. Monounsaturated fatty acids (MUFA) represented 39.6 % (mainly oleic acid), and polyunsaturated fatty acids (PUFA) 6.5% (predominantly linoleic acid). In *J. communis*, germacrene D (29.79 %) and germacrene B (12.48 %) were the main volatiles. The extract showed a PUFA-rich profile (37.6 %), with contributions from n-3 (15.3 %) and n-6 fatty acids (22.3 %).

The cytotoxic effect of both extracts was evaluated using MTT assays on primary human dermal fibroblasts (HDF) and immortalized keratinocytes (HaCaT). *J. communis* extract was non-cytotoxic at concentrations up to 781 ng/mL (24 h) and 391 ng/mL (48 h) in HDF cells, while *F. vulgare* extract maintained HDF viability above 94 % at concentrations up to 0.4 mg/mL. In HaCaT cells, both extracts slightly increased viability, with *F. vulgare* reaching 119.94 % at 3.13 µg/mL after 48 h. Further analyses include antioxidant activity assays (ABTS, SOD, catalase), as well as mechanistic assays to explore proteasome function and autophagy.

This study highlights the chemical richness and skin-related bioactivity of supercritical extracts from fennel and juniper, supporting their potential inclusion in regenerative and anti-aging skincare formulations.

Acknowledgements. This work received support and help from FCT/MCTES (LA/P/0008/2020 DOI 10.54499/LA/P/0008/2020, UIDP/50006/2020 DOI 10.54499/UIDP/50006/2020, and UIDB/50006/2020 DOI 10.54499/UIDB/50006/2020) and program CEEC IND5ed (<https://doi.org/10.54499/2022.04909.CEECIND/CP1725/CT0014>).

ENZYMATIC SYNTHESIS OF GLUCOLIPIDS FOR SUSTAINABLE CONSUMER PRODUCTS

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Biosurfactants are surface-active compounds produced by microorganisms, and they have become very important in our daily lives due to their unique and distinctive properties (Figure 1). In the food industry, biosurfactants are used as emulsifiers and stabilizers in products like ice cream, salad dressings, and bakery items, enhancing texture and shelf life. In household cleaning products, they serve as effective, eco-friendly alternatives to chemical surfactants, providing excellent cleaning and foaming properties while being gentler on the environment. The personal care and cosmetics sector utilizes biosurfactants in products such as shampoos, body washes, and skincare formulations, benefiting from their mildness and compatibility with human skin. Glucolipids are gaining traction as environmentally friendly biosurfactants with potential applications in the food, detergent, and personal care industries.^[1] This research aims to optimize enzymatic process for glucolipid synthesis using α -transglucosylases from the GH70 family. For that purpose, pH and temperature dependence of the enzyme will be investigated and kinetic measurements will be carried out.

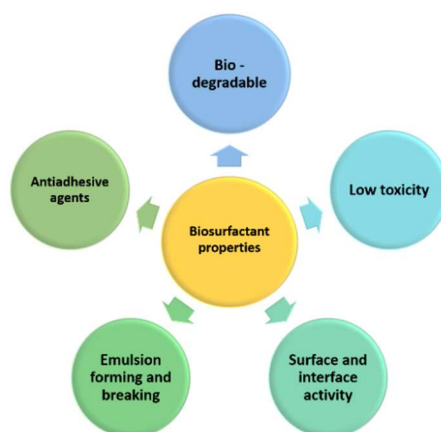


Figure 1. Unique and distinct properties of biosurfactants

Acknowledgements. The Croatian Science Foundation supports this work through the Career Development Project for Young Researchers.

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CROATIAN WHEAT VARIETIES AND BETA GLUCAN CONTENT

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Glucans are glucose polymers that can be found in cereals. They consist of linear mixed (1→4) (1→3)-linked β-D-glucans, in which blocks of (1→4)-linked β-Glcp units are separated by single (1→3)-linkages. Cereal β-glucans are known to differ in their tri- to tetra-mer ratio, the share of longer cellulosic fragments, and the ratio between the two types of glycosidic bonds. Glucans are also found in wheat and wheat malt, but to a much lesser extent. However, they are significant for brewing. They generally get degraded during malting and mashing, but if they “survive” these stages, they can end up in wort and beer. The commonly found glucans in wheat and wheat malt are β-glucans. β-glucans are β-linked (1,3, and 1,4) glucose polymers, while α-glucans are α-linked glucose polymers, colloquially called dextrins. Glucans can be found in cell walls and the endosperm, just as AXs. However, during the malting process, the cell wall gets degraded via enzymatic activity (β-glucanase), and β-glucan molecules get released from the cell wall. The endosperm cell walls are complex structures made up of hemicelluloses and gums. This paper aims to give a short overview on glucans in Croatian wheat varieties.

Acknowledgements. This work has been supported by internal competitive research project “Assessment of quantitative traits in small grain cereals germplasm considering climate change (CLIM-CEREALS-QUANT)” of the Agricultural Institute Osijek.

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ACTIVATION OF LPMO IN LOW-TEMPERATURE DEEP EUTECTIC SOLVENT

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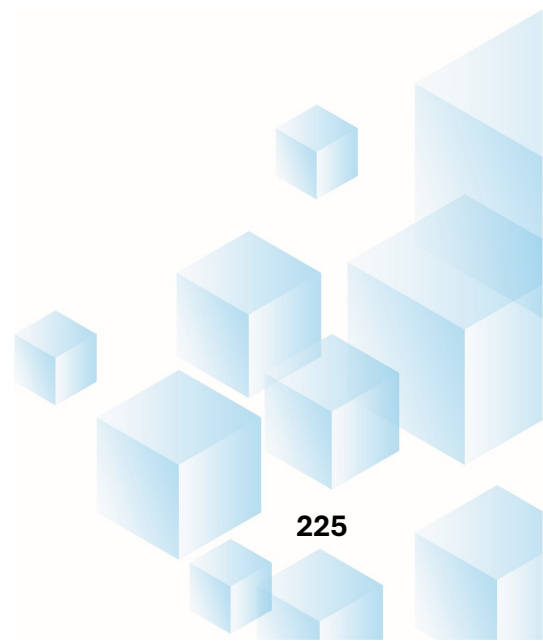
This work investigated the activity of the LPMO enzyme in low-temperature deep eutectic solvents and developed two simple and robust mathematical models to predict the use of solvents with the most suitable physicochemical properties of their components for the LPMO biocatalytic reaction. Easily accessible, non-toxic, and relatively inexpensive components were selected to create the deep eutectic solvents (DES) according to the principles of green chemistry and sustainable development. The activity of LPMO was initially spectrophotometrically tested in NaAc buffer pH 6.4 for comparison. Then, the enzyme activity was tested in prepared solvents using the same method with buffer as a blank. Furthermore, the deep eutectic solvents were mathematically described using the COSMO-RS software package. The obtained values were grouped into 10 intervals to create a sigma profile of the solvents. Based on these intervals, multiple linear regression models were developed using the Statistica 13.0 software package.

Acknowledgements. This work has been supported by bilateral collaborations between Croatia and Austria BIL-HR-AUT-2024-2025/19; Croatian Science Foundation grant number IP-2022-10-3075 (project under title 'Biorefinery system for biofuels and biochemicals production from non-food lignocelulosic raw materials *Biorefinery-NFLRM*').



POSTERS

MATERIALS AND NANOTECHNOLOGY



CHALLENGES OF GLASS AS A PRIMARY PACKAGING MATERIAL IN PHARMACEUTICAL INDUSTRY

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Glass is a chemically inert material in most neutral or slightly acidic environments. However, alkaline solutions can react with the silicate structure of glass, causing the release of sodium and/or potassium alkali ions into the solution. The extent of leaching and stability are influenced by factors such as the composition of the glass, as well as the temperature, concentration, and pH of the solution. The aim is to test the hydrolytic resistance of glass packaging, which determines the quality of glass for use in the pharmaceutical industry. The release of alkali ions from the glass structure, the appearance of delaminated particles in the solution and morphological changes on the inner surface are monitored. These tests aid in selecting the ideal glass material for specific formulations, ultimately helping to extend the product's shelf life. Observations focus on the presence of visible particles, pH shifts, and the leaching of elements from the glass. Delamination of glass, particularly in alkaline media, is a common issue, and signs of delamination include a pitted or 'broken' appearance on the inner surface of the container. The figure 1 illustrates these damaged areas on the inner surface and the delaminated particles found in the solution. In uncoated vials, an increase in pH and leachable glass components in solution has been observed, which is a first indication of a change in the chemical composition of the glass surface and increases the tendency to delamination. A hydrophilic or hydrophobic surface modification of the inner surface of glass vials increased the hydrolytic resistance and thus reduced the tendency for glass delamination.

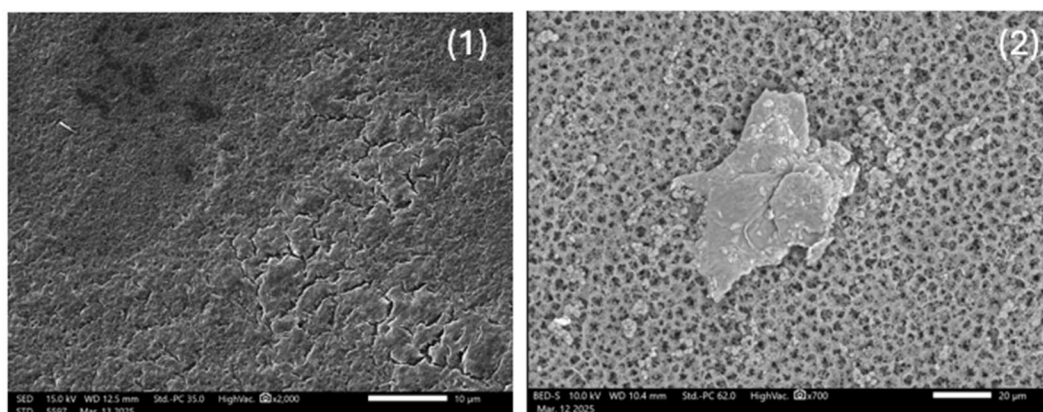


Figure 1. SEM images of: surface of delaminated glass vial (1) and delaminated particle in solution in the vial (2)

Acknowledgements. This work was fully supported by Pliva d.o.o.

FABRICATION AND PROPERTIES OF COC/Cu COMPOSITE FILAMENTS

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The development of composite filaments for 3D printing has gained significant attention due to their enhanced mechanical and thermal properties. Cyclo-olefin copolymer (COC), a high-performance polymer known for its excellent transparency, low moisture absorption, high chemical resistance, and high thermal stability, serves as the matrix material. Copper powder with micro-sized particles, chosen for its excellent thermal and electrical conductivity, was blended with COC granules in an extruder. The resulting mixture was pelletized and re-extruded to produce filaments suitable for 3D printing applications.

Mechanical properties of the 3D printed samples were assessed through standard tensile test, to evaluate the effect of copper incorporation on the material's strength and durability. Additionally, thermal properties of the composites were analyzed using differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), and melt flow rate (MFR) measurements. The DSC and TGA results provide insight into the thermal behavior and stability of the COC/Cu composites, while MFR tests reveal the processing characteristics critical for filament extrusion.

This study is significant as it provides valuable insights into the potential of COC/Cu composites for 3D printing applications in fields that require enhanced thermal and electrical conductivity, such as electronics, automotive, and aerospace industries. The findings from this work could lead to the development of high-performance, multifunctional composite filaments that meet the demands of advanced manufacturing and functional 3D printed components.



Figure 1. Filaments of COC/Cu composites.

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

INFLUENCE OF 3D PRINTING PARAMETERS ON THE MECHANICAL PROPERTIES OF 17-4 PH STAINLESS STEEL PARTS

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17-4 PH stainless steel is a crucial material in chemical engineering, offering high strength, corrosion resistance, and heat treatability, making it suitable for reactor components, heat exchangers, and filtration systems. The development of metal-polymer composite filaments for fused filament fabrication (FFF) has enabled cost-effective and accessible 3D printing of metal parts, followed by debinding and sintering to obtain fully metallic structures. However, the mechanical performance of the final part is highly dependent on printing parameters, polymer binder removal, and sintering conditions.

This study investigates the mechanical properties of 17-4 PH stainless steel composite parts fabricated using FFF and post-processed through thermal debinding and sintering. The effects of printing parameters, such as layer height, print speed, and extrusion temperature, on the final mechanical properties were analysed.

The findings emphasize the critical role of process optimization in achieving high mechanical reliability in sintered FFF printed 17-4 PH stainless steel. Understanding these relationships is essential for ensuring structural integrity in chemically demanding environments. This research contributes to the advancement of additive manufacturing for functional metal components, offering a sustainable and scalable approach for industrial applications in chemical engineering.



Figure 1. Microreactors 3D printed of 17-4 PH composite material

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



THE ROLE OF SIZE-SELECTED METAL NANOCCLUSERS IN CATALYTIC CO₂ MITIGATION

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With the growing need to address climate change, the development of efficient and affordable catalysts for greenhouse gas reduction has become crucial. One promising research direction involves size-selected copper tetramer nanoclusters deposited on metal-oxide surface. These systems have demonstrated high catalytic efficiency in CO₂ hydrogenation and conversion into valuable C1 products. Based on a density functional theory (DFT) approach, we propose a reaction mechanism for methanation on Cu₄O₂ supported by Zr_nO_{2n} (n=12).^[1] Catalyst tunability is further explored through the doping strategy by replacing a single Cu atom in the cluster with a Pd atom, which is known to facilitate H₂ dissociation.^[2] The dual role of the copper-based cluster and the significance of the support are examined.

Theoretical and complementary experimental results confirm the high activity of the copper–zirconia catalyst, reveal the influence of the substrate morphology, and offer fundamental insight into the mechanism of CO₂ conversion, thus showing a new way to tune the catalytic activity of deposited nanocluster catalysts.

Acknowledgements. This work has been supported by Cosy COST Action “European Cooperation in Science and Technology – Confined Molecular Systems: from the new generation of materials to the stars”.

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Fe-SUBSTITUTED SrTiO₃: A ROUTE TOWARD TAILORED ELECTRONIC AND OPTICAL PROPERTIES

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Strontium titanate (SrTiO₃) is a wide-bandgap (≈ 3.3 eV) perovskite oxide known for its high dielectric constant and tunable physical properties, making it attractive for applications in photocatalysis, electronics, and optoelectronics.^[1,2] In this study, we explore the effects of iron (Fe) substitution at the titanium (Ti) sites on the structural, optical, and electronic properties of SrTiO₃. Fe doped SrTiO₃ samples were prepared *via* a facile hydrothermal route and characterized using powder X-ray diffraction (P-XRD), scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), UV-vis diffuse reflectance spectroscopy (UV-DRS), and photoelectrochemical (PEC) measurements. Fe incorporation induces noticeable changes in lattice parameters and introduces mid-gap states, resulting in bandgap narrowing and enhanced visible light absorption. These modifications significantly improve the material's photoelectrochemical performance. The findings demonstrate that Fe-doped SrTiO₃ offers a tunable platform for developing next-generation functional oxides for solar energy conversion and related applications.

Acknowledgements. This work has been supported by Croatian Science Foundation under project: Solar-assisted photocatalytic degradation of perfluorinated compounds in water SoAPperF (IPS-2022-02-4780).

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EXPLORING 1-ETHYL-3-METHYLIMIDAZOLIUM BIS(TRIFLUOROMETHYLSULFONYL)IMIDE IONIC LIQUID AS ADVANCED ELECTROLYTE FOR CALCIUM-OXYGEN BATTERIES

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Calcium-oxygen (Ca-O₂) batteries are emerging as a promising next-generation energy storage technology due to the high abundance of calcium, its low cost and its high theoretical energy density.^[1] These batteries operate through the reversible electrochemical reaction between calcium and oxygen, similar to lithium-oxygen (Li-O₂) batteries, but with the potential for improved safety and resource availability. However, their development faces significant challenges, including the instability of calcium metal in conventional electrolytes, sluggish oxygen reduction and evolution reactions (ORR/OER) and the formation of different discharge products that hinder rechargeability.^[2] To overcome these issues, researchers are exploring novel electrolyte systems, such as ionic liquids, to enhance calcium plating/stripping efficiency and improve overall battery performance. If successfully developed, Ca-O₂ batteries could offer a viable alternative for high-energy applications, contributing to the advancement of sustainable energy storage technologies. Here in, we investigated the potential application of 1-ethyl-3-methylimidazolium bis (trifluoromethylsulfonyl)imide [EMIM][TFSI] in DMSO as electrolyte for oxygen reduction and oxidation, without and with different calcium salts (calcium trifluoromethanesulfonate (Ca(OTf)₂), calcium tetrafluoroborate (Ca(BF₄)₂) and calcium bis (trifluoromethanesulfonyl)imid (Ca(TFSI)₂).

Acknowledgements. This work has been supported by NATO SPS programme, under project number SPS G5910. N. Z. would like to thank the Croatian Science Foundation for financial support through the MOBDOL-2023-12 programme, Funded by the European Union – NextGenerationEU.

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SYNTHESIS AND CHARACTERIZATION OF MESOPOROUS ZINC OXIDE DOPED WITH COPPER AND NICKEL

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Zinc oxide is a material recognized for its exceptional photocatalytic properties, enabling its potential application in various fields of science and the industry. Due to its non-toxicity and environmental sustainability, it is used as a photocatalyst for the degradation of various harmful organic compounds, such as organic dyes in wastewater. This study focuses on the synthesis of zinc oxide and zinc oxide doped with copper and nickel using the soft-template method, which involves the use of surfactants or polymers as templates for ZnO precipitation. The soft template is removed through thermal treatment, resulting in the formation of a stable and catalytically active mesoporous material. The prepared samples were characterized by X-ray diffraction analysis (XRD), attenuated total reflectance Fourier transform infrared spectroscopy (FTIR-ATR), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDS), and UV-Vis diffuse reflectance spectroscopy (UV-Vis DRS). The photocatalytic performance of the synthesized materials was evaluated through the degradation of the organic dye rhodamine B (RhB) ($c_0 = 10 \text{ mg L}^{-1}$) under UV light. The prepared samples exhibited excellent photocatalytic performance, indicating strong potential for application in the purification of wastewater containing organic dyes such as rhodamine B.^[1,2]

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ENHANCING DSSC PERFORMANCE WITH NATURAL DYES AND NOBLE METAL NANOCCLUSERS

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This research explores dye-sensitized solar cells (DSSCs) enhanced with bio-nano hybrids combining natural anthocyanin dyes and noble metal quantum clusters. These hybrids, designed within the computational quantum chemistry methods (DFT/TDDFT), aim to improve light absorption and charge transfer through donor-acceptor interactions. This research focuses on bio-nano hybrids for dye-sensitized solar cells (DSSCs), combining natural anthocyanin dyes—specifically cyanidin—with noble metal nanoclusters (Ag, Au). Quantum chemical simulations (DFT/TDDFT) show that complexation of cyanidin with noble metal nanoclusters enhances light absorption, increases oscillator strength, and improves charge injection driving force (ΔG_{inject}), indicating improved photovoltaic potential. These effects arise from donor-acceptor interactions and π - π^* coupling between the dye and nanocluster. A small-scale DSSC prototype is being developed to test efficiency, stability, and photoconversion performance^[1-6]. This study proposes a sustainable nanomaterial strategy to improve DSSC functionality using non-toxic, plant-based components.

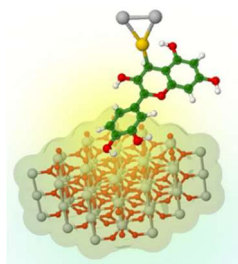


Figure 1. Schematic representation of cyanidine@NC (adapted from^[2] and^[3])

Acknowledgements. This research was supported by the project STIM – REI, Contract Number: KK.01.1.1.01.0003, funded by the European Union through the European Regional Development Fund – the Operational Programme Competitiveness and Cohesion 2014–2020 (KK.01.1.1.01).

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MECHANOCHEMISTRY FOR UNIQUE FLUORIDE-FREE MXENE

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MXenes, a family of transition metal carbides and nitrides, have emerged as one of the fastest-growing groups of 2D materials. They are represented by the chemical formula $M_{n+1}X_nT_x$ ($n=2-4$), where M represents transition metals like Sc, Ti, Zr, Hf, V and Nb, X is carbon and/or nitrogen, and T stands for surface termination groups (-OH, -F, -O or -Cl). MXenes are synthesized via wet chemical etching of the $M_{n+1}AX_n$ (MAX) phase, where the A-layer (typically Al) is selectively removed using fluoride-based solutions. However, this method presents significant safety, handling, and environmental challenges, limiting production scalability. As a promising alternative, mechanochemistry (MC) offers a green and scalable route for MXene synthesis, eliminating the need for hazardous solvents and enabling a safer production process.

In this work, we prepare fluoride-free $Ti_3C_2T_x$ MXene using a MC method followed by post-treatment process necessary to obtain delaminated MXene layers. The product was characterized using Raman spectroscopy (RAMAN), scanning electron microscopy (SEM) with energy dispersive X-ray spectroscopy (EDX) and low-energy ion scattering (LEIS). LEIS, with its high surface sensitivity, provided detailed insights into the elemental distribution of the outermost atomic layer and the composition of the first 10 nm of sub-surface material. The results showed that mechanochemically synthesized MXene is characterized by a unique structure that is mainly confined to the MAX phase in the sub-surface. The chemically etched MXene showed a more homogeneous elemental distribution throughout the depth, indicating structural differences between mechanochemically and chemically synthesized MXene.

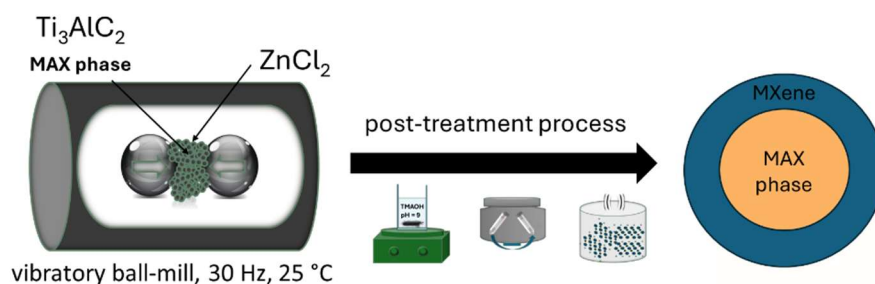


Figure 1. Schematic illustration of the mechanochemical synthesis of unique MXene structure.

Acknowledgements. This work has been supported by the Foundation of the Croatian Academy of Sciences and Arts for the project “Green Synthesis of 2D Transition Metal Carbides: An Innovative Approach for Sustainable Production and Application”.



UTILIZATION OF IONIC LIQUIDS IN NEXT-GENERATION CARBON BASED SUPERCAPACITORS

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Due to the increasing global demand for electrical energy, the need for energy storage has also grown. Supercapacitors can store energy through mechanisms of electric double-layer capacitance (EDLC) or pseudocapacitance. Supercapacitors possess a higher specific power in comparison with batteries (10–20 kW/kg), charge rapidly, do not lose capacity over time, maintain stable performance at higher temperatures, offer improved environmental compatibility, and demonstrate higher energy density compared to traditional capacitors (4–5 Wh/kg). In this study, carbon-based supercapacitor systems were electrochemically characterized with the addition of ionic liquids to the base electrolyte in order to improve the properties of the supercapacitors, with an emphasis on investigating the influence of the cations and anions of the ionic liquids. For this purpose, tested capacitors were prepared from carbon electrodes with tetraethylammonium tetrafluoroborate (TEABF_4) in acetonitrile (ACN) as the electrolyte to which varying proportions of the following ionic liquids were added: 1-ethyl-3-methylimidazolium bis(fluorosulfonyl)imide (EMFSI), *N*-butyl-*N*-propylpyrrolidinium bis(fluorosulfonyl)imide (Py_{14}FSI), 1-butyl-3-methylimidazolium tetrafluoroborate (BMIBF_4), and 1-butyl-3-methylimidazolium hexafluorophosphate (BMIPF_6). The tested systems were characterized using standard electrochemical techniques such as electrochemical impedance spectroscopy, cyclic voltammetry, and galvanostatic charge-discharge measurements. The research showed changes in the current response shape of the cyclic voltammogram as well as changes in the voltage profile depending on the percentage of ionic liquid added to the base electrolyte. Furthermore, the addition of ionic liquids significantly reduced the electrolyte resistance. This demonstrated that an optimal amount of ionic liquid in the base electrolyte can significantly enhance the energy storage capability of supercapacitors, thus opening avenues for further research.

Acknowledgements. This work was financially supported by the project NATO SPS G5910 : High-energy calcium-oxygen batteries.

INFLUENCE OF BLENDING PARAMETERS ON THE STRUCTURAL AND THERMAL PROPERTIES OF PLA/PGA SYSTEMS FOR DRUG DELIVERY APPLICATIONS

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Drug delivery systems based on biodegradable polymers such as poly(lactic acid) (PLA) and poly(glycolic acid) (PGA) are gaining more and more attention due to their biocompatibility and potential influence on extended drug release.^[1] These systems are comprised of a suitable polymeric carrier in which the desired active pharmaceutical ingredient is dispersed.^[2] The biocompatibility and biodegradability of PGA and PLA already makes them suitable for biomedical applications, such as degradable sutures and tissue engineering.^[3] Therefore, the goal of the study was to develop efficient polymeric blends comprising these two biodegradable polymers. To achieve such a goal, a major step was to optimize their blending conditions. The optimization of the blending conditions was carried out using a Box-Behnken experimental design. Thermal properties of the polymeric blends were studied using differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA), while polymeric molecular masses were analyzed using gel permeation chromatography (GPC). Results of the study show that the blending conditions have a significant impact on the properties of the final blends and need to be taken into consideration when preparing such systems.

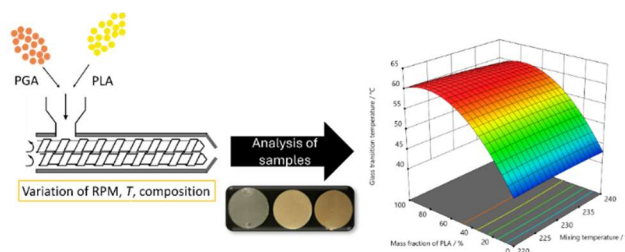


Figure 1. Process chart: the rotational speed of the extruder, temperature of mixing and composition variation; properties of the polymer mixtures analysis, and graphic chart of response surfaces.

Acknowledgements. This work is part of the project “Development and characterization of complex prolonged release drug delivery systems based on biodegradable polymers” (NPOO.C3.2.R3-I1.04.0126) funded by NextGenerationEU.

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POLYMER SEMICONDUCTOR THIN FILMS BASED ON DINITROSOBIPHENYL MOIETY

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Polymer semiconductors composed of a carbon-based π -conjugated backbone have attracted great interest due to their potential applications in organic electronic devices.^[1] Aromatic dinitroso compounds are known for their ability to spontaneously form one-dimensional (1D) azodioxy oligomers or polymers. Recent experimental and computational studies indicated that such 1D azodioxy polymers could be used as building blocks for organic semiconductors.^[2,3] However, for possible application of these systems in organic electronic devices, the detailed study of the influence of various experimental parameters on the surface morphology and optoelectronic properties of the deposited thin films of azodioxy polymers is crucial.

In this work, we deposited 4,4'-dinitrosobiphenyl polymers using drop-casting and spin-coating on Au(111), highly oriented pyrolytic graphite (HOPG) and Si substrates. The comparison of the Raman spectra of the films with the bulk Raman spectrum of powder sample indicated formation of azodioxy polymers in drop-casted and spin-coated samples on all three substrates. The influence of deposition methods and substrates on the morphology and optoelectronic properties of films were investigated by atomic force microscopy (AFM), ellipsometry and photoluminescence measurements. The band gaps of the deposited samples are lower compared to the band gap of the powder sample, which can be attributed to the surface-induced change in the torsion angle of the polymer, as suggested by DFT calculations. Furthermore, the band gap values of drop-casted samples are lower for each substrate compared to spin-coated samples, supporting the hypothesis that the spin-coating method inhibits molecular relaxation due to rapid solvent evaporation.

Acknowledgements. This work has been fully supported by the Croatian Science Foundation under the project IP-2020-02-4467.

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TAILORING MECHANICAL PERFORMANCE OF EPOXY COMPOSITES USING DICYANAMIDE-BASED IONIC LIQUID MIXTURES

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Natural fiber-reinforced epoxy composites are gaining attention as sustainable alternatives to conventional materials, especially in applications where mechanical performance and processing efficiency are key. In this study, we present a novel approach to tailoring the mechanical properties of flax-fiber reinforced epoxy composites using dicyanamide-based ionic liquid (IL) mixtures as both curing agents and functional modifiers.

Ionic liquids are organic salts that remain liquid at or near room temperature and are known for their tunable physicochemical properties, thermal stability, and ability to act as multifunctional additives in polymer systems.^[1] Three designed ILs: 1-hexyl-3-methylimidazolium dicyanamide, 1-hexyl-1,4-diazabicyclo-[2.2.2]octan-1-ium dicyanamide and trimethyloctadecylammonium dicyanamide (figure 1) were synthesized and combined into binary and ternary systems. These IL mixtures were evaluated for their ability to initiate epoxy resin crosslinking and simultaneously enhance mechanical properties such as tensile and bending strength. Differential Scanning Calorimetry (DSC) revealed altered polymerization profiles and reduced total enthalpy for IL mixtures compared to single-IL systems, indicating a shift toward more controlled and possibly multi-pathway curing.

Mechanical testing confirmed the dual functionality of the IL systems: selected mixtures significantly improved tensile strength and bending modulus, while others promoted structural integrity under strain by preventing catastrophic failure. The results highlight the potential of IL mixtures not only as efficient curing agents but also as tunable modifiers for optimizing the performance and safety of natural fiber-reinforced thermoset composites.^[2]

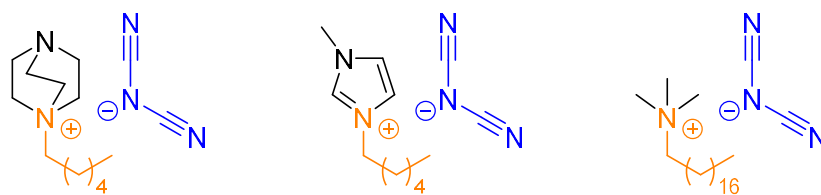


Figure 1. Structures of ionic liquids.

Acknowledgements. This research was funded by the National Science Centre: project SONATA BIS 7 (2017/26/E/ST8/01059).

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NEW SURFACE PASSIVATING IONOGEL TECHNOLOGY FOR MESA-TYPE DETECTOR STRUCTURES (PASION PROJECT)

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Mesa-type detectors (e.g. IR detectors) are attracting constant attention due to wide range of applications, from astronomy, diagnostics, night-vision, thermal-vision, optical fiber communication, to security and defense. Unfortunately, they can have significant disadvantage, namely, surface area leakage current (“surface dark current”) occurrence, which dominates over bulk leakage mechanisms and is a main limiter of device performance. The PASION project aims to develop a universal, based on selected ionic liquids of specific structure^[1,2,3] ionogel material platform for these detectors, and particularly for a dense array detector passivation, where the sidewalls area is significant. On the one hand, the passivating layer should minimize the effects caused by plasma/wet etching of the epitaxial structure layers (such as dangling bonds, impurities or structural defects), and on the other hand, it should not constitute a significant complication of the entire detector manufacturing process, ensuring both the efficiency of process and the minimization of costs and risks.

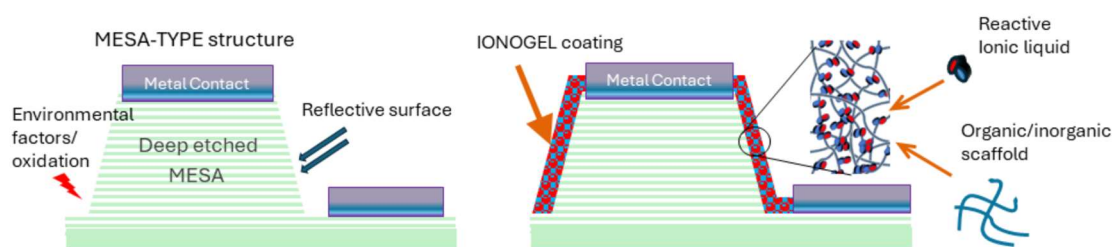


Figure 1. Ionogel passivation concept: passivating ionic liquid in the organic/inorganic matrix placed on the side walls of the deep etched mesa structure.

Acknowledgements. This research is funded by the National Science Centre OPUS 27 (UMO-2024/53/B/ST8/02113).

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TAILORING PROPERTIES OF Sr-FERRITE AND DOPED IRON OXIDE NANOPARTICLES FOR HYPERTHERMIA EFFECT

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Magnetic iron oxide nanoparticles (MNPs) are promising materials for medical applications, specifically magnetic hyperthermia on cancer cells – localized heating of cancer cells under an alternating magnetic field. The key points for magnetic hyperthermia are the use of materials with a high specific absorption rate (SAR), defined as the amount of energy converted into heat per time and per mass of magnetic material. To improve SAR, particle size, size distribution, shape, composition and surface area should be controlled, as all these parameters can influence the magnetic properties of MNPs. Some authors have shown that cubic, ring-shaped and anisotropic disk-shaped MNPs have significantly higher SAR values compared to the corresponding spherical MNPs. Recently, Sr-ferrite has emerged as a promising material for magnetic hyperthermia due to its high crystalline anisotropy, excellent magnetic properties and non-toxicity.

Sr-ferrite and Sr-doped magnetite NPs were synthesized hydrothermally with alkaline solutions of FeCl_3 and SrCl_2 precursors to investigate their phase composition, size-dependent magnetic properties and specific absorption rate (SAR). The main synthesis parameters, including $\text{Fe}^{3+}/\text{Sr}^{2+}$ ratio, pH, temperature, reaction time and polymers were systematically investigated.

Different synthesis conditions yielded plate-like hexagonal Sr-ferrite disks with a broad size distribution and an average thickness of 40–80 nm, small Sr-ferrite particles (40 nm), 50–100 nm plate-shaped Sr-doped magnetite, and spherical superparamagnetic Sr-doped magnetite NPs (10–13 nm). The formation of monophasic Sr-ferrite required very high pH and high temperatures ($\geq 200^\circ\text{C}$), while mixtures of Sr-ferrite, hematite, goethite and Sr-doped magnetite were formed at lower synthesis temperatures. Longer synthesis times at higher temperatures improved the phase purity and uniformity of the Sr-ferrite particles, as confirmed by FE-SEM microscopy. On the other hand, significantly smaller Sr-ferrite NPs were synthesized by shortening the reaction time at high temperatures. Stabilization using polymers (DEAE-dextran, PVA) resulted in very small Sr-doped magnetite NPs, caused by the partial reduction of Fe^{3+} with the polymer. Characterization by SQUID magnetometry and Mössbauer spectroscopy showed superparamagnetic behavior in Sr-doped magnetite NPs. The measured SAR values indicate promising properties for hyperthermia treatment. Physisorption measurements of the plate-like Sr-ferrite NPs indicate macroporous or non-porous materials with a plate-like morphology characterized by slit-shaped pores, as evidenced by the type H3 hysteresis pattern. These results show that synthesis parameters significantly affect particle properties essential for the hyperthermia effect on cancer cells.

Acknowledgements. This work has been supported by Croatian Science Foundation under the project IP-2022-10-3687 (RadMagnNanoHyperT).

FULLY PRINTED MODULARIZED MICROFLUIDIC SETUP FOR *IN SITU* ANALYTICAL MONITORING BASED ON ELECTROCHEMICAL DETECTION OF METHYLENE BLUE

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This work presents a fully printed, adaptable microfluidic setup convenient for tracking chemical processes that are unsuitable for continuous monitoring with a single sensor, or for which it is important to ensure minimal sample losses. Planar printed three electrode systems were used for direct electrochemical detection of methylene blue as the model analyte.

Methylene blue has a tendency to strongly adsorb on the electrode surface, which affects long term monitoring with the same sensor. The system was instead designed to enable tracking the process throughput by allowing hot swapping of the used planar printed three electrode system with a new one without interrupting or disassembling the system. Different modules have been prepared to enable easy adjustment of the sample volume according to needs. Transparent cell components with microchannels were 3D-printed by using Digital Light Processing (DLP), while the flexible components were 3D-printed by using Fused Filament Fabrication (FFF).

Electrochemical detection was conducted via differential pulse voltammetry and square wave voltammetry. Methylene Blue (MB) was dissolved in phosphate buffer aqueous solutions (pH range 5-8, concentration range 10^{-9} - 10^{-4} M) and its properties examined using square wave voltammetry, differential pulse voltammetry, linear sweep voltammetry and cyclic voltammetry. Interelectrode reproducibility, which is crucial for this system design, has been tested by measuring calibration curves on different, identically produced and processed printed electrodes and comparing them against each other. Pretreatment and post-measuring treatment options were explored by using polarization at a fixed potential to enhance the electrochemical signal and evaluate possible regeneration of the sensing system.

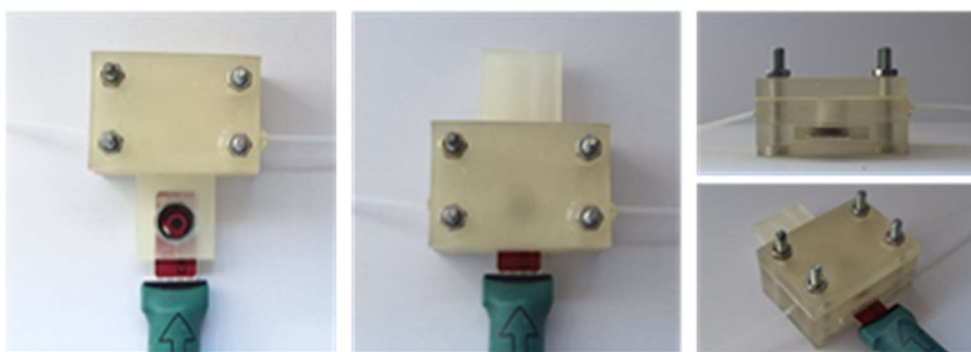


Figure 1. Fully printed modularized microfluidic setup

Acknowledgements. This work has been supported by the Croatian Science Foundation under grants HRZZ-UIP-2020-02-9139, HRZZ-IP-2022-10-8004, HRZZ-DOK-NPOO-2023-10-1144.

SURFACE MODIFICATION OF TITANIUM IMPLANTS WITH ELECTRODEPOSITED MULTIFUNCTIONAL CALCIUM PHOSPHATE COATINGS

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The need for durable, high-performance implant materials has grown with increasing longevity and quality-of-life standards, with titanium alloys being widely used due to their mechanical strength, biocompatibility and corrosion resistance.^[1,2] However, being bioinert, they offer limited bone interaction. Calcium phosphate (CaP) coatings, which mimic bone chemistry and support bone growth, are used to enhance osseointegration, improving the mechanical stability and long-term performance of implants.^[1,2] The CaP coatings were synthesized on the TiAlNb alloy using an electrochemical deposition technique. Despite standing out among various deposition techniques, there still remain difficulties in ability to finely control the characteristics of CaP coatings, which was the main topic of this study. Employing various electrochemical and structural spectroscopic techniques the optimization of electrodeposition process variables was performed with an emphasis on achieving consistent crystal structure and morphology and enhanced corrosion resistance.

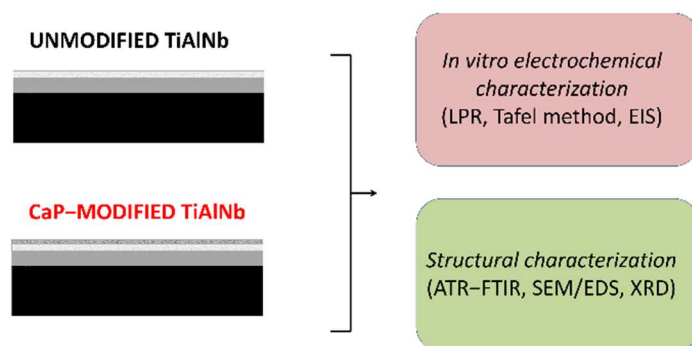


Figure 1. Illustrative diagram of the CaP coating preparation and electrochemical and structural characterization methods.

Acknowledgements. The research was conducted as part of the project “Biomimetic multifunctional calcium phosphate coatings with enhanced anticorrosion protection”, funded by the Croatian Academy of Sciences and Arts (HAZU) Foundation.

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CONDUCTIVE PEDOT-THERMOPLASTIC ELASTOMER FILMS FOR STRETCHABLE ELECTRONICS APPLICATIONS

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This research focuses on the synthesis and characterization of intrinsically stretchable and conductive composite films of poly(3,4-ethylenedioxythiophene) (PEDOT) and the thermo-plastic elastomer sulfonated polystyrene-block-poly(ethylene-ran-butylene)-block-polystyrene (S-SEBS). The aim was to develop materials for applications in flexible electronics, in particular for the fabrication of simple sensors to evaluate their effectiveness in detecting biological signals in the real world. The synthesis of the macroinitiator PEDOT-Br was optimized by adjusting the proportions of S-SEBS. Poly(acrylate-urethane) chains were then grafted onto PEDOT-Br to produce a self-healing polymer. These materials exhibited an electrical conductivity of about 3 S/cm and over 300 % stretchability, meeting the requirements for wearable bioelectronic devices. These materials were validated by using them as electrodes in electromyogram (EMG) measurements on human skin. EMG tests showed significant changes in signal intensity compared to background noise during muscle contractions. This confirmed not only the practical functionality of the PEDOT-Br and grafted PEDOT-g-PAU materials as electrodes, but also their ability to record the electrical activity of muscles accurately. The clarity and consistency of EMG data obtained with these novel polymer films indicate their considerable potential for use in clinical and fitness settings where monitoring muscle activity is critical. Their ability to maintain performance under mechanical stress underscores their suitability for real-world applications in wearable technology.

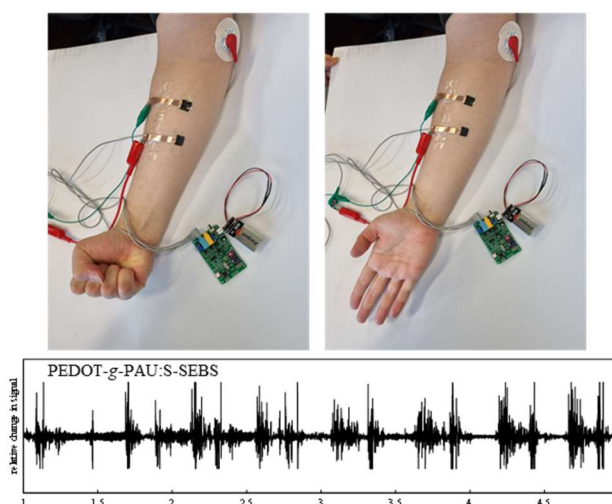


Figure 1. EMG signal acquired from forearm muscle using the grafted PEDOT-g-PAU:S-SEBS film as a stretchable on-skin electrode during repeated muscle contractions.

Acknowledgements. This work has been supported by Croatian Science Foundation.

FORMULATION OF DASATINIB-LOADED CYCLODEXTRIN NANOSPONGES FOR TARGETED DRUG DELIVERY

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Targeted drug delivery systems have emerged as a promising strategy to enhance the efficacy and safety of chemotherapeutic agents. Dasatinib, a tyrosine kinase inhibitor used in the treatment of chronic myeloid leukemia and Philadelphia chromosome-positive acute lymphoblastic leukemia, is associated with serious side effects, including cardiotoxicity, primarily due to its systemic exposure and rapid release. To address these challenges, β -cyclodextrin-based nanosponges were synthesized using diphenyl carbonate as a cross-linking agent to form a porous, three-dimensional network capable of encapsulating dasatinib. Cyclodextrin nanosponges represent highly promising drug delivery systems due to their high surface area, tunable porosity, and capacity to form inclusion complexes with hydrophobic drug molecules, thereby effectively modifying drug release profiles. Various analytical techniques were used to investigate the thermal behavior, crystallinity, chemical interactions, morphology, porosity, and drug loading efficiency of the prepared nanosponges. The nanosponges were subsequently incorporated into tablet formulations containing appropriate excipients to assess drug release characteristics. *In vitro* release studies demonstrated that dasatinib was released in a sustained and controlled manner from the nanosponge-based tablets, suggesting a significant potential for reducing dose-related toxicities and improving therapeutic outcomes. This delivery system offers a promising approach for enhancing the safety and efficacy of dasatinib, with potential applicability to other hydrophobic anticancer agents.

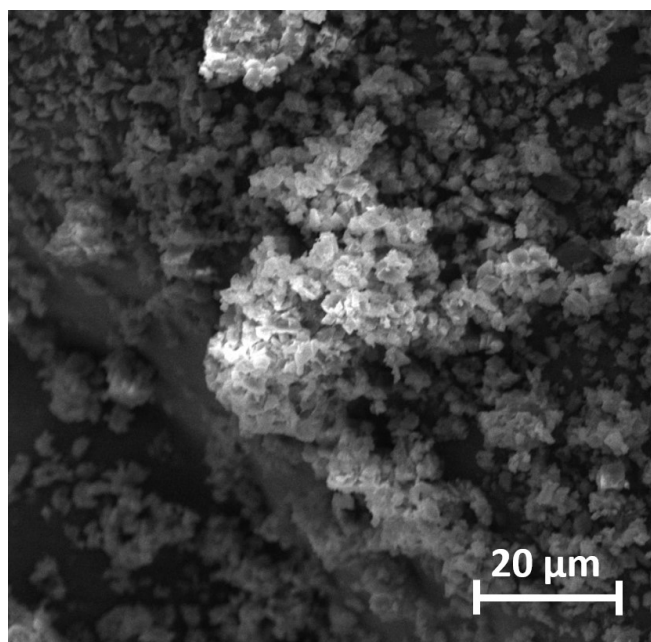


Figure 1. Micrograph of the obtained β -cyclodextrin-based nanosponges.

ENHANCING LITHIUM-ION BATTERY PERFORMANCE WITH SILICON–GRAPHITE COMPOSITE NEGATIVE ELECTRODES

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The increasing reliance on renewable energy sources present a significant challenge in energy storage due to inconsistency of the production of the energy. One of the most promising solution is usage of the lithium-ion batteries. These type of the batteries, compared with other secondary batteries, offer high energy and power density due to favourable properties of the lithium metal including low atomic mass, ionic radii and lowest reduction potential (−3.01 V). These properties positioned lithium ion batteries as the current state of the art in energy storage technology. Among various potential negative electrode materials, graphite is most widely used due to its ability to reversibly intercalate lithium, high cycling stability and theoretical capacity of 375 mAh/g. However, with growing electronic and automotive sector, demands for battery performance are far more than what graphite can offer. Possible solution is application of different kind of active material, in particular the silicon which is well known for the enormous capacity, of 4200 mAh/g, that even exceeds capacity of the lithium metal. Even though the silicon possesses highest known capacity for lithium storage, it is broadly reported that silicon undergoes to structural changes during each cycle, leading to pulverisation of the electrode. Instead of focusing on development of entirely new electrode material, composite negative electrodes based on silicon-graphite mixture present promising strategy to enhance the capacity without sacrificing the stability of the electrode. Although application of this kind of the composite could mark breakthrough in the battery industry, it is necessary to carefully design the electrode composite to achieve synergistical performance of both materials. Scope of the work is to find best ratio of the silicon and the graphite to achieve the electrode of high energy and power density. Different composites of the silicon and graphite was prepared with different ratio of the initial materials altering from pure components to 50:50 ratio. All components are prepared in type of the electrode slurry with carbon black and PVDF, and NMP as the solvent. Once electrodes were prepared, by coating and drying procedures, there were assembled inside of the Swagelok test cell as a working electrode and lithium as counter and reference electrodes. Electrochemical evaluation was performed using standard electrochemical testing including electrochemical impedance spectroscopy, galvanostatic charge and discharge and cyclic voltammetry. Following preparation of the electrodes and electrochemical testing, physical characterisation was conducted using X-ray diffraction (XRD), scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDS). Results of the research suggest that small amount of the silicon significantly increase the capacity of the graphite electrode without pulverisation phenomenon while large amounts of silicon decrease overall cyclability of the electrode.

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

SURFACE MODIFICATION OF Ti-6Al-4V ALLOY

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The most widely used material for orthopedic implants is the commercially available titanium alloy Ti-6Al-4V. Titanium alloys in general show excellent mechanical properties, corrosion resistance and biocompatibility among similar metallic biomaterials. However, adhesion of bacteria and biofilm formation on the implant's surface post-implantation is one of the main causes for revision surgeries in patients. One of the proposed solutions is modifying the surface of the metallic biomaterial with antibacterial agents such as copper.^[1,2] By containing the antibacterial agent to the surface, the mechanical and structural properties of the bulk material remain unchanged.^[3]

The purpose of this study is to assess impact of laser surface alloying of Ti-6Al-4V with copper on the microstructure, element distribution and microstructural properties e.g. microhardness. Thermodynamic modeling was performed using Thermo-Calc software based on CALPHAD method, and phase stability in equilibrium conditions was determined. Surface microstructure and distribution of Ti₂Cu phase were analysed by Optical Microscopy (OM) and Scanning Electron Microscopy (SEM), equipped with an energy dispersive X-ray spectroscopy (EDS) detector. A correlation between laser beam optimization, distribution of intermetallic phase and microhardness was determined.

Acknowledgements. The scientific paper was created during the implementation of the project The Development of an Innovative Antibacterial Material for Hip Prosthesis – AntibacHip – NPOO.C3.2.R3-I1.04.0324, financed by the EU – Next Generation EU.

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SPARK ABLATION COUPLED WITH AEROSOL DIRECT WRITING IN THIN FILM FABRICATION

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Spark ablation is a novel method capable of synthesizing stable nanoparticles below 20 nm, even in the quantum confinement range. While being an extremely material efficient and purely solid state, many aspects of this technique remain unassessed^[1]. In this work, we study the ablation of the target material, investigating the chemical and morphological aspects of thin film formation during aerosol direct writing of particles synthesized by spark plasma in a one-step process^[2]. The studied systems mainly involve titanium but also include copper and molybdenum. We utilize structural characterization techniques, such as SAED, XRD, XPS and Raman spectroscopy to study the influence of processing parameters (oxygen content, power, gas flow regime) on the chemical properties of the synthesized material. It was revealed that all of the oxide materials exhibit a highly oxygen deficient but crystalline structure. Moreover, we correlate the obtained structural information to optical properties of the thin films and also discuss the influence of plasma chemical composition on the final product of various syntheses. Morphology is investigated via TEM, FE-SEM and AFM to estimate the size, porosity and shape of the synthesized particles. It was found that many systems can produce single particles of sizes as small as 5 nm with most of the agglomerates being around 10–30 nm. It was also discovered that spark plasma induces certain reactivity in nitrogen by atomisation which plays a pivotal role in solid-state synthesis of thin films by this technique. Finally, a general thin film formation mechanism is proposed.

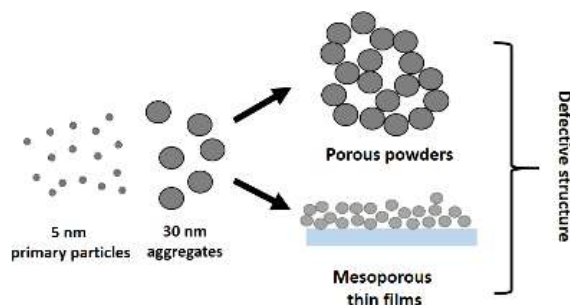


Figure 1. Schematic presentation of the experimental part and particle growth during spark ablation.

Acknowledgements. UIP-2019-04-2367 of The Croatian Science Foundation and COST CA1825 are gratefully acknowledged.

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INFLUENCE OF LiBOB CONCENTRATION ON THE STRUCTURE AND THERMAL PROPERTIES OF POLY(ETHYLENE-OXIDE)/LITHIUM MONTMORILLONITE NANOCOMPOSITE

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In this work, the influence of adding lithium bis(oxalate)borate (LiBOB) salt and lithium montmorillonite (LiMMT) on the glass transition temperature, melting temperature, and crystal structure of poly(ethylene oxide) (PEO) was investigated. Differential Scanning Calorimetry (DSC) and Fourier Transform Infrared Spectroscopy (FTIR) were used to analyze the material properties. Nanocomposite polymer electrolytes were prepared by mixing PEO with LiMMT in a weight ratio of 60/40, with the addition of LiBOB salt in various Li/EO molar ratios (defined as the molar ratio of lithium ions from the salt to the oxygen atoms in the ethylene oxide units). DSC analysis showed that the addition of LiBOB led to increased glass transition temperatures, indicating the formation of a PEO:LiBOB complex. Furthermore, the addition of LiBOB completely disrupted the crystallinity of PEO in the sample with Li/EO molar ratios of 1/7. Samples with Li/EO molar ratios of 1/9, 1/16, 1/32, and 1/40 showed endothermic peaks corresponding to the melting of the PEO crystalline phase, with melting temperatures lower than that of pure PEO. FTIR analysis confirmed that the crystallinity of PEO in the polymer electrolyte was influenced to varying extents by the concentration of LiBOB. Based on the obtained results, the system with the highest potential for application as a polymer electrolyte was determined.

ENHANCEMENT OF ANTIMICROBIAL PROPERTIES OF DECM-BASED HYDROGELS FOR APPLICATION IN SKIN TISSUE ENGINEERING

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Chronic wounds and skin injuries present significant clinical challenges due to the high risk of infection and impaired tissue regeneration. In skin tissue engineering, hydrogels derived from decellularized extracellular matrix (dECM) have gained attention for their biocompatibility, native tissue mimicry, and ability to support cellular adhesion and proliferation. However, their lack of intrinsic antimicrobial activity limits their efficacy in infected wound environments^[1]. Natural bioactive compounds such as allicin, a sulfur-containing molecule derived from garlic, and curcumin, a polyphenolic compound found in turmeric, have demonstrated potent antimicrobial, anti-inflammatory, and antioxidant properties. Integrating these agents into dECM hydrogels may provide a dual benefit, structural support for tissue regeneration and localized antimicrobial activity, to improve wound healing outcomes^[2,3].

dECM hydrogels were prepared from porcine tissue and characterized for their physical, chemical, and biological properties. Allicin and curcumin were incorporated individually in dECM-based hydrogel containing 5% w/v chitosan to assess antimicrobial effects. Chitosan was added to enhance the mechanical and antimicrobial properties of the hydrogel in an amount that demonstrated the best cell adhesion and viability. The resulting multicomponent hydrogels were tested against *Escherichia coli* using the minimum inhibitory concentration assay. The multicomponent hydrogels were characterized by their thermal (differential scanning calorimetry, DSC), mechanical (rheological testing), and chemical (Fourier transformed infrared spectroscopy, FTIR) properties to assess the structural integrity and successful incorporation of bioactive molecules. In vitro cytocompatibility was assessed using human dermal fibroblasts and keratinocytes through live/dead staining and metabolic activity (Alcian Blue™ assay).

Results demonstrated that both allicin and curcumin improved the antimicrobial performance of dECM hydrogels. Addition of curcumin changes the rheological behavior of hydrogels where the addition of both allicin and curcumin increases viscosity. Addition of bioactive molecules does not affect the thermal stability of hydrogel in temperature range for application in skin tissue engineering which is physiological conditions. It is confirmed via FTIR spectra that there is no chemical interaction between allicin and curcumin with the hydrogel matrix. These findings suggest that dECM-based hydrogels with allicin and curcumin represent a promising multifunctional platform for infection-preventing skin tissue scaffolds. Future work will focus on the optimization of concentration and biocompatibility of hydrogels prepared in this manner.

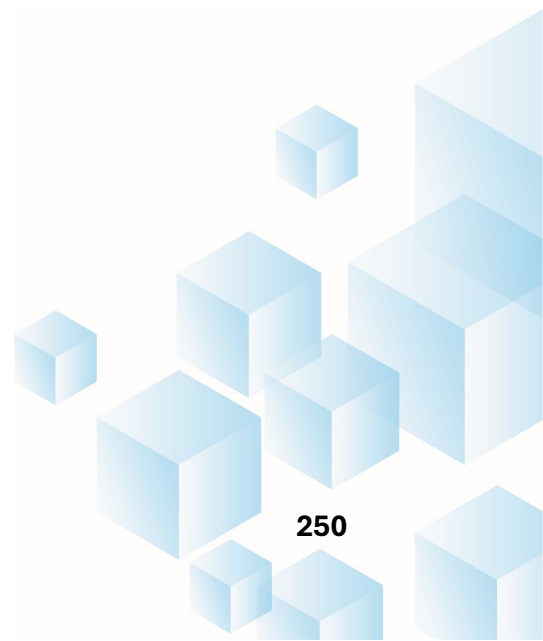
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POSTERS

ENVIRONMENTAL ENGINEERING AND SUSTAINABLE TECHNOLOGIES



ISOLATION AND IDENTIFICATION OF MICROORGANISMS FROM ACTIVATED SLUDGE POLLUTED WITH ANTIVIRALS

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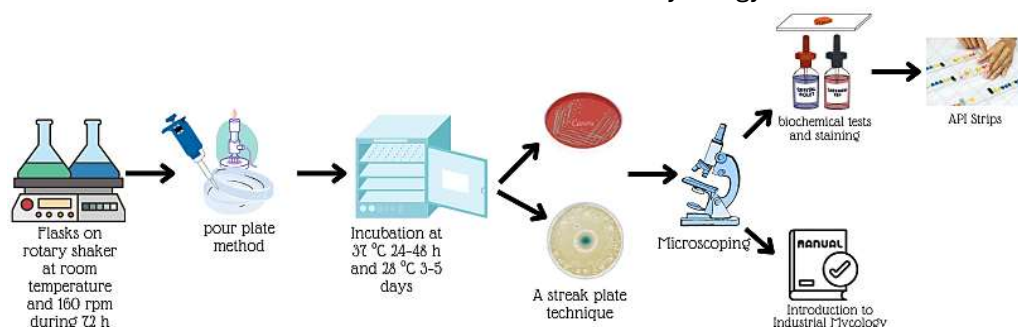
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In this study, the isolation and identification of microorganisms from activated sludge containing antiviral substances was performed. The activated sludge was collected from a municipal wastewater treatment plant in Zagreb, Croatia. In sterilized 250 mL Erlenmeyer flasks, 86 mL of the activated sludge was added with 14 mL of antiviral substances and shaken at 160 rpm for 72 hours at room temperature. After 72 hours, the colony forming units (CFU) of bacteria and fungi on the general purpose media (nutrient agar for bacteria and malt agar for fungi) were determined using the pour plate method. After incubation, the number of colonies on the agar plates was determined; the CFU for bacteria was $1.1 \cdot 10^5$ cells/mL, while the CFU for fungi was $2.6 \cdot 10^4$ cells/mL. The morphologically different bacterial and fungal colonies, which dominated on the nutrient agar and malt agar plates, were collected and transferred to the nutrient agar and malt agar plates and incubated at 37 °C for 24–48 hours and 28 °C for 3–5 days, respectively. Biochemical tests (catalase, oxidase and nitrate reductase), KOH test, Gram and Schaeffer-Fulton staining and motility test were performed on the pure bacterial cultures obtained. The cell morphology of the bacteria was observed under a light microscope, while identification was carried out using API (Analytical profile index, bioMérieux, France). According to the API results, *Brevundimonas vesicularis* (93.7 %), *Comamonas testosteroni* (86.8 %), *Bacillus amylolique-faciens* (99.9 %) and *Bacillus mycoides* (80.4 %) were identified. Yeast was identified using API 20 C aux (*Trichosporon mucoides*, 63.8 %), while the morphological characteristics of molds (*Fusarium* sp.) were determined using the methods described in the Introduction to Industrial Mycology.^[1]



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

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IT DEVICES AS DETECTORS IN SURFACE WATER QUALITY MONITORING

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This paper presents the application of IT devices as detectors in colorimetric chemical analyzes by determination in real water samples in nature. It is possible to develop a simple method of applying IT devices in chemical analyzes and, consequently, in the monitoring of environmental quality indicators, to include a wider population in these activities and thus to practice citizen science. This work represents the unification and continuation of previous research and developed methods for the application of IT devices for monitoring water quality indicators in nature. The aim of this research is to examine the physico-chemical parameters of the water in the lower course of the Neretva River at 4 locations where, during earlier research,^[1,2] the occurrence of increased salinity was determined and in the use of IT devices as detectors.

The performance of two different approaches is compared. The first approach is the Beer-Lambert principle, the second approach is based on the evanescent field absorption from an uncoated U-bend sensing region of an optical fiber. Variations in the salinity level of the surrounding medium of the fiber sensing region affect the absorption of the evanescent field and this can be monitored by a smartphone. The smartphone sensor has the ability to measure salinity level variations of as low as 0.1 parts per thousand (ppt) with high accuracy and repeatability,^[3,4]

The system could be a low-cost tool for measuring water quality in various rural and urban locations. The entire system is cost-effective, portable, and easy to use by students, recreationalists, and the general population for the purpose of popularizing science and practicing citizen science.

Acknowledgements. This work was supported by the Federal Ministry of Education and Science of the Federation of Bosnia and Herzegovina (Grants No. 05-35-4543-1/24, December 18th 2024).

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LIGHT-DRIVEN DEGRADATION OF PFAS USING Fe-MODIFIED SrTiO_3 PHOTOCATALYSTS

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In recent years, poly- and perfluoroalkyl substances (PFAS) have gained increasing attention due to their extreme persistence in the environment, their mobility and their potential harmful effects on human health and ecosystems. Due to their strong carbon–fluorine bonds, they are highly resistant to conventional remediation technologies, posing a major challenge for environmental treatment.^[1,2] This study investigates the potential of Fe-doped strontium titanate (Fe-SrTiO_3) as photocatalysts for the degradation of PFAS in the context of advanced oxidation/reduction (AO/RP) processes. The photocatalysts were synthesised with Fe molar ratios of 0.03, 0.05, and 0.07 to investigate the influence of dopant concentration on photocatalytic performance. The materials were characterised using photoluminescence (PL) and diffuse reflectance spectroscopy (DRS) to evaluate the charge carrier behaviour and light absorption properties, while zeta potential measurements provided insight into the surface charge properties. The photocatalytic activity was tested under both simulated solar and UV-A irradiation in a batch reactor system. The degradation of PFAS was monitored by LC-MS/MS to quantify the concentration changes over time. This work aims to evaluate the effects of Fe doping on the photocatalytic efficiency of SrTiO_3 in AO/RP applications, which is relevant for water treatment strategies to combat persistent fluorinated compounds.

Acknowledgements. This work has been supported by Croatian Science Foundation under project: Solar-assisted photocatalytic degradation of perfluorinated compounds in water – SoAPperF (IPS-2022-02-4780)

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INVESTIGATION OF THE CORROSION-INHIBITING PROPERTIES OF ROSEMARY EXTRACT FOR ALUMINUM

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Corrosion inhibitors are essential for extending the life of materials, improving safety and reducing maintenance costs in various industries. Aluminum is widely used in areas such as food packaging (especially in the form of foils), construction, automotive and aerospace due to its diverse and promising properties. With increasing concern over the environmental impact of synthetic inhibitors, research has focused on sustainable, plant-based alternatives. Among these, rosemary extract has emerged as a promising candidate due to its natural corrosion-inhibiting compounds.

In this study, rosemary extract was obtained by microwave-assisted extraction at different durations of 5, 10, 20, 40, and 60 minutes. The chemical composition of the extracts was analyzed by UV-visible and Raman spectroscopy. The anticorrosive effect was evaluated by electrochemical methods in a 3 % NaCl solution to simulate a corrosive environment.

The results showed that the rosemary extract effectively suppressed aluminum corrosion, indicating its suitability as an environmentally friendly corrosion inhibitor. The protective effect is attributed to the presence of bioactive components such as phenolic acids, terpenoids and flavonoids, which adsorb to the metal surface and form a passive barrier layer. This research supports the further development of green corrosion inhibitors and provides insights for further research in this field.



BRIDGING THE GAPS: GREEN STARTUP ACCELERATORS AND SUSTAINABILITY INNOVATION IN SERBIA

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Startups are innovative enterprises operating under high risk, impacting economy and society through new business models. The sustainable development shift emphasizes green startups' role in innovation and environmental protection. Green startups are among the fastest-growing sectors globally. Serbia's startup ecosystem was valued at €980 million (2020-2022) according to the 2023 "Startup Genome" report, excluding self-funded startups. Serbia has 200-400 startups, mainly in Belgrade (71%), Novi Sad (15%) and Niš (4%). Serbia ranks 54th in the "Global Innovation Index 2021" among moderate innovators. However, the ecosystem lacks systematic development strategy.

Green startups lack private sector investment, relying mainly on international donors but struggling to scale without local funding. Regulations and administrative barriers hinder green innovation. The "Green Up Hub" analysis reveals only 3 of 20 entrepreneurship programs include environmental sustainability. The academic sector remains underutilized. Serbian green startups face limited access to international markets and EU platforms due to administrative hurdles.

To foster green innovation in Serbia's startup ecosystem, the following measures are recommended: Systematic data collection on green startups and developing accelerators for sustainable sectors, Integration of sustainability principles into entrepreneurship education, Regulatory support for environmental laws and EU alignment, Investment incentives to promote green innovation and Enhanced science-industry links for research commercialization. At the moment, the *Global GreenChem Innovation and Network Program* is developing a *Green Chemistry Accelerator* to support sustainable startups and bridging the identified gaps. This accelerator will provide a model for creating a green startup community that delivers sustainable solutions and demonstrates viable alternatives to hazardous processes.

Acknowledgements. This research has been financially supported by the Ministry of Science, Technological Development and Innovation of Republic of Serbia (Contract No. 451-03-136/2025-03/200026) and UNIDO/GEF/University YALE "Global Greenchem Innovation and Network Programme" – GGINP. This work is related to the implementation of the United Nations Sustainable Development Goal 9 – Industry, Innovation and Infrastructure.



HARNESSING MICROBIAL POWER FOR SUSTAINABLE REMEDiation IN CIRCULAR ECONOMY

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The transition from a linear to a circular economy underlines the need to close material loops and minimize environmental impact. Bioremediation is in line with these goals by converting pollutants into less harmful or inert forms through natural biological processes. Compared to conventional methods, it requires less energy and resources and results in minimal secondary pollution. Bioremediation is generally more economical as less excavation, transportation and energy-intensive treatments are required. It is particularly effective for organic contaminants such as petroleum hydrocarbons and achieves high degradation rates under optimal conditions (temperature, pH, oxygen and nutrients). However, its applicability is limited when it comes to persistent, non-biodegradable pollutants such as certain heavy metals and radioactive substances, for which conventional technologies are still required.

In a 45-day laboratory study, the degradation of motor oil was investigated using bacterial strains isolated from petroleum-contaminated sites. Three strains — *Stenotrophomonas* sp., *Rhodococcus* sp. and *Bacillus* sp. — were tested for their efficiency in degrading residual oil over time. Residual oil concentrations (mg) and the corresponding percentages of biodegradation were measured every 15 days. On day 15, *Stenotrophomonas* sp. degraded about 62.73 % of the engine oil, *Rhodococcus* sp. showed a degradation rate of 51.22 %, while *Bacillus* sp. was the least efficient at this stage, degrading only 31.21 % of the engine oil. At day 30, the efficiency of *Stenotrophomonas* sp. increased to 70.91 %, *Rhodococcus* sp. also reached a biodegradation rate of 70.91%, while *Bacillus* sp. showed a modest improvement to 36.36 % degradation. After 45 days, *Bacillus* sp. showed a significant increase in biodegradability, reaching the highest rate among the three strains at 95.45 %, with only 1.5 mg of oil remaining. *Rhodococcus* sp. followed with a degradation rate of 84.90 %, while *Stenotrophomonas* sp. achieved a degradation rate of 76.63 %, leaving 7.8 mg. *Bacillus* sp. showed the highest degradation rate after 45 days, demonstrating the potential of indigenous microbial populations to improve remediation in oil-contaminated environments.

Bioremediation offers a sustainable solution for the treatment of biodegradable pollutants and is an important part of circular economy strategies. While not universally applicable, it is promising for site-specific environmental management. With the help of research and supporting measures, bioremediation can become the key to sustainable remediation.

Acknowledgements. This research has been financially supported by the Ministry of Science, Technological Development and Innovation of Republic of Serbia (Contract No. 451-03-136/2025-03/200026). This work is related to the implementation of the United Nations Sustainable Development Goal 15 – Life on Land.



WINTER LEVELS OF METALS IN ZAGREB AIR DURING 2014 AND 2024


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Particulate matter and levels of metals, which are some of its components, are some of the important air quality parameters in Europe and its monitoring, limit values in the air, as well as obligation to make measures and plans to reduce concentrations are defined in the EU Directive 2024/2881 on ambient air quality and cleaner air for Europe (recast). Levels of metals in Zagreb air are regularly monitored in particulate matter with an aerodynamic diameter less than 10 μm , PM_{10} . Elevated values of PM_{10} particulate matter are usually found in the winter period of the year due to increased emissions during heating season and meteorological conditions determined by the geographical location of the town. The aim of this paper was to analyse and compare the PM_{10} and As, Cd, Cu, Fe, Mn, Ni, Pb and Zn levels at an urban station in the western part of Zagreb during the winters of 2014 and 2024. Mass concentrations of PM_{10} particles were determined by gravimetry while the metal content was analysed using inductively coupled plasma mass spectrometry. Data were processed for samples collected from 1st January to 27th March of 2014 and 2024. The results showed a 22 % reduction in the mean value of PM_{10} for 2024. The number of days with a 24-hour limit value of 50 $\mu\text{g}/\text{m}^3$ was also reduced from 27 days in 2014 to 14 days in 2024. A significant decrease in 2024, ranging from 25 % to 38 %, was found in the mass concentrations of As, Cd, Cu, Ni, Pb and Zn. The level of manganese did not differ between years while the mean iron level was 40 % higher in 2024. The differences between working and non-working days in 2024 were also examined. Although the measuring station is influenced by different emission sources, no significant difference in levels was found between working and non-working days except for Ni, Fe and Mn.

Acknowledgements. This work was performed using the facilities and equipment funded within the European Regional Development Fund project KK.01.1.1.02.0007 “Research and Education Centre of Environmental Health and Radiation Protection – Reconstruction and Expansion of the Institute for Medical Research and Occupational Health” and Next Generation EU (Program Contract of 8 December 2023, Class: 643-02/23-01/00016, Reg. no. 533-03-23-0006)-EnvironPollutHealth. Measurements of PM_{10} and metals in PM_{10} were carried out at monitoring station of the local air quality monitoring network funded by the City of Zagreb.



SWEET AND SOUR CHERRY PITS AS SUSTAINABLE GREEN SORBENTS FOR THE TREATMENT OF HEAVY METAL-CONTAMINATED WATER

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Sweet cherry and sour cherry pits were used as green, readily available sorbents for the treatment of zinc(II)-contaminated water of varying degrees of pollution. The experiments were conducted in batch mode at initial zinc(II) concentrations ranging from 0.5 to 5 mmol/L, at 230 rpm, at a solid-liquid ratio of 1 g / 100 mL, at room temperature for 24 hours. Monitoring of the pH value after sorption did not show any possibility of zinc(II) precipitation, indicating that the zinc removal was solely a result of the sorption process. The sorption capacity of sweet cherry pits ranged from 0.022 to 0.038 mmol/g, while that of sour cherry pits ranged from 0.018 to 0.061 mmol/g, depending on the initial zinc(II) concentration. The maximum removal efficiency was achieved for the lowest zinc(II) concentration and equalled 49.5 % for sweet cherry pits and 41.3 % for sour cherry pits, while the highest capacity was achieved, as expected, for the highest initial Zn(II) concentration. Sour cherry pits showed a higher capacity compared to sweet cherry pits, indicating different sorption behaviour of the materials, despite similar composition.^[1,2] According to the obtained results, both pits can serve as potential sorbents in water treatment, especially for lower concentrations of pollutants. Moreover, it is worth nothing that the tested pits were used in their original form without any modifications, which makes their use even more environmentally friendly and cost-effective. In order to increase the removal efficiency, future research should focus on optimizing the process conditions, especially regarding the pH value, which significantly affects the availability of functional groups present on the surface of the material. Overall, the use of industrial by-products contributes to the goals of circular economy, green transition and more sustainable agricultural waste management, while reducing the need for expensive synthetic adsorbents.

Acknowledgements. Thanks to the RETSCH GmbH for the generous donation of a new MM 200 to enable science.

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TUNING PROPERTIES OF PLA/PHBV BLENDS WITH BIOPLASTICIZERS FOR FOOD PACKAGING

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The widespread use of non-biodegradable synthetic plastics in food packaging has led to serious environmental concerns. For this reason, sustainable alternatives such as polylactide (PLA) and poly(3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV) have gained increasing attention due to their renewable origin and biodegradability. In this study, PLA/PHBV blends (75:25 wt%) were prepared using a Brabender kneader and plasticized with 5, 10, and 15 wt% acetyltributyl citrate (ATBC) and polyethylene glycol (PEG 600) to improve miscibility and adjust material properties. The blends were extensively characterized, including morphological, thermal, rheological, mechanical, and barrier property analyses. The addition of the bioplasticizer improved phase compatibility and lowered the glass transition temperature, indicating improved chain mobility and miscibility between PLA and PHBV, while maintaining overall thermal stability. Rheological tests confirmed reduced viscosity and improved processability, while mechanical tests showed reduced brittleness and increased elongation, indicating improved ductility. However, an increase in oxygen transmission rate was observed, which can be attributed to a trade-off in barrier performance due to increased free volume and a decrease in polymer crystallinity as a result of plasticization. Overall, the results highlight the potential of plasticized PLA/PHBV blends as viable, biodegradable alternatives for food packaging with tunable properties that can be optimized according to specific application requirements.

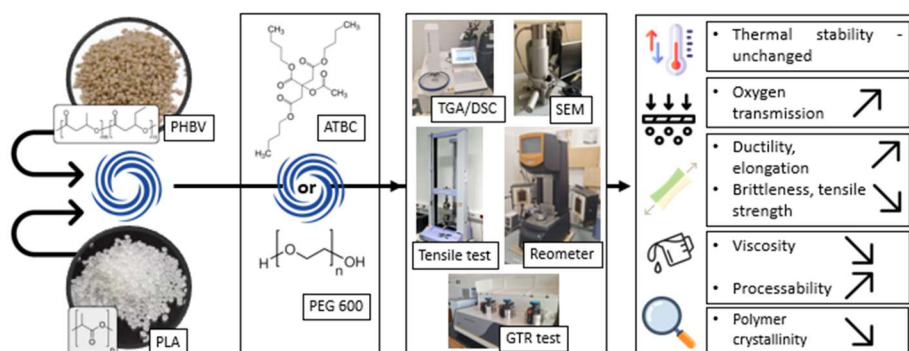


Figure 1. Preparation and characterization of PLA/PHBV blends with plasticizers.

Acknowledgements. This research was carried out as part of the project “Production and development of compostable packaging from waste biomass for the packaging of industrially processed food products” (NPOO.C3.2.R3-IL.04.0059) financed by the National Recovery and Resilience Plan (financed by the European Union, NextGenerationEU).

COMPARISON OF SELECTED VOLATILE ORGANIC COMPOUNDS IN ZAGREB CITY HOUSEHOLDS ACROSS TWO SEASONS

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Volatile organic compounds (VOCs) are a typical example of indoor air pollutants, and their effects on human health have made indoor air quality a significant concern. VOCs originate from both biogenic and anthropogenic sources and can form secondary pollutants, such as ozone and aerosols. According to studies, indoor VOC concentrations are often higher than outdoor levels, emphasising the importance of assessing and exploring their effects on human health.^[1] This work aims to present levels of selected VOCs in indoor air of Zagreb households that are known to have predominantly indoor sources, such as various solvents, disinfection by products, cleaning products, deodorants and antiperspirants, lubricants, degreasers, adhesives, paints, coatings, fragrances, and cigarette smoke. The sampling was conducted in ten households during both the winter and summer periods of 2024. The following compounds were measured: chloroform, trichloroethylene, tetrachloroethylene, 1,4-dichlorobenzene, 2-methylpentane, 2-methylhexane, methylcyclopentane, methylcyclohexane, styrene, and heptane. The results indicated that the levels of all of the measured VOCs in households were higher during winter, which is consistent with previous findings from the literature.^[2] Given the preliminary results obtained in this study, further measurements of VOCs in households will be carried out, taking into account the seasonality of their levels.

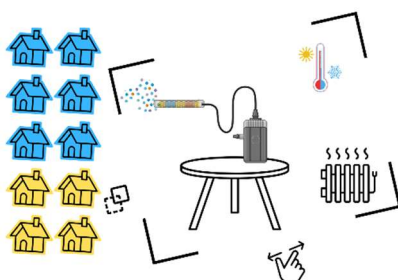


Figure 1. Scheme of the VOC active sampling in households.

Acknowledgements. This work has been funded by the European Union's Horizon Europe research and innovation programme under Grant Agreement No. 101057497 (EDIAQI) and supported by Programme Contract European Union – Next Generation EU No. 533-03-23-0006 (EnvironPollutHealth). This study was performed using the facilities and equipment funded by the European Regional Development Fund project KK.01.1.1.02.0007 (ReC-IMI).

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BIOMARKER FINGERPRINT AS A FORENSIC TOOL FOR OIL SPILL SOURCE IDENTIFICATION IN ALLUVIAL SEDIMENTS

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Oil pollutants are among the widespread contaminants in the world. Their content and composition is influenced by both, the content of the original crude oil or its derivative, and by the environmental conditions at the location of their spillage. Although the environmental conditions can change significantly the content of oil pollutants, their biomarker fingerprint can remain intact and therefore can be used for the source identification.

The aim of this study was application of saturated biomarkers for oil spill source identification in alluvial sediments. The investigated location is located in the alluvial plain of the Sava River, in the vicinity of the heating plant in New Belgrade, Serbia, and it is covering the surface area of 300 000 m².

Surface soil and sediment samples were collected at several microlocations from this locality. From these samples extractable organic matter was isolated with dichloromethane using a Soxhlet apparatus. Saturated hydrocarbons were isolated from the extracts using a column chromatography and analyzed by GC-MS. The instrumental analysis included typical petroleum biomarkers: *n*-alkanes in the ($m/z = 71$), steranes ($m/z = 217$) and terpanes ($m/z = 191$). The analytical procedure employed was described in our previous papers.^[1,2]

The distribution of the *n*-alkanes revealed that most of the samples contained a mixture of an oil pollutant and a native organic matter. Their ratio varied depending on the distance from the heating plant, which was the only suspected source of oil pollution in this area. The analyses of steranes and terpanes showed that, at some locations, different oil pollutants were present. These results suggested that multiple discharges of the oil pollutants to the surrounding soil occurred over the years.

According to these results it can be concluded that biomarker fingerprint can be a useful tool for oil spill identification and source discrimination in alluvial sediments.

Acknowledgements. This research has been financially supported by the Ministry of Science, Technological Development and Innovation of Republic of Serbia (Contract No. 451-03-136/2025-03/200026 and Contract No. 451-03-65/2024-03/200169). This work is related to the implementation of the United Nations Sustainable Development Goal 15 – Life on Land.

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PESTICIDES BURDEN IN SURFACE WATERS ADJACENT TO SMALL AGRICULTURAL HOLDINGS IN EASTERN SERBIA

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Extensive usage of pesticides during agricultural practices can cause a pollution of soil but it can also cause a pollution of surface and ground waters.^[1] In the current research, the aim was investigation of the presence and concentration level of pesticides in surface waters adjacent to small agricultural holdings in eastern Serbia.

The water samples analyzed in this study were sampled from five representative locations. In the water samples, pesticides were analyzed with gas chromatography – mass spectrometry (GC-MS) technique in the selected ion monitoring mode using one target and three qualifier ions for each analyte. Also, a series of samples with spikes was used to confirm the extraction efficiency of the method.

The results confirmed presence of pp-DDE (in concentration range from not detectable (ND) to 28.92 $\mu\text{g kg}^{-1}$), fludioxonil (from ND to 166.81 $\mu\text{g kg}^{-1}$), metalaxyl (from ND to 164.03 $\mu\text{g kg}^{-1}$), azinophos ethyl (from ND to 334.02 $\mu\text{g kg}^{-1}$), tetrahydroptalimide (from ND to 38.07 $\mu\text{g kg}^{-1}$), difenconazole (from ND to 75.23 $\mu\text{g kg}^{-1}$), resmethrin (from ND to 54.23 $\mu\text{g kg}^{-1}$), fenvelarate (from ND to 263.20 $\mu\text{g kg}^{-1}$), diazinon (from ND to 145.56 $\mu\text{g kg}^{-1}$), linden (from ND to 74.2 $\mu\text{g kg}^{-1}$), carbaryl (from ND to 30,61 $\mu\text{g kg}^{-1}$), cypermethrin (from ND to 159.62 $\mu\text{g kg}^{-1}$), delta HCH (from ND to 37.48 $\mu\text{g kg}^{-1}$), myclobutanil (from ND to 275.53 $\mu\text{g kg}^{-1}$), krezoxym methyl (from ND to 185.47 $\mu\text{g kg}^{-1}$), azoxystrobin (from ND to 16.32 $\mu\text{g kg}^{-1}$), and hexachlorobenzene (from 10.02 to 23.12 $\mu\text{g kg}^{-1}$).

The number of the pesticides detected and their amounts indicate that these waters were exposed to a serious input of these pesticides and point to the need for continuous monitoring of the pesticides in this area.

Acknowledgements. This research has been financially supported by the Ministry of Science, Technological Development and Innovation of Republic of Serbia (Contract No. 451-03-136/2025-03/200026, 451-03-47/2025-01/200030 and 451-03-68/2025-14/200168). This work is related to the implementation of the United Nations Sustainable Development Goals 6 – Clean Water and Sanitation, 14 – Life Below Water, and 15 – Life on Land.

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ENHANCING RO MEMBRANE SELECTIVITY FOR *N*-NITROSAMINE AND BORIC ACID REJECTION VIA 1,10-DIAMINODECANES PLUGGING

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Disinfection by-products (DBPs), particularly *N*-nitrosamines (NTRs) such as *N*-nitrosodimethylamine (NDMA), pose significant health risks due to their carcinogenicity and poor removal by conventional reverse osmosis (RO) membranes.^[1] Similarly, boric acid – an uncharged form of boron commonly found in desalinated water – frequently exceeds WHO and agricultural standards after single-pass RO treatment.^[2] This study evaluated the *in-situ* modification of five commercial RO membranes (ACM4, BW30XFRLE, AK, UTC73HA, ACM5) using 1,10-diaminodecane (1,10-DI), a linear alkyl diamine applied at 0.5 and 2.0 mM. The molecular plug approach reduced membrane pore size and altered surface properties, enhancing selectivity. Water permeability decreased by 10–34 % (0.5 mM) and 5–44 % (2.0 mM), remaining within acceptable operational ranges. Notably, NDMA rejection improved by up to 15 % and boric acid rejection by up to 24.1 %. These results highlight the potential of *in-situ* molecular plugging with 1,10-DI as a practical strategy to improve RO performance for challenging small, neutral contaminants while preserving operational viability.

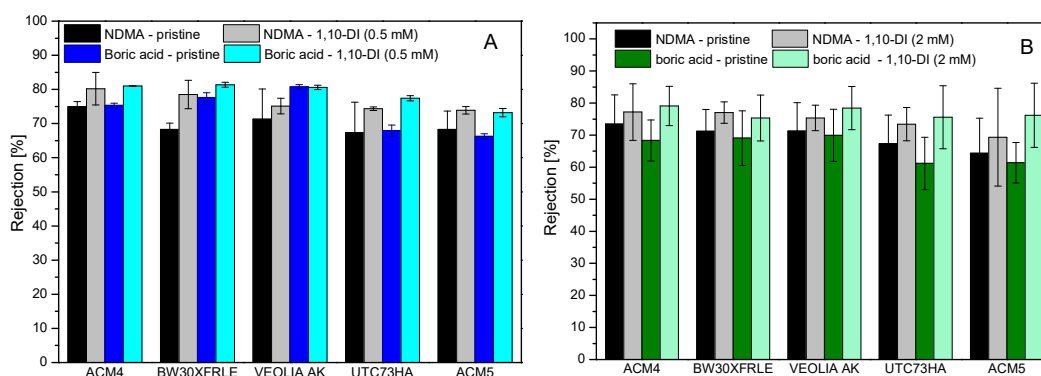


Figure 1. Impact of molecular plugging with 1,10-DI on NDMA and boric acid rejection by RO membranes using plugging solution concentrations of (A) 0.5 mM and (B) 2 mM.

Acknowledgements. This work was supported by the Croatian Science Foundation under the project number [HRZZ-IP-2024-05-7383].

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COMPARATIVE CHARACTERIZATION OF FLUIDIZED BED FLY ASH AND CONVENTIONAL FLY ASH FOR USE IN SELF-COMPACTING CONCRETE

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Self-compacting concrete (SCC) is a type of concrete that flows to completely fill the formwork without the use of additional vibrating devices.^[1] Fly ash (FA) is a powdered mineral additive for concrete produced by the combustion of coal in power plants.^[2] Fly ash obtained by high-temperature combustion technology is most often used as mineral additives in concrete mixtures, and is produced by combustion at temperatures up to 1750 °C. Morphologically, these amorphous particles are characterized by their spherical shape and smooth surface^[2,3]. However, fluidized bed combustion technology is increasingly being used today, where the combustion temperature reaches around 900 °C, which saves energy during the process itself. Due to the significantly lower combustion temperature, the particles of fly ash obtained in this way are irregular in shape and contain more crystalline phases. The use of fluidized bed fly ash is currently not standardized for traditional concrete, including self-compacting concrete.^[3] It is known that the most important properties of fly ash as a mineral additive for concrete production are: particle fineness, moisture content, loss on ignition and chemical composition.^[4] The aim of this work is to compare the properties of different fly ash samples using laser diffraction (*which involves determining the size of particles as well as their distribution*), X-ray fluorescence spectroscopy (XRF) (*to determine the chemical composition*) and scanning electron microscopy (SEM) (*insight into the morphology, microstructure and texture of the samples*) methods, to determine the key differences between fluidized bed fly ash and conventional fly ash used as a mineral additive in cement for the production of self-compacting concrete.

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FROM AIRBORNE PARTICLES TO SOIL DEPOSITS: UNDERSTANDING THE DISTRIBUTION OF PAHS AND HEAVY METALS

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Air and soil pollution by polycyclic aromatic hydrocarbons (PAHs) and heavy metals presents a complex environmental challenge, especially in urban and peri-urban settings influenced by different emission sources. This study explores the spatial and temporal distribution of PAHs and heavy metals in PM₁₀ particles and surface soils across the Zagreb region, Croatia, integrating data from multiple monitoring campaigns conducted over several years. Explainable machine learning (ML) models, including Random Forest (RF), Nonnegative Matrix Factorization (NMF), and Principal Component Analysis (PCA), were applied to evaluate the influence of traffic, industrial activity, meteorological conditions, and land use patterns on pollutant concentrations and accumulation trends. The analysis reveals that concentrations in PM₁₀ are connected to seasonal dynamics, with elevated levels of PAHs and certain metals during colder months. This is primarily due to increased emissions from residential heating, combined with atmospheric stability conditions, such as temperature inversions, that limit vertical mixing and lead to the accumulation of pollutants near the ground. In contrast, soil contamination appears more stable over time but reflect spatial gradients linked to historical deposition, traffic proximity, and industrial zones. Temperature, precipitation, and wind speed emerged as main drivers of pollutant variability in air.

The combined air-soil perspective offers new understanding of pollutant behavior, mobility, and persistence in the environment. These findings revealed the need for integrated air and soil monitoring strategies and demonstrate the value of interpretable ML in guiding environmental risk assessment and targeted mitigation efforts.

Acknowledgements. This work is supported by Next Generation EU under the EnvironPollutHealth project, Program Contract of 8 Dec 2023, Class: 643-02/23-01/00016, Reg. no. 533-03-23-0006. We gratefully acknowledge the use of facilities and equipment at the Institute for Medical Research and Occupational Health, made possible through the European Regional Development Fund project KK.01.1.1.02.0007: *Research and Education Centre of Environmental Health and Radiation Protection – Reconstruction and Expansion of the Institute for Medical Research and Occupational Health*.



APPLICATION OF ATR-FTIR SPECTROSCOPY FOR THE IDENTIFICATION OF MICROPLASTICS

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The mass production and use of plastic began in the 1950s. Since then, enormous quantities of plastic waste have found their way into the world's seas and oceans, which today represent a global environmental problem. The term microplastic was coined in 2004 in the paper by R. C. Thompson et al, Lost at Sea: Where Is All the Plastic?, Science 304 (2004) 838, in which microplastics are defined as particles smaller than 5 mm. Since then, the number of studies dealing with the distribution, toxicology and analytical methods of microplastics has increased exponentially. ATR-FTIR (Attenuated Total Reflectance Fourier Transform Infrared) spectroscopy is a commonly used analytical method for the identification of microplastics as it is fast, simple and non-destructive. It should be noted that IR spectroscopy is very effective when analysing pure substances—which is never the case with plastic waste samples. In addition, ATR-FTIR spectroscopy only analyses the surface of a sample. As microplastic particles often spend long periods of time in the ocean, organic contaminants can be deposited on their surface, which poses an additional challenge for the analysis.

In this study, microplastic samples collected with a net from the sea surface in the Bay of Kotor were analysed. ATR-FTIR spectroscopy and polarisation microscopy were used for the analysis. The limitations of the ATR technique were identified in terms of particle size and pre-treatment of the microplastic samples. The study showed the importance of good sample preparation for FTIR analysis. In contrast to previous studies, where the protocol of Kovač-Viršek et al.^[1] was used, in the current study a complete preliminary degradation of the organic matter (chemical digestion) was applied to remove the organic matter that might be retained on the surface of the sample. By comparing the samples, we conclude that the quality of polymer categorisation by FTIR has improved significantly. Therefore, it is recommended to follow the protocol of Galgani et al.^[2], prepared by the MSFD Technical Group on Marine Litter, for all further investigations.

Acknowledgements. This work has been supported by the project MEDiverSEAty – “In quest of the human dimensions of MEDiterranean Marine Biodiversity”, funded by HORIZON-TMA-MSCA-DN.

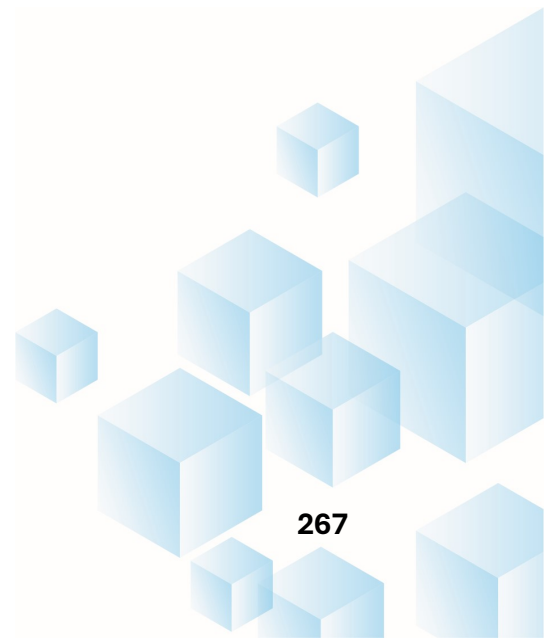
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POSTERS

EDUCATION





ADOPTION OF EDUCATIONAL OUTCOMES IN CHEMISTRY THROUGH THE EXTRA-CURRICULAR ACTIVITY “ORCHARDISTS GROUP” USING THE EXAMPLE OF DETERMINING THE STREIF INDEX

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Achieving learning outcomes in chemistry is the primary task of teaching chemistry in primary schools. Based on the chemistry curriculum for primary schools, four macroconcepts have been identified (substances, changes and processes, energy, and the scientific approach).^[1] Learning outcomes are achieved through regular classes, but also through extracurricular activities.

The school curriculum consists of the development of extracurricular programs and activities that schools will implement according to students' preferences. The aim of the paper is to take a closer look at the experiences in integrating extra-curricular activities into the school curriculum extracurricular activity “Orchardists Group” in the Sveti Martin na Muri Primary School as one of the possibilities of achieving learning outcomes in chemistry using the examples of the procedures for determining the ripeness of apple fruits (Streif index). The Streif index combines three indicators of ripeness and quality of fruits. These are fruit hardness, sugar content and starch index according to the Ctifl scale.

The extracurricular activity “Orchardists Group” is not a mandatory part of the students’ workload, but it can be recognized by students as fulfilling their obligations at school. The students have the opportunity to assess their own work, the work of other students, and the work of their teacher. This develops the students’ ability of self-assessment and criticism, but also the teachers’ openness to the opinions and viewpoints of their students.^[2] In accordance with the Regulations on Assessment and the parameters assessed in chemistry teaching (mastery of chemical, scientific competence), it is possible to reward and encourage such a way of working with a good grade created by the teacher, driven by the activity and motivation of the students.^[3]

The implementation of the planned activities has adhered to many of the guidelines of the national curriculum, and especially the chemistry curriculum. The learning outcomes achieved by students through the listed activities are in fact fundamental competencies that will be important for them in their further education and life.

Acknowledgements. This work has been supported by the Ministry of Science, Education and Youth.

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FROM THEORY TO PRACTISE: SCIENTIA PROJECTS AS A MODEL FOR MODERN STEM TEACHING

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In order to improve the pedagogical skills and practises of chemistry and biology teachers and to motivate students, a series of activities were carried out with second and third grade students at the School of Science in Split as part of the Scientia projects. The Scientia 1 and 2 projects were designed and implemented with the aim of strengthening and expanding the interests, competences and skills of gifted students. In addition, through co-operation with the Faculty of Chemistry and Technology and the Faculty of Science, avenues were opened for teacher activities in the field of natural science. Through learning according to the principles of project work, applying scientific methods and developing creativity, self-confidence and motivation in students, the project made a significant contribution to motivation, the development of skills and attitudes suitable for lifelong learning, based on critical thinking, the presentation of arguments and the development of co-operation and responsibility. The aim of this article is to demonstrate the importance of interdisciplinary work in relation to current trends in teaching and research – modular teaching/STEM. The activities designed in the subjects of chemistry, biology, physics and computer science were problem and research orientated and included theoretical and practical aspects of the work. Soft skills and communication skills, self-concept and stress management skills were promoted through simple laboratory techniques, but also through the use of spectrophotometry, ultrasound and microwave methods in extraction and analysis. Both students and teachers actively participated in the workshops, acquiring knowledge and tools for working with gifted students and passing on their knowledge when working with other children.

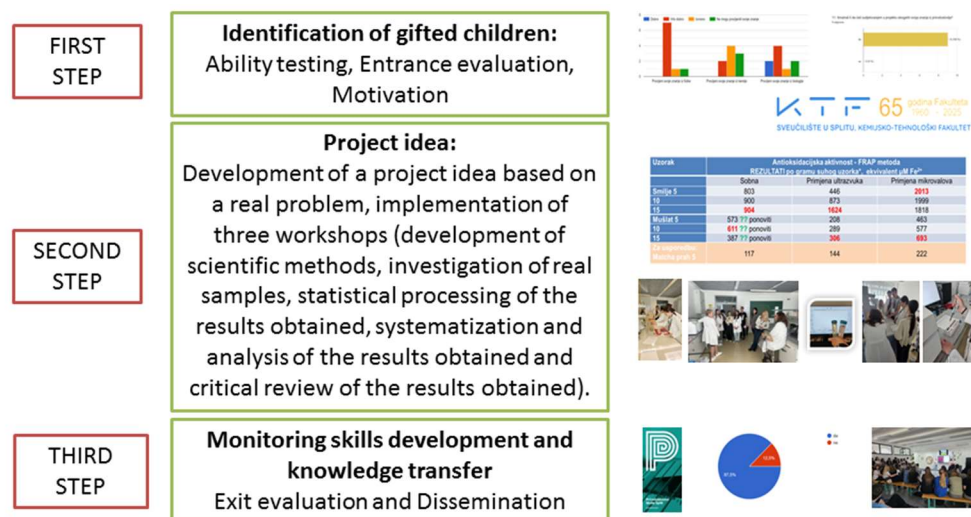


Figure 1. Steps in project implementation.

AI AND CHEMISTRY – SMART SCIENCE OF THE FUTURE

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In today's world, artificial intelligence (AI) is increasingly used in science, including chemistry. This project introduces 7th and 8th grade students to the basics of AI and its applications in chemical research and everyday life. Activities include recognizing substances using AI-powered applications, simulating chemical reactions with digital tools, and analyzing experimental data using simple AI systems. Students develop critical thinking, digital skills, and an understanding of the link between technology and science. The project promotes interdisciplinary learning, scientific literacy, and awareness of future learning and career opportunities in STEM. Learning outcomes achieved during the project include: OŠ. A.1.3. The student uses AI to support learning; and OŠ. A.1.4. The student creates simple digital content with the help of AI. As part of the project, students create simple applications such as chatbots, object recognition apps, experiment generators, and video content. In our work, we used the programs Copilot, Perplexity, Chat GPT, InvideoAI, Teachable Machine, Snatchbot and tried many other AI applications that could help students learn chemistry content. At the same time, using AI tools, they checked the results and learned critical thinking when using AI tools

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INTRODUCING ADVANCED ANALYTICAL METHODS TO HIGH SCHOOL STUDENTS: CAN DIFFERENT CANDLE WAXES BE DISTINGUISHED BY ^1H NMR SPECTROSCOPY?

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Second-year high school students learned during a course in organic chemistry that candle wax can be made from various alternative materials apart from paraffin. With proper guidance, they have prepared or acquired four different types of candle wax: paraffin, beeswax, soy wax, and the used cooking vegetable oil wax – which was synthesized in the school laboratory by following commonly available instructions found online.^[1]

After the candle making, students were curious about wax content and analytical methods used to distinguish various waxes. Apart from more widespread methods such as FTIR or HPLC, an opportunity arose to make ^1H NMR analysis at the NMR Lab of the Department of Chemistry, Faculty of Science, University of Zagreb. After the initial literature search of similar studies,^[2,3] the samples were prepared. The analysis was carried out in CHCl_3 as a solvent, and spectra have been obtained. Although the full analysis and assignment of wax components were beyond the student's level of comprehension, the spectra showed visible differences between waxes and proved that waxes can be distinguished by this method. With further guidance, students learned that some signals in the spectra can be easier to interpret than others and that they may indicate the presence of specific compounds in the wax samples.

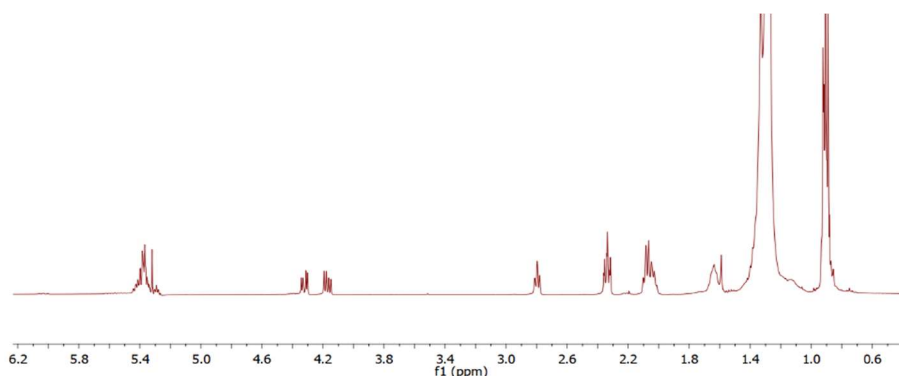


Figure 1. ^1H NMR spectrum of candle wax made from waste cooking oil (dissolved in CHCl_3)

Acknowledgements. This work could not be possible without resources provided by the NMR Laboratory of the Department of Chemistry, Faculty of Science, University of Zagreb. A special thanks goes to Dr. Katarina Leko for her advisement, guidance and measurements.

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A JOURNEY THROUGH TIME – A CHEMISTRY LESSON WITH THE HELP OF ARTIFICIAL INTELLIGENCE

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In recent decades, we have witnessed an incredibly rapid development of technology that is transforming the way we live, communicate, and work. Digitalization has touched nearly every aspect of human daily life. Among all technological advancements, artificial intelligence (AI) stands out in particular — a technology that enables computers to “think”, analyze data, make decisions, and behave in ways that, to some extent, mimic human intelligence.

A successful example of applying artificial intelligence in education was demonstrated during a seventh-grade chemistry class. Students reviewed the history of chemistry through an interactive and dynamic approach that incorporated games, movement, and digital tools. A key role was played by a virtual character named Mirko—a time traveler created with the help of AI, who acted as a guide and motivator. Mirko interacted with students, encouraged collaboration, and facilitated understanding of the material. Students “activated” the time machine through physical activities and traveled through three historical periods of chemistry. First, they arrived in the age of alchemy, where they used association games to discover concepts such as Barbara of Cilli, the philosopher’s stone, and the elixir of life, developing their logical thinking and verbal expression. The next stop was Lavoisier’s laboratory in 1785, where students, through questions and riddles, reviewed key contributions of this scientist to modern chemistry. The third time jump brought them to the year 1975, where they used a quiz to reinforce their knowledge about Croatian Nobel laureates Ružička and Prelog.

This teaching method combined tradition and technology, boosting motivation, collaboration, and deeper content understanding, while offering a vision of an AI-based future of education. Artificial intelligence in schools offers great potential—it can ease teachers’ workloads, enable personalized learning, and help students acquire knowledge more effectively. However, it is crucial to view AI as support, not a replacement for teachers. Teachers still play the central role in the educational process—not only as knowledge transmitters but also as mentors, leaders, and role models. Human empathy, understanding, and the teacher-student relationship remain the irreplaceable foundations of quality education.

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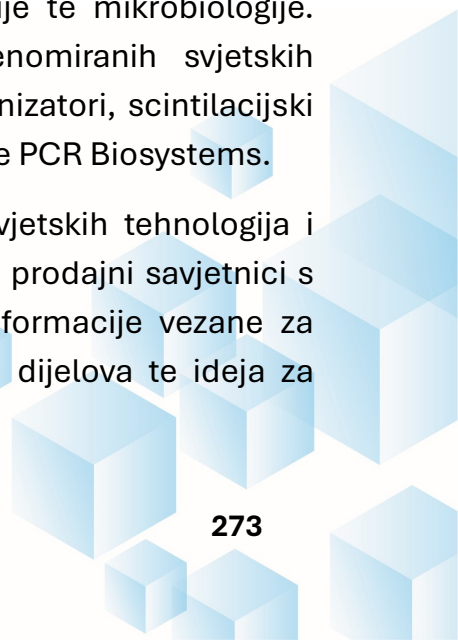
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Odjel Analitike tvrtke Jasika d.o.o. specijaliziran je za distribuciju laboratorijske opreme brojnih renomiranih svjetskih proizvođača od kojih izdvajamo PerkinElmer u područjima molekularne spektroskopije (UV-Vis, FT-IR, FT-IR mikroskopija, fluorimetrija), termalne analize (DSC, TGA, STA, TMA i DMA), kromatografije (GC, LC, GC-MS, LC-MS/MS), hipernacijskih sustava (IR-TGA, TGA-GC/MS, IR-TGA-GC/MS) te anorganskih tehnika analize (AAS, ICP-OES i ICP-MS), Berghof (uređaji za mikrovalnu digestiju i ekstrakciju, visokotlačni i niskotlačni reaktori te pročišćivači kiselina), Cole-Parmer (SpexSamplePrep - homogenizatori, kriogeni mlinovi te SpexCertiPrep standardi i *custom made* standardi), Labtech (generatori plinova, centrifuge, uparivači, ekstraktori, kupelji) te Evoqua (uređaji za pročišćavanje vode). Odjel Analitike također obuhvaća i *Life Science* program namijenjen za istraživačke i dijagnostičke institucije u poljima biokemije, molekularne i stanične biologije, protočne citometrije te mikrobiologije. Program se specijalizirao za distribuciju opreme brojnih renomiranih svjetskih proizvođača poput Revvity (čitači mikrotitarskih pločica, homogenizatori, scintilacijski brojači, NGS reagensi), eBioscience (ELISA, protutijela), Luminex te PCR Biosystems.

Naš dinamičan tim stručnjaka uvest će Vas u svijet vodećih svjetskih tehnologija i inovacija te upravo za Vaše potrebe predložiti najbolje rješenje, a prodajni savjetnici s dugogodišnjim iskustvom stoje Vam na raspolaganju za sve informacije vezane za program prodaje instrumenata, potrošnog materijala i rezervnih dijelova te ideja za provedbu projekata.

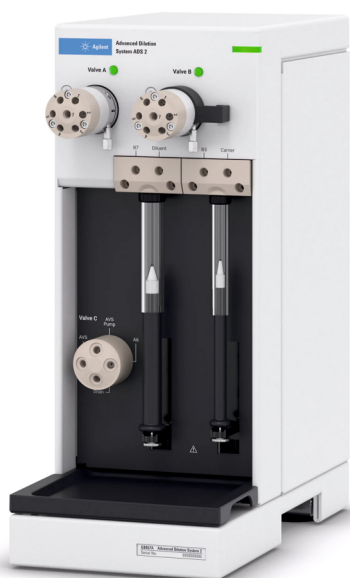




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Agilentov ADS 2 (Advanced Dilution System) preuzima najdosadniji dio posla u laboratoriju i pretvara ga u potpuno automatiziran, pouzdan proces. Od kalibracija do over-range uzoraka - sve ide brže i preciznije. U potpunosti se integrira s Agilent ICP-MS i ICP-OES instrumentima, donoseći veću produktivnost i sigurnost rada. Kompaktan dizajn i integracija s Agilent softverom čine ga idealnim dodatkom svakom ICP laboratoriju.

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Doprinos društvu kroz znanost i tehnologiju

Shimadzu je vodeći svjetski proizvođač analitičkih i mjernih instrumenata. Nudimo sofisticirana i optimalna rješenja neophodna za istraživanje, razvoj i kontrolu kvalitete.

Naša rješenja!

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



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



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



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



Spektrofotometri mjere intenzitet svjetlosti koju apsorbiraju ili emitiraju kemijske tvari.



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



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



KONTAKTIRAJTE NAS!

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