THE **CROATIAN CHEMICAL SOCIETY**
PROUDLY PRESENTS

THE COMPILATION OF THIS YEAR'S NEW

SOLUTIONS IN CHEMISTRY

1–5 September 2026 · Rijeka, Croatia

RIJEKA PULA HKD2026



CELEBRATING **100 YEARS** OF THE

HKD 1926 CROATIAN CHEMICAL SOCIETY

BOOK OF ABSTRACTS

SOLUTIONS IN CHEMISTRY

RIJEKA PULA HKD2026

SOLUTIONS IN CHEMISTRY 2026 × RICHEM 2026

1–5 September 2026

Faculty of Biotechnology and Drug Development

Rijeka, Croatia

BOOK OF ABSTRACTS

IMPRESSUM

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EDITORS
Iva Rezić Meštrović, Marina Šekutor, Andrea Usenik, Franka Sunjka, Luka Klemen, Donna Danijela Dragun

CONFERENCE VENUE
Faculty of Biotechnology and Drug Development
Radmile Matejčić 2, 51000 Rijeka, Croatia

solutionsinchemistry.hkd.hr
sic@hkd.hr

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ORGANISER

Croatian Chemical Society
Horvatovac 102a
HR-10000 Zagreb, Croatia
T: +385 1 4606-163
e-mail: sic@hkd.hr
web: sic.hkd.hr

PROGRAMME BOOK EDITORS

Iva Rezić Meštrović
Marina Šekutor
Andrea Usenik
Franka Sunjka
Luka Klemen
Donna Danijela Dragun

Welcome from the Chairmen of the Organising Committees

On behalf of the Organising Committees, it is our great pleasure to welcome you to the Solutions in Chemistry (SiC 2026) and Summer Conference of the Croatian Chemical Society Rijeka-Pula (RiChem 2026), taking place in Rijeka from 1 to 5 September 2026.

This year's meeting brings together two closely connected scientific events, with parts of their programmes running in parallel. Their joint programme provides a broader forum for the exchange of scientific knowledge, ideas, and experience, offering participants an opportunity to engage with colleagues from different areas of chemistry and related disciplines.
It is particularly worth mentioning that the conferences are devoted to celebrating the 100th anniversary of the Croatian Chemical Society.

Both conferences place strong emphasis on interdisciplinarity, innovation, and the application of chemistry in areas such as advanced materials, environmental protection, and sustainable technologies. By bringing together researchers, educators, students, and industrial professionals, we aim to foster sharing their expertise, encourage new collaborations, and facilitate the transfer of knowledge, ideas, and technologies from fundamental research to practical applications. We hope that this will be particularly valuable for younger researchers and will strengthen the links between academic institutions and industry.

A number of plenary, invited, and section lectures will be delivered by world-renowned scientists, along with various presentations by our sponsors. These will provide insights into current challenges and developments in chemical science and industry, as well as opportunities to learn and obtain new skills from leading researchers, educators, and entrepreneurs. In addition, participants will have a chance to find out more about the latest instruments and consumables presented by our numerous sponsors, whose support we greatly appreciate. The poster session will give everyone the opportunity to present their work, from undergraduate students to experienced scientists working in diverse fields of chemistry and chemical engineering. The education section will be held as well, focusing on new approaches to teaching the next generation of chemists. This year's new features are two panel discussions dedicated to the future of chemistry and the rapid development of chemical education.

Finally, we hope that the conferences will offer not only a stimulating scientific experience but also an opportunity to enjoy the hospitality and unique atmosphere of Rijeka, the *City that Flows*. We encourage participants to take part in various social events, meet colleagues in an informal manner, exchange ideas, and establish new friendships while discovering the rich cultural heritage of the city on the Kvarner Bay and tasting its local delicacies.

LET'S FIND THE NEW SOLUTIONS IN CHEMISTRY!

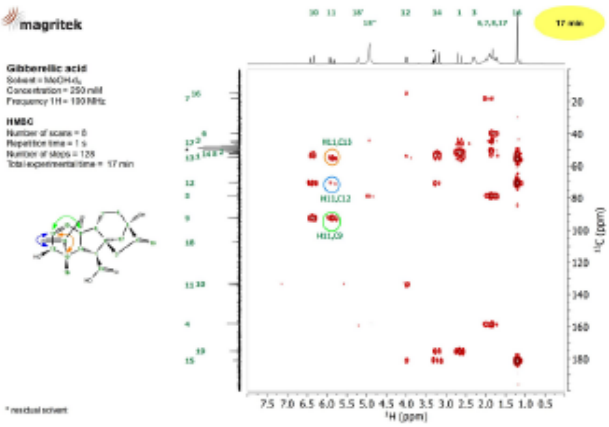
Dean Marković, Ernest Meštrović, Vladislav Tomišić

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New solutions since last Solutions!

In less than two years, quite a lot has happened - quietly, instrument by instrument, release by release – while most of us were looking somewhere else. Since the doors closed on the last Solutions in Chemistry in November 2024, Agilent has shipped 12 new instruments, consumables, and software releases across liquid and gas chromatography, mass spectrometry, vacuum technology, and the lab of the future.

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CONFERENCE PROGRAMME

DAY 1 • TUESDAY, 1 September

12:00 – 14:00	**REGISTRATION** (SiC2026)

14:00 – 14:30	**OPENING CEREMONY**

SECTION I · Big Hall, Faculty of Civil Engineering · CHAIR: Vladislav Tomišić

14:30 – 15:15	**PLENARY**	**Stefan Kubik** Supramolecular Chemistry in Water – Lessons from Cyclic Peptides and Calixarenes
15:15 – 15:45	**INVITED**	**Katharina Edkins** Solution structure of drugs – Can we understand crystallisation and enhanced solubility?
15:45 – 16:05	**SECTION**	**Valerije Vrček** Light as an NMR Variable: Coaxial Photo-NMR for Clean *In Situ* Mechanistic Studies
16:05 – 16:25	**SECTION**	**Andrea Usenik** Does the *Basket* Fluoresce? Origins and Applications of the Intrinsic Calixarene Fluorescence
16:25 – 16:45	**SECTION**	**Nawal Al Hakawati** From Supramolecular Anion Recognition to CO_2 Capture

16:45 – 17:15	☕ **COFFEE BREAK** ☕

SECTION II · Big Hall, Faculty of Civil Engineering · CHAIR: Marina Šekutor

17:15 – 18:00	**PLENARY**	**Pablo Pinacho** Solutions for Chemical Problems from Rotational Spectroscopy
18:00 – 18:20	**SECTION**	**Krešimir Molčanov** Two-Electron Multicentre Bonding (*Pancake Bonding*) in Two Novel Salts of TCNQ Radical Anion with Low Partial Charges
18:20 – 18:40	**SECTION**	**Irena Dokli** Biocatalytic Synthesis of Chiral Propargylic Alcohols Through HHDH-Catalyzed Cascade Reactions

18:40 –	**WELCOME PARTY** Wine tasting + music

DAY 2 • WEDNESDAY, 2 September

SECTION III · Faculty of Biotechnology and Drug Development · CHAIR: Mirna Petković Didović

09:15 – 9:45	**INVITED**	**Māris Turks** Nitrogen-Rich Diazines and Annulated Diazines as Novel Energetic Materials
9:45 – 10:15	**INVITED**	**Damjan Makuc** Honey Authentication: Origin Determination and Structural Characterization of Glycosides by NMR
10:15 – 10:25	**YOUNG RES.**	**Donna Danijela Dragun** Next-Generation Formulations for Improved Phytopharmaceutical Efficacy
10:25 – 10:35	**YOUNG RES.**	**Martina Jović** When Diversity Becomes a Solution: Morin and Gallic Acid in Next-Generation PCL Nanofibers

10:35 – 11:00	☕ **COFFEE BREAK** ☕

SECTION IV · Faculty of Biotechnology and Drug Development · CHAIR: Predrag Novak

11:00 – 11:30	**INVITED**	**Nikola Sakač** Optical Biosensors: Magnetic Solutions for Environmental and Food Safety
11:30 – 11:45	**SECTION**	**Benjamin Vella** The Influence of Trace Water on the Solution Aggregation of Drug Molecules towards Crystallisation
11:45 – 12:00	**SECTION**	**Abbie O. R. Madden** Structure of Water-Dimethylformamide Mixtures and Potential Effects on Crystallisation
12:00 – 12:15	**SECTION**	**Nikola Jakupec** Formation of O···π 'Lamp Motifs' in Modified 2,3-Dichloro-5,6-Dicyano-*p*-Benzoquinone Facilitated by Protonated Polycyanometalates: Mechanism and Structure
12:15 – 12:35	**SPONSOR**(ALTIUM)	**Ema Podravski** Software Solutions that Connect Your Lab

12:35 – 15:00	🍽 **LUNCH BREAK** 🍽

SECTION V · Faculty of Biotechnology and Drug Development · CHAIR: Andrea Usenik

15:00 – 16:00	**PLENARY**	**Morten Meldal** Structure through Clicking
16:00 – 16:45	**PLENARY**	**Valerie Gabelica** Mass Spectrometry of Biomolecular Architectures
16:45 – 17:15	**INVITED**	**Robert Vianello** We Will Dock You: Accelerating Drug Design with Computational Chemistry

SECTION VI · Faculty of Biotechnology and Drug Development · MODERATORS: Andrea Usenik and Donna Danijela Dragun

17:15 – 18:45	**PANEL**	**PANEL DISCUSSION** Chemistry is Powering the Future

18:45 – 20:00	🍽 **DINNER BREAK** 🍽

SECTION VII · Beertija Pub (Slavka Krautzeka 12) · CHAIR: Nikola Bregović

20:00 – 20:30	**PUB LECTURE**	**Vladimir Stilinović**: From 0 to 3D

20:30 – 22:00	**CONFERENCE PARTY** There will be #Solutions · @ Beertija Pub

DAY 3 · THURSDAY, 3 September

SECTION VIII · Faculty of Biotechnology and Drug Development · CHAIR: Ernest Meštrović

09:15 – 10:00	**PLENARY**	**Moniek Tromp** The Quest for Sustainable and Circular Battery Technologies – Operando X-Ray Techniques Probing Dynamic Processes in Batteries
10:00 – 10:30	**INVITED**	**Ivana Murković Steinberg, Matthew D. Steinberg, Gerhard J. Mohr** Wearable Sensors for Multimodal Optical Monitoring of Epidermal Biomarkers
10:30 – 11:00	☕ **COFFEE BREAK** ☕	

SECTION IX · Faculty of Biotechnology and Drug Development · CHAIR: Nikola Bregović

11:00 – 11:45	**PLENARY**	**Ana Sunčana Smith** The Effect of Self-Organisation of Liquid Interfaces on Associated Transport and Reactivity
11:45 – 12:15	**INVITED**	**Anamarija Knežević** Designer Amphiphiles: From Self-Assembly to Functional Nanoreactors in Water
12:15 – 12:30	**SECTION**	**Hüma Yilmaz** A Phosphorescent Quantum Dot–Hydrogel Hybrid Platform for Biocompatible Optical Sensors
12:30 – 12:45	**SECTION**	**Deepak Joshy** Validation of Wearable Optical Biochemical Sensors Using Phantoms Representing Diverse Skin Tones
12:45 – 13:00	**SECTION**	**Milenko Korica** *N,O*-Donor Macrocyclic Ligands as Building Blocks for Silver Coordination Polymers and Inclusion Compounds
13:00 – 15:00	🍽 **LUNCH BREAK** 🍽	

SECTION X · Faculty of Biotechnology and Drug Development · CHAIR: Nikolina Vidović

15:00 – 15:45	**PLENARY**	**Catarina de Carvalho Esteves** Functional Coatings as Sustainable Solutions
15:45 – 16:00	**SECTION**	**Leila Motiei** Detecting and Modulating Proteins with Multifunctional Molecular Probes
16:00 – 16:10	**YOUNG RES.**	**Lucija Vrban Đerek** Predictive Atomistic Modeling of Antitumor Drug Encapsulation Within Supramolecular Hosts
16:30 – 18:30	**POSTERS OVER COFFEE** Poster session × coffee break **posters P1-P49**	
18:30 – 20:30	**PUB QUIZ** Do you have the #Solutions? @ InnovaLab	

DAY 4 · FRIDAY, 4 September

08:00 – 09:15	**REGISTRATION** (RiChem2026)	

SECTION EDU · Faculty of Biotechnology and Drug Development · CHAIRS: Vladimir Stilinović and Orjen Petković

09:15 – 10:00	**PLENARY**	**Natasa Brouwer-Zupancic** Future-ready Chemistry Teaching in Higher Education
10:00 – 10:30	**INVITED**	**Geert-Jan Graulus** The Future-Proof Materials Scientist: Lessons from the Interdisciplinary Master in Materiomics
10:30 – 10:50	**SECTION**	**Jurica Bauer** Empowering Students to Investigate Sustainability: from Chemistry Laboratories to Indoor Air Quality
10:50 – 11:10	**SECTION**	**Catarina de Carvalho Esteves** An Approach For Students With a Multidisciplinary Profile: Nanomaterials Chemistry
11:10 – 11:30	☕ **COFFEE BREAK** ☕	

SECTION EDU · Faculty of Biotechnology and Drug Development · CHAIRS: Vladimir Stilinović and Orjen Petković

11:30 – 12:00	**Questionnaire for Teachers**: Overview of the Current Chemistry Curriculum in Schools - Preliminary Results

SECTION EDU · Faculty of Biotechnology and Drug Development · MODERATORS: Vladimir Stilinović and Orjen Petković

12:00 – 13:30	**PANEL**	**PANEL DISCUSSION** Education 4.0: Training Chemists for an Interdisciplinary World
13:30 – 15:00	🍽 **LUNCH BREAK** 🍽	
15:00 – 17:00	**POSTERS** Poster session **posters P50-P100**	
17:00 – 19:30	**TOUR OF TRSAT** Guided walking tour	
19:30 – 20:00	**SHORT BREAK**	
20:00 – 22:00	**CONFERENCE DINNER** @ Aquarium Restaurant	

DAY 5 · SATURDAY, 5 September

SECTION XI · Faculty of Biotechnology and Drug Development · CHAIR: Dean Marković

09:00 – 09:45	**PLENARY**	**Nuno Maulide** Be Positive: Using Carbocations to Advance Organic Synthesis
09:45 – 10:15	**INVITED**	**Moisés Canle** Toward Photocatalytic Green Flow Technologies to Fight Diffuse Pollution
10:15 – 10:30	**SPONSOR**(CERIC-ERIC)	**Marcello Turconi** CERIC-ERIC: a distributed Research Infrastructure for materials characterisation
10:30 – 11:00	**COFFEE BREAK**	

SECTION XII · Faculty of Biotechnology and Drug Development · CHAIR: Mirna Petković Didović

11:00 – 11:30	**SPONSOR**(JGL)	**Ana Čikoš** Loading Latanoprost into Micelles: the NMR Perspective
11:30 – 12:00	**INVITED**	**Blaž Likozar** Designing Catalytic Processes for Bio-based, CO_2-derived or Recycled Speciality Chemicals by Modelling
12:00 – 12:30	**AWARD**	**Leopold Ružička Award Milena Mlakić** Resveratrol Inspired Diarylethenes as Multifunctional Neuroprotective Agents
12:30 – 12:45	**SECTION**	**Dairo José Hernández Páez** Topological Analysis of Molecular Potential Energy Surfaces Using Sublevel Persistent Homology
12:45 – 13:00	**SECTION**	**Deepkumar Joshi** Substituent Effects, Biological Activity and Drug-Likeness: A Medicinal Chemistry based Study
13:00 – 13:10	**YOUNG RES.**	**Iva Karneluti** Hydrogel-Coated Colourimetric Face Sheet Mask for Monitoring Skin pH
13:10 – 13:25	**SHORT BREAK**	

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14:05 – 14:15	**YOUNG RES.**	**Katarina Kordej** Indole-3-Carbaldehyde Schiff Bases: From Synthesis to Antimicrobial Activity
14:15 – 14:25	**YOUNG RES.**	**Paula Ćurić** Synthesis and Biological Activity of Novel Indole Derivatives
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14:35 – 14:45	**YOUNG RES.**	**Katarina Marija Drmić** Degradation of Sulfamethoxazole and Venlafaxine During Chlorination
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Posters P1 – P49: Thursday, 3 September can be placed in the morning (Wednesday, 2 September) and must be removed immediately after the first poster session ends.

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PLENARY LECTURES

SUPRAMOLECULAR CHEMISTRY IN WATER – LESSONS FROM CYCLIC PEPTIDES AND CALIXARENES

Stefan Kubik

Department of Chemistry – Organic Chemistry, RPTU University Kaiserslautern-Landau,
Erwin-Schrödinger-Straße 54, 67663 Kaiserslautern, Germany
* stefan.kubik@rptu.de

Research on characterizing and controlling molecular recognition processes is central to supramolecular chemistry. These binding processes depend heavily on the medium, and achieving molecular recognition in water is sometimes considered a particular challenge that has emerged only recently. This is only partly true. While activities in this field have indeed increased in recent years, supramolecular chemistry in water began decades ago with research on cyclodextrins, predating even work on crown ethers. Moreover, numerous early synthetic receptors work effectively in water. However, these systems were not primarily developed to characterize the influence of water on their behavior.

The ability of water to bring apolar solutes together has also long been recognized. In recent years, however, our understanding of the impact of solutes on water structure and the interplay between water reorganization and molecular recognition has increased considerably. These developments also had an impact on supramolecular chemistry, enabling the more reliable design of receptors that operate in water with remarkable efficiency.[1]

In my lecture, I will briefly summarize the basic principles of molecular recognition in water to show how, unlike most other solvents, water can actively mediate recognition processes. Rather than merely posing a challenge, water can therefore create unique opportunities for molecular recognition. I will use two examples from my own group to illustrate this aspect.

First, I will present our work on a class of hybrid cyclophane-cyclopeptide receptors with an alternating sequence of natural and non-natural amino acids. Of the many macrocyclic receptors we have prepared, one was found to efficiently bind inorganic anions, including halides and sulfate, in aqueous media. Complex formation relies on hydrogen bonding, making the strong interaction of this cyclopeptide with highly hydrated anions in water particularly surprising. I will discuss our efforts to elucidate the driving force of this behavior and present work aimed at functional systems and structural control.[2]

The second example concerns a calix[4]arene derivative that forms discrete dimeric capsules in water capable of encapsulating alkanes and cycloalkanes. The direct attractive interactions that mediate complex formation are weak, involving a combination of aromatic and dispersion interactions. Thus, the self-assembly of these capsules relies heavily on the ability of water molecules to bring solutes together, ultimately affording well-defined, discrete structures.[3]

These two examples are only a small part of the broad range of current worldwide research activities in this field. In the long term, advances in our understanding and control of molecular recognition in water may help bring supramolecular systems closer to practical applications.

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SOLUTIONS FOR CHEMICAL PROBLEMS FROM ROTATIONAL SPECTROSCOPY

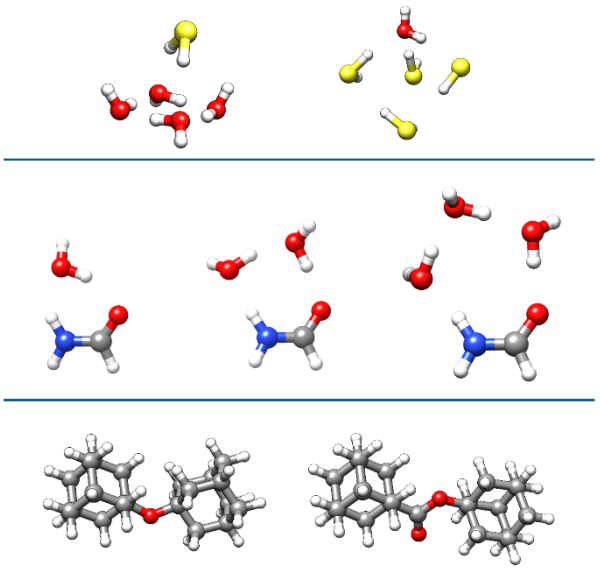
Pablo Pinacho

Department of Physical Chemistry and Inorganic Chemistry, IU-CINQUIMA University of Valladolid, Paso Belén 7, 47011 Valladolid, Spain

* pablo.pinacho@uva.es

Despite well-stablished as a technique to extract accurate, unperturbed molecular structures for isolated molecules and clusters, rotational spectroscopy remains underutilized in standard chemistry laboratories. Instrumental developments in the last decades, as the broadband Chirped-Pulse mode coupled with supersonic jet expansions, combined with state-of-the-art quantum chemical computations, allow to solve fundamental questions on molecular structure and interaction networks in the gas phase.

This talk addresses three chemical problems solved via rotational spectroscopy. First, the evaluation of H_2S capability to establish hydrogen bonding. The precise structural determination of the H_2S clusters provide empirical evidence of sulfur's dual capability to act simultaneously as a proton donor and acceptor, analogous to water. Second, the unambiguous detection and characterization of Resonance-Assisted Hydrogen Bonding (RAHB) effects, enabling the direct empirical quantification of structural deformations. Finally, an example of the sensitivity of modern spectrometers, which allow for the analysis of intricate multi-conformational landscapes, large non-covalent architectures, or heavy molecules in the example of large adamantyl derivatives.



STRUCTURE THROUGH CLICKING

Marie-Thérèse C. Choukér, Yuan Zhang, Christoffer Warming, Mads L. Ramsing, Sára M.T. Mellemgaard, Christian Kofoed, Kai Holland-Nell, Morten Meldal*

Department of Chemistry, Faculty of Science, University of Copenhagen, Universitetsparken 5, 2100 København, Denmark

* meldal@chem.ku.dk

In the design of recognition molecules based on peptides and miniproteins it is important to be able to lock active structural populations into the active form. The lecture will discuss the design and assembly of β-bodies and mini-proteins with recognition functions and show how these can be designed with incorporation of amino acids with alkynes and azides in the sidechains for post assembly clicking by CuAAC to promote a structural motif. This will be illustrated with examples of design of molecules that recognize Alzheimer fibrils, act as antibiotics or have enzymatic activity. With the increasing importance of novel drugs based on active peptide structures and hormones there is a growing need for cell penetrating peptides to bring pharmaceutically active substances targeting intracellular targets as cargo into the cells. We present a study of a small library of click cyclized peptides that interact with cell surface components and mediate internalization. One of the library components proved to be a powerful CPP entering cells by a dynamin and energy dependent pathway leading to endocytosis and cellular import even of larger proteins such as GFP. Furthermore, alkylation of the arginines responsible for cell surface interaction to increase the hydrophobicity of the CPP by a new approach, increased the release of cargo from the endosomes.

MASS SPECTROMETRY OF BIOMOLECULAR ARCHITECTURES

Valerie Gabelica

School of Pharmaceutical Sciences, Faculty of Science, University of Geneva, Rue Michel-Servet 1 1206 Geneva

* valerie.gabelica@unige.ch

Mass spectrometry is widely recognized as an essential analytical tool for determining molecular masses and compositions. Originally developed as a method to identify molecules and characterize chemical reactions, its remarkable advances in sensitivity, resolution, speed, and accuracy have transformed it into a versatile technique used throughout chemistry, biology, medicine, and materials science. Today, mass spectrometry not only reveals *what molecules are present*, but can also provide insights into *how molecules are organized and interact*. This lecture will highlight how mass spectrometry can probe biomolecular architectures, from folded macromolecules to non-covalent assemblies. Native mass spectrometry preserves molecular interactions during transfer from solution to the gas phase, allowing direct characterization of complex composition, stoichiometry, and binding equilibria.

Recent developments have greatly expanded the structural information accessible by mass spectrometry. Coupling with ion mobility spectrometry separates ions according to their size and shape, providing insights into molecular conformation, while gas-phase ion spectroscopy offers a powerful means to probe local structural motifs and intermolecular interactions. Together, these approaches enable the characterization of complex biomolecular systems in unprecedented detail. Examples will be drawn from studies of nucleic acid supramolecular assemblies, nucleic acid-ligand interactions, and synthetic foldamers. These case studies illustrate how modern mass spectrometry can address fundamental questions in structural chemistry and molecular biophysics, bridging the gap between molecular composition and higher-order organization. The lecture will highlight both the opportunities and the challenges of using mass spectrometry to explore the architectures that underpin biomolecular function.

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THE QUEST FOR SUSTAINABLE AND CIRCULAR BATTERY TECHNOLOGIES - OPERANDO X-RAY TECHNIQUES PROBING DYNAMIC PROCESSES IN BATTERIES

Moniek Tromp

Zernike Institute for Advanced Materials, Materials Chemistry, Faculty of Science and Engineering, University of Groningen, Nijenborgh 3, 9747 AG Groningen

* Moniek.Tromp@rug.nl

Batteries are of key importance in the energy transition, i.e. for mobility as well as for a temporary (intermediate) storage of excess energy (e.g. stabilise the grid). Li ion batteries are widely used in applications such as mobile phones and laptops, and will likely be key to future electromobility due to their low weight. Alternatively, more sustainable batteries are essential to enable the significant increase in demand as well as their differing applications and requirements (incl. local and grid storage), while reducing pressure on climate and environment.

Rational design of novel battery chemistries and technologies requires a detailed understanding of the charge, discharge and deactivation mechanisms, preferably quantitative and spatially resolved. X-ray techniques (spectroscopy and scattering) are characterisation techniques which provide detailed structural and electronic information on the material under investigation, in a time- and spatially resolved manner. These operando spectro-electroechemical investigations provide insights in the type, location and reversibility of the intermediates formed in and on electrodes and/or electrolytes as a function of state-of-charge and position in the battery. Obtained insights in cycling and deactiviation mechanisms for different battery types, i.e. Li-ion and Li-S, as well as more sustainable battery technologies like Ni-Fe and Fe-air, will be discussed and the strategy towards new sustainable batteries explained.

THE EFFECT OF SELF-ORGANISATION OF LIQUID INTERFACES ON ASSOCIATED TRANSPORT AND REACTIVITY

Ana Sunčana Smith

Division of Physical Chemistry, Ruđer Bošković Institute, Bijenička 54, HR-10000 Zagreb, Croatia
Institute of Theoretical Physics, FAU Erlangen–Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany
* smith@physik.fau.de

In this presentation, I will discuss how chemical reactions occurring at liquid interfaces may be affected by the organisation of the interface itself, in the context of supported ionic liquid catalysis. To resolve these effects, I will present the computational tools we developed to probe interfacial behaviour under reaction conditions. I will show that the organisation, surface tension, and transport of reactants and products are affected by the interface compared to the bulk liquid, and that the interface itself changes under reaction conditions. In particular, I will examine how solvation and diffusivity near the interface differ from bulk behaviour, and how these differences shape the local environment experienced by reacting species. Finally, I will show that the positioning of reactants and, in particular, the catalyst, can be manipulated through interface design, which in turn can improve the overall turnover of the reaction.

FUNCTIONAL COATINGS AS SUSTAINABLE SOLUTIONS

Catarina de Carvalho Esteves

Coatings, Surfaces & Interfaces, Laboratory of Physical Chemistry, Chemical Engineering and Chemistry Department, Eindhoven University of Technology, Het Kranenveld 14, 5612 AZ Eindhoven, The Netherlands

*a.c.c.esteves@tue.nl

The urgent materials and energy transition require a critical change in the way we currently use, produce and dispose of materials. The application of coatings over products and devices improves their performance and durability, preventing early disposal of the full product. Thus, protective coatings extend materials and products lifetime, maximize energy efficiency, slow-down waste accumulation and contribute to curb CO_2 emissions. Furthermore, new functions can be added to a product via the application of functional coatings, creating more sustainable alternatives, for example adding barrier properties,[1,2] improving performance and extending lifetime[3,4], or preventing early degradation, via a self-healing function.[5,6]

I will discuss how research in the functional coatings field can enable sustainable solutions and coatings with added-value functions. I will present a few study cases on how to include new sustainable strategies in well-established coating systems and formulations, for example by improving mechanical[3,4] or barrier properties;[1,2] and illustrate how to incorporate self-healing strategies on polymer coatings,[5,6] to extend materials and products lifetime at high performance.

These reserach cases will demonstrate the high potential for industry and academia players to work together on the current materials and energy transition, and highlight all players in the chemistry and coatings value-chain are required to embrace this change.

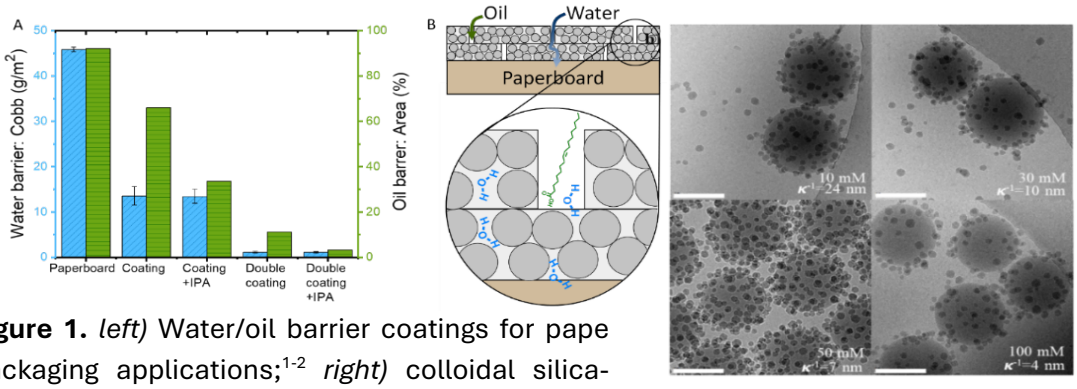


Figure 1. *left)* Water/oil barrier coatings for pape packaging applications;[1-2] *right)* colloidal silica-polymer composites designed to improve waterborne coatings mechanical performance.[3-4]

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FUTURE-READY CHEMISTRY TEACHING IN HIGHER EDUCATION

Nataša Brouwer–Zupančić

University of Amsterdam, Teaching and Learning Centre, Postbus 19268, 1000 GG Amsterdam, The Netherlands

* natasa.brouwer@uva.nl

Chemistry graduates are urgently needed to help address global socio-economic, political, and environmental challenges. This demands sustainable, continuous, discipline-based, future-oriented professional development for university chemistry teachers. Universities offer generic pedagogical training and, in some countries, compulsory teaching certification, which leads to higher quality of university teaching. A teaching-practice-oriented university teaching qualification program stimulates participants to continue to professionalise after they achieved their certificate.[1] Yet this is not enough to ensure that we apply chemistry knowledge to its full potential in a changing world.

In this lecture, I argue for continuous professional development (CPD) that respects local needs and is embedded in international communities of practice for sustainable teaching development. I will present the European Chemistry Thematic Network (ECTN) Eurolecturer Academy (ELA), an innovative European platform that supports the ongoing development and recognition of teaching competences in chemistry higher education.[2] A flagship initiative is the STEM-CPD Summer School, which prepares participants to act as CPD Ambassadors who design and implement professional-development activities within their own institutions, combining top-down support with bottom-up innovation in order to foster relevant, student-centred active-learning teaching practices.[3] I will discuss the importance of alignment between learning goals, learning activities, and assessment to support the development of the skills students need to succeed in an uncertain future. While active learning is increasingly adopted, the arrival of GenAI has often led assessment practices to fall back on traditional, high-stakes examinations that are not aligned with these approaches. I will share our experiences with IguideME (I guide My Education), an AI- and learning-analytics-based tool that supports students' self-regulation and provides lecturers with actionable insight into course design and individual learning processes.[4]

Together, these initiatives illustrate how a coherent CPD ecosystem can offer concrete solutions for the future of chemistry higher education.

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BE POSITIVE: USING CARBOCATIONS TO ADVANCE ORGANIC SYNTHESIS

Nuno Maulide

Institute of Organic Chemistry, University of Vienna, Währinger Straβe 38, 1090 Wien, Austria

* nuno.maulide@univie.ac.at

The turn of the century brought about a pressing need for new, efficient and clean strategies for the chemical synthesis of biorelevant compounds. Our group has studied the use of various molecular rearrangements and atom-economical transformations as particularly appealing means towards the streamlined synthesis of complex small molecule targets.

In this lecture, we will present an overview of our research in these areas focusing on the chemistries of carbocations – underappreciated intermediates in synthesis. We shall present examples from our work showcasing how they can provide efficient solutions for the discovery of unusual reactivity or concise total synthesis.

We furthermore will discuss innovative approaches to reactions that might come a step closer towards “ideality”.

INVITED LECTURES

SOLUTION STRUCTURE OF DRUGS – CAN WE UNDERSTAND CRYSTALLISATION AND ENHANCED SOLUBILITY

Katharina Edkins

Strathclyde Institute of Pharmacy and Biomedical Sciences, University of Strathclyde, RW501j, Robertson Wing, 161 Cathedral Street, Glasgow G4 0RE, UK

* katharina.edkins@strath.ac.uk

Pharmaceutical materials have to be safe for the patient while also delivering the drug payload with tight control. This starts with the crystalline drug material itself, which has a significant influence on the dissolution behaviour and hence the bioavailability of the final formulation. It is currently impossible to predict the outcome of a crystallisation experiment before performing it. In this presentation, I will show our approach to understand solution structure using supramolecular host-guest analytics and neutron total scattering, and how our results can help to understand and tailor the crystallisation outcome.

The first example is the co-crystal of caffeine with benzoic acid, which has been shown to have nucleation inhibition. We have shown that solution aggregation measurements can explain the lack of nucleation and open up a pathway to predict which solvents can be exchanged to still obtain the same co-crystal form.[1]

The second example investigates the increased solubility of caffeine in the presence of sodium benzoate. By using neutron total scattering and tethered Monte Carlo simulations, we could gauge the molecular interactions in solution and propose a mechanism, with which the solubility increase can be explained.[2]

Lastly, I will present how solution aggregation could be used to mask the bitter taste of an antiretroviral drug in pediatric formulations.[3]

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NITROGEN-RICH DIAZINES AND ANNULATED DIAZINES AS NOVEL ENERGETIC MATERIALS

Māris Turks,* Kristaps Valkovskis, Dāgs Dāvis Līpiņš, Irina Novosjolova

Faculty of Natural Sciences and Technology, Riga Technical University, P. Valdena Str. 3, Riga, LV-1048, Latvia

* maris.turks@rtu.lv

The development of next-generation energetic materials requires a careful balance between high detonation performance, thermal stability, environmental compatibility, and reduced sensitivity to mechanical stimuli. Nitrogen-rich heterocycles have emerged as privileged molecular scaffolds owing to their high positive heats of formation, dense crystal packing, and the ability to establish extensive intermolecular interactions.[1] Among these, diazines, annulated diazines, and structurally related nucleobase-derived heterocycles represent particularly attractive platforms.[2] Their rigid planar architectures, high nitrogen content, and well-defined hydrogen-bonding motifs enable rational molecular engineering aimed at simultaneously enhancing energetic performance and safety. Herein, we present two complementary molecular design strategies. The first utilizes nitrogen enrichment and ring annulation to develop highly energetic fused diazine frameworks. We have developed the metal-free primary explosive (C_6N_{16}, **DBTP**), which combines a planar nitrogen-rich framework with high density (1.79 g cm^{-3}), excellent thermal stability (T_{onset} = 201 °C), a high heat of formation (5631 kJ kg^{-1}), and calculated detonation parameters of D = 8001 m s^{-1} and P = 24.2 GPa.[3] Importantly, **DBTP** successfully initiates PETN detonators while exhibiting good UV stability, negligible aqueous solubility and hygroscopicity, and substantially reduced aquatic toxicity compared with conventional lead-based primary explosives, demonstrating its potential as a sustainable heavy-metal-free replacement. The second strategy exploits bio-inspired nucleobase scaffolds through selective azido and nitro functionalization of purine and uracil derivatives while retaining their intrinsic hydrogen-bonding capability. Furthermore, co-crystallization of energetic nucleobase analogues, exemplified by the co-crystal of 2,8-diazidoadenine and 5-nitrotetrazolouracil, affords an unprecedented planar hydrogen-bonded tetramer, demonstrating that supramolecular crystal engineering provides an effective strategy for tuning crystal packing, stability, and energetic performance. This non-canonical supramolecular motif offers new opportunities to manipulate crystal packing, stability, and detonation characteristics without altering molecular composition, highlighting co-crystallization as a promising strategy for optimizing energetic performance through supramolecular design. In summary, nitrogen-rich diazines, annulated diazines, and nucleobase-derived fused azines are versatile platforms for the development of high-performance energetic materials. By integrating molecular design through nitrogen enrichment and annulation with hydrogen-bond-directed crystal engineering and supramolecular assembly, this work provides new design principles for environmentally benign, high-energy, and intrinsically safer energetic materials suitable for future primary explosive technologies.

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HONEY AUTHENTICATION: ORIGIN DETERMINATION AND STRUCTURAL CHARACTERIZATION OF GLYCOSIDES BY NMR

Damjan Makuc,*[a] Monika Škrjanc,[a,b] Janez Plavec[a,b,c]

[a] Slovenian NMR Centre, National Institute of Chemistry, Hajdrihova 19, SI-1000 Ljubljana, Slovenia,
[b] Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113, SI-1000, Ljubljana, Slovenia, [c] EN- FIST Centre of Excellence, Trg Osvobodilne fronte 13, SI-1000 Ljubljana, Slovenia
* damjan.makuc@ki.si

Identifying honey glycosides is important because of their potential biological activities and their value as botanical markers. In this study, NMR profiling of Slovenian honey was combined with multivariate statistical analysis to investigate differences in chemical composition among honey samples of various botanical and geographical origins. The NMR fingerprints enabled reliable classification of honey samples primarily according to their botanical origin, while geographical origin had a considerably smaller influence on the observed chemical variability. Characteristic spectral markers responsible for distinguishing individual honey types were identified, providing valuable insights into the compounds that define their unique chemical profiles.

During this analysis, a previously uncharacterized signal was consistently observed in linden honey, prompting further investigation and the identification of a novel glycoside. The discovery of new glycosides improves our understanding of the molecular composition of honey and its potential biological functions. The higher abundance of the newly identified glycoside in linden honey compared with other botanical origins highlights its potential as a chemical marker for honey authentication. Furthermore, this work demonstrates the applicability of NMR spectroscopy, combined with chemometric analysis, as a powerful approach for the characterization, authentication, and discovery of novel compounds in complex food matrices.

OPTICAL BIOSENSORS: MAGNETIC SOLUTIONS FOR ENVIRONMENTAL AND FOOD SAFETY

Nikola Sakač,[a] Daniele Marra,[b] Raffaele Velotta,[b] Bartolomeo Della Ventura[b]

[a] Faculty of Geotechnical Engineering, University of Zagreb, Hallerova aleja 7, 42000 Varaždin, Croatia,

[b] Department of Physics, Federico II University of Naples, Via Cinthia 21, 80126 Naples, Italy

* nsakac@gfv.unizg.hr

Conventional gold nanoparticle-based colorimetric biosensors, while widely used for optical detection, were found to face fundamental limitations: passive diffusion restricted binding kinetics, active control for particle manipulation was lacking, and separation from complex matrices remained challenging. Here, core-shell Fe_3O_4@Au nanoparticles were developed to overcome these constraints, transforming standard plasmonic sensing into a versatile, actively controllable platform for food and environmental safety applications.

Three distinct advantages over conventional LSPR-based detection were introduced by the magnetic core. First, active micromixing was achieved under a rotating magnetic field, generating controlled nanoparticle stirring that drastically enhanced analyte-induced aggregation kinetics by overcoming diffusion-limited binding. Second, magnetophoretic separation was enabled, allowing rapid purification and preconcentration of target-bound nanoparticles from complex sample matrices—a capability that was not available with conventional gold nanoparticles. Third, magnetic steering was utilized to provide spatial control over nanoparticle positioning, facilitating washing steps and signal optimization without centrifugation or filtration.

The multifunctional platform was validated through two complementary biosensing applications. For the mycotoxin deoxynivalenol (DON), antibody-functionalized Fe_3O_4@Au nanoparticles were employed for magnetophoretic migration-based detection. Analyte-induced aggregation was found to increase aggregate size proportionally to DON concentration, accelerating magnetic migration velocity—a readout mechanism that was entirely dependent on the magnetic core. A detection limit of 0.5 ppm was achieved by the sensor, exceeding regulatory thresholds for many foods, while matrix interferences were eliminated through magnetic washing.

For glyphosate detection in tap water, active micromixing was enabled by the magnetic core, enhancing diffusion and aggregation kinetics.[1] A 500-fold improvement in sensitivity was observed compared to passive conditions. Optical transduction was provided by the localized surface plasmon resonance (LSPR) of the gold shell, while oriented antibody tethering was ensured through photochemical immobilization. A detection limit of 20 $ng \cdot L^{-1}$ was achieved by the biosensor, well below the European Union's 0.1 $\mu g \cdot L^{-1}$ regulatory limit—demonstrating that standard colorimetric assays were transformed into ultra-sensitive platforms through magnetic enhancement.

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WE WILL DOCK YOU: ACCELERATING DRUG DESIGN WITH COMPUTATIONAL CHEMISTRY

Robert Vianello

Laboratory for the Computational Design and Synthesis of Functional Materials, Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička cesta 54, HR-10000 Zagreb, Croatia

* robert.vianello@irb.hr

Computational chemistry has become an indispensable tool in modern drug discovery, enabling the rational design of biologically active molecules based on the three-dimensional structures of their targets. By integrating these techniques with experimental approaches, it is possible to gain detailed insights into binding mechanisms, facilitating efficient identification and optimization of new therapeutic agents. These strategies reduce the time and cost of drug development while improving our understanding of structure-activity relationships. Tubulin polymerization inhibitors represent a cornerstone of anticancer therapy, as they disrupt microtubule dynamics essential for cancer cell growth. This lecture highlights our recent research efforts in the design, synthesis, and evaluation of benzazole-based compounds as potent tubulin-targeting agents (Figure 1). These chemically versatile scaffolds play an important role in medicinal chemistry,[1] offering a platform for the development of innovative bioactive molecules.

Using classical and microwave-assisted synthesis, we prepared *N*-derived benzimidazole acrylonitriles (Figure 1, X = C–H) with submicromolar antiproliferative activity (IC_{50} 0.2–0.6 μM) and favorable selectivity.[2] Mechanistic studies confirmed inhibition of tubulin assembly and induction of mitotic arrest. Computational analyses identified critical protein-ligand interactions, guiding the design of improved analogues. In particular, replacement of the benzimidazole phenyl ring with pyridine led to imidazo[4,5-*b*]pyridines (Figure 1, X = N) with enhanced potency (IC_{50} ~0.04 μM), reduced toxicity, and cell migration inhibition.[3] Advanced computations revealed multiple binding modes at the colchicine site and alternative tubulin regions (Figure 2), underlining the versatility of these ligands. Since microtubule anomalies are, beyond oncology, linked to neuropsychiatric disorders, future perspectives, including repurposing for post-COVID neurological sequelae, will also be discussed.[4]

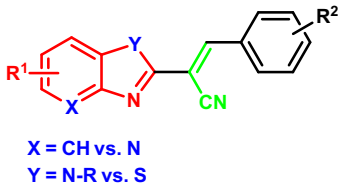


Figure 1. General chemical structure of studied ligands that interfere with the tubulin polymerization.

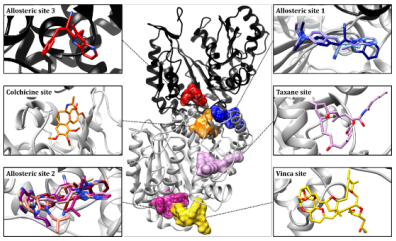


Figure 2. Various ligand binding sites on the α- (in black) and β-subunits (in gray) in the tubulin dimer, as identified through the docking and molecular dynamics simulations.

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WEARABLE SENSORS FOR MULTIMODAL OPTICAL MONITORING OF EPIDERMAL BIOMARKERS

Ivana Murković Steinberg,[a] Matthew D. Steinberg,[a] Gerhard J. Mohr[b]

[a] Faculty of Chemical Engineering and Technology, University of Zagreb, Trg Marka Marulića 19, 10000 Zagreb, Croatia, [b] Joanneum Research, Leonhardstrasse 59 A-8010 Graz, Austria
* imurkov@fkit.unizg.hr

The design of wearable (bio)chemical sensors presents significant multidisciplinary challenges spanning device ergonomics, chemistry, physics, and electronics, with particular emphasis on material and chemical architectures that must ensure reversibility, reproducibility, and biocompatibility[1]. This presentation outlines our current research on the development of optically responsive nanomaterials and associated sensing strategies aimed at integration into low-cost wearable platforms.

Furthermore, the talk introduces a novel research direction within the WearSense project, focused on multimodal biomarker monitoring. This approach combines the optical measurement of biochemical and physical parameters obtained both from the skin surface, via on-skin colourimetric sensing patches[2], and from subdermal tissue based on photoplethysmography (PPG) and pulse oximetry methods.

Key challenges associated with this approach will be discussed, including the development of photonic sensing schemes and materials, the application of diffuse reflectance spectroscopy to skin, and the design of multi-wavelength wearable optoelectronic devices. Additional considerations include the fabrication of representative skin tissue phantoms, the establishment of robust data collection protocols, and the implementation of advanced data analysis techniques for signal extraction and sensor validation.

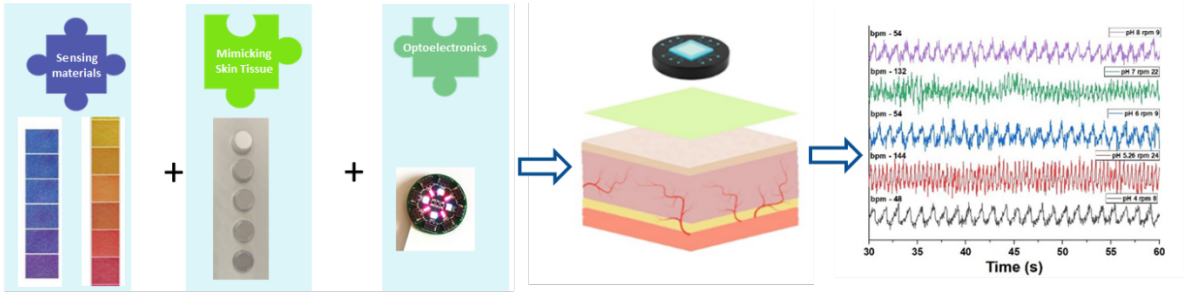


Figure 1. Multimodal optical wearable sensing platform combining colourimetric skin patches and subdermal PPG-based measurements for integrated biochemical and physical biomarker monitoring.

ACKNOWLEDGEMENTS This work is supported by the Croatian Science Foundation under the project *WearSense* HRZZ IP-2022-10-2595.

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DESIGNER AMPHIPHILES: FROM SELF-ASSEMBLY TO FUNCTIONAL NANOREACTORS IN WATER

Anamarija Knežević, Antonija Ožegović, Emina Debogović, Karlo Petrić, Ivan Lisjak, Aleks Logožar

Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb

* anamarija.knezevic@irb.hr

The self-assembly of amphiphilic molecules in aqueous media has emerged as a versatile strategy for constructing functional nanostructures with applications ranging from biomedicine to catalysis and organic synthesis.[1] In particular, non-ionic amphiphiles offer attractive features such as chemical stability, structural tunability, and the ability to form well-defined supramolecular assemblies, such as micelles, vesicles, and nanofibers, through hydrophobic interactions, hydrogen bonding, and π–π stacking.[2] These dynamic nanostructures provide confined reaction environments that can influence reaction efficiency and selectivity, and even enabling transformations that are otherwise challenging under conventional conditions.[3]

This lecture will present our recent work on the design, synthesis, and characterization of a new generation of non-ionic amphiphiles that self-assemble into micellar and tubular supramolecular architectures in water (Figure 1). Particular emphasis will be placed on the relationship between molecular structure and self-assembly, the development of pH-responsive supramolecular systems, and the characterization of the resulting nanostructures using spectroscopic, calorimetric, and microscopic techniques. Finally, the potential of these self-assembled systems as nanoreactors for organic transformations in aqueous media will be discussed, highlighting new opportunities for supramolecular catalysis and synthetic chemistry.

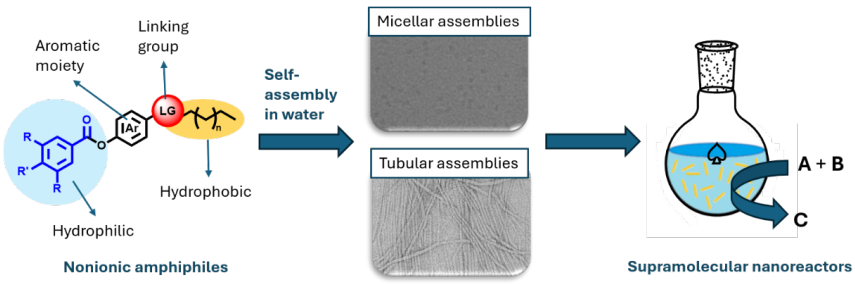


Figure 1. Self-assembly of nonionic amphiphiles into micellar and tubular assemblies for use as supramolecular nanoreactors.

ACKNOWLEDGEMENTS This work has been financially supported by STARTNOW project (NPOO.C3.2.R2-I1.06.0042) funded by the European Union under the NextGenerationEU Programme.

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THE FUTURE-PROOF MATERIALS SCIENTIST: LESSONS FROM THE INTERDISCIPLINARY MASTER IN MATERIOMICS

Geert-Jan Graulus,[a,b] Dorien Baeten,[b] Sarah Doumen,[b] An Hardy[a,b]

[a] Institute for Materials Research (IUMAT), UHasselt, Agoralaan building D, 3590 Diepenbeek, Belgium,
[b] Faculty of Sciences, UHasselt, Agoralaan building D, 3590 Diepenbeek, Belgium
* geertjan.graulus@uhasselt.be

Materials science is becoming increasingly multi- and interdisciplinary. The rapid succession of advances demands educational models that keep pace and prepare graduates to work across disciplinary boundaries. However, many university programs remain siloed. This contribution introduces the *Master's in Materiomics* programme at Hasselt University.

The programme uniquely bridges the gap between materials chemistry and materials physics, while simultaneously training students in both experimental and computational methods. By applying a research-based approach (i.e., a strong emphasis on project-based learning), the programme encourages students to transcend their own educational backgrounds. To prepare graduates for evolving research and industrial ecosystems, the programme offers four specialisation tracks (pillars): materials for energy applications, materials for healthcare, sustainable materials and materials for quantum technologies, thereby aligning with ongoing research within the Institute for Materials Science (IUMAT), the Data Science Institute (DSI) and the faculty of sciences (X-Lab) at Hasselt University.

In the talk, we analyse the curriculum and discuss the design choices with respect to the programme's objective of training versatile interdisciplinary scientists equipped to tackle STEM talent shortages, translational problem-solving, and societal expectations regarding sustainability. Our approach to assessing the interdisciplinary learning process, guided by boundary-crossing theory, will also be discussed in more detail.[1] Finally, we outline key challenges in scaling an integrative programme and propose practical design principles to guide future curriculum development.

ACKNOWLEDGEMENTS The MSc in Materiomics at Hasselt University was developed in close collaboration with industry and policymakers to create a future-proof curriculum. We acknowledge all participants in these fruitful discussions and thank the members of the educational management team (current and former) for incorporating the input received into the curriculum design.

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TOWARD PHOTOCATALYTIC GREEN FLOW TECHNOLOGIES TO FIGHT DIFFUSE POLLUTION

Moisés Canle, M.I. Fernández Pérez, Z. Marín, D.R. Ramos, J.A. Santaballa
Universidade da Coruña, Grupo React!, Facultade de Ciencias & CICA, E-15071 A Coruña, Spain

* moises.canle@udc.es

Industrialization and social development have led to the presence of a variety of pollutants in the environment, which may cause harmful effects on living beings and many other detrimental impacts.[1] Thus, their presence in the environment has been reported as an emerging risk.[2]

Innovative photocatalytic composites have been developed for sunlight-driven photodegradation of organic pollutants in waters.[3] Natural clays and TiO_2 were used to produce bulky aggregates that can be filtered out by gravity and reused a large number of times.[4] The physicochemical characterisation of this material allowed a better understanding of its catalytic activity. Experiments with different families of pollutants, and different aqueous matrices have shown the versatility of these photocatalytic composites, which, together with their low cost and ease of production may allow wide use for water, sewage and wastewater treatment, including the medium scale. These binary composites have shown very good photocatalytic activity. This approach has recently been extended to the production of mechanically stable thin photocatalytic films supported onto inert materials, with excellent efficiency results.[5] Other photocatalytic hetero-systems have been tested as well, with good results.

The use of these bulky photocatalysts is very simple, as polluted water can simply be treated in a shallow, sunny pool or basin with the bottom covered with the catalytic material, and the photodegradation increases with the photocatalyst load, until the surface exposed to light is completely covered. The large size of the pellets allows their easy recovery, while their efficiency is not affected. They are mechanically stable, as they do not have any detachable catalytic film. Good catalytic activity has been proved for the removal of a number of chemicals in different aqueous matrices, including seawater. This material is inexpensive and can easily be produced. It is promising for larger scale use in solar photocatalytic waters treatment as a cheap, green, easily recoverable and efficient reusable composite photocatalyst.

The use of thin films of these composite materials allows to produce different types of systems that allow batch photocatalytic treatment that can be coupled to synergistic natural-based solutions such as constructed wetlands to boost the efficiency of the process. Eventually, we have managed to develop the technology for a flow photocatalytic system where the thin film is deposited inside a cylindrical tubing, where different parameters can be optimized.

ACKNOWLEDGEMENTS This research was carried out in the framework of grant PID2021-127898OB-I00 (WAntRed), funded by MICIU/AEI and "ERDF: A way of making Europe". Financial support was also provided by the regional government of the Xunta de Galicia through project GRC/ED431C 2023/33.

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DESIGNING CATALYTIC PROCESSES FOR BIO-BASED, CO_2-DERIVED OR RECYCLED SPECIALITY CHEMICALS BY MODELLING

Blaž Likozar

Kemijski inštitut, University of Ljubljana, Hajdrihova 19, p.p. 660 SI-1001 Ljubljana

* blaz.likozar@ki.si

More than 90% of traditional chemical processes integrated catalysis, while we are nowadays faced with unconventional new feedstocks (CO_2, biomass, the recycling of plastics...), energy (electrification instead of natural gas powering) and operation (a demand for flexibility or resilience). The latter requires experiments to go hand in hand with the models at various involved scales, making it optimal, should the be linked as muti-scale. Presentation will walk through a few intriguing cases, where such tandem methodology yields compelling design, description or optimisation results, when it comes to catalysis, reactions, processes... What is more, methodology can also be translated to solubility, extraction and separation unit operations, integrated downstream.

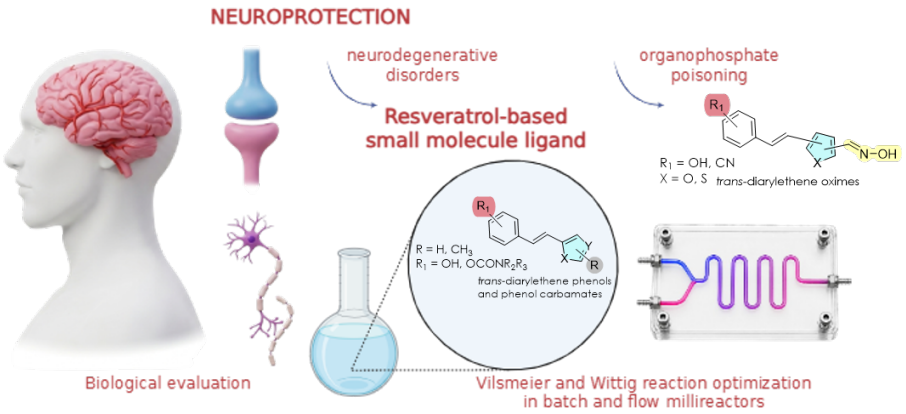
RESVERATROL-INSPIRED DIARYLETHENES AS MULTIFUNCTIONAL NEUROPROTECTIVE AGENTS

Milena Mlakić

Department of Organic Chemistry, University of Zagreb Faculty of Chemical Engineering and Technology, Trg Marka Marulića 19, HR-10 000 Zagreb, Croatia

* mdragojev@fkit.unizg.hr

The development of resveratrol-inspired small molecules represents a promising strategy for the discovery of novel therapeutic agents targeting cholinesterase enzymes, particularly acetylcholinesterase (AChE) and butyrylcholinesterase (BChE), which play key roles in the cholinergic dysfunction associated with neurodegenerative disorders.[1,2] In our studies, the design, synthesis, and biological evaluation of a series of novel resveratrol-based diarylethene derivatives incorporating diverse heterocyclic scaffolds, including thiophene, oxazole, benzimidazole, furan, triazole, thiazole and pyranone are described. The synthesized compounds were evaluated as potential AChE and BChE inhibitors, with selected oxime-analogues additionally investigated for their ability to reactivate organophosphate-inhibited cholinesterases.[3] Resveratrol-based triazoles and carbamates demonstrated promising BChE inhibitory and antioxidant activities, while selected heteroaryl-arylethenes exhibited favorable selectivity profiles toward BChE. Computational studies, including molecular docking and molecular dynamics simulations, were employed to elucidate the molecular basis of enzyme-ligand interactions and to assess binding stability within the BChE active site. Selected compounds were further subjected to in silico safety assessment and experimental cytotoxicity evaluation. To improve the efficiency and sustainability of the synthetic procedures, conventional batch reactions were complemented by flow chemistry and photochemical approaches. Flow millireactors provided improved conversion and isomer selectivity in key Wittig and Vilsmeier transformations, while custom-designed 3D-printed photochemical reactors enabled rapid and accessible synthesis of selected photocyclization products. Overall, the results demonstrate the potential of resveratrol-inspired diarylethene scaffolds as versatile platforms for the development of cholinesterase-targeting compounds and highlight the advantages of integrating modern synthetic technologies with biological and computational evaluation.



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PUB LECTURE

FROM 0 TO 3D

Vladimir Stilinović

Department of Chemistry, University of Zagreb Faculty of Science, Horvatovac 102a, 10000 Zagreb, Croatia

* vstilinovic@chem.pmf.hr

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SECTION LECTURES

LIGHT AS AN NMR VARIABLE: COAXIAL PHOTO-NMR FOR CLEAN IN SITU MECHANISTIC STUDIES

Valerije Vrček, Antonio Ljulj, Davor Šakić

University of Zagreb Faculty of Pharmacy and Biochemistry, Ante Kovačića 1, Zagreb, Croatia
*valerije.vrcek@pharma.unizg.hr

Light is one of the cleanest ways to initiate, perturb, or control chemical systems, but in NMR spectroscopy it is often treated only as an external stimulus rather than as a well-defined experimental parameter. We describe a Photo-NMR platform designed to close this gap by combining controlled photon delivery with real-time molecular observation. The system was developed around a Varian INOVA 400 MHz spectrometer and uses optical-fiber light delivery from externally positioned irradiation sources, including UV and visible LEDs as well as broadband halogen illumination.

The key design element is not simply the introduction of light into an NMR tube, but the separation of optical function from chemical reactivity. A coaxial 3 mm-in-5 mm tube arrangement places the optical fiber along the central axis while keeping it physically isolated from the reaction mixture. This architecture enables internal irradiation without exposing the fiber, its surface, or its coatings to solvents, reagents, radicals, nanoparticles, or other reactive components. In this way, the experiment retains the advantages of in situ illumination while minimizing contamination, adsorption, and uncontrolled surface effects.

A sandblasted fiber tip disperses light within the active NMR volume, while radiometric characterization allows irradiance to be quantified and reported. Illumination can therefore be treated as a reproducible variable rather than an approximate condition. This is essential for studies in which the relationship between light dose, molecular structure, and reaction progress must be followed directly.

The platform is now being extended toward comparative Photo-NMR experiments on an Oxford X-Pulse 90 MHz benchtop spectrometer. This development will allow the same irradiation architecture and experimental logic to be evaluated across high-field and benchtop NMR environments, broadening access to in situ photochemical NMR studies. Applications include photolysis of bioactive compounds, radical reactions, porphyrin and photodynamic systems, nanoparticle-mediated photochemistry, upconverting nanoparticles, and complex matrices such as olive oil. Overall, the approach provides a scalable route from photon input to NMR-resolved chemical mechanism.

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DOES THE *BASKET* FLUORESCE? ORIGINS AND APPLICATIONS OF THE INTRINSIC CALIXARENE FLUORESCENCE

A. Usenik,[a] F. Sunjka,[a] L. Klemen,[a] K. Kukina Gradečak,[a] M. Belovari,[b] M. Jurković,[b] K. Leko,[a] N. Cindro,[a] G. Horvat,[a] I. Piantanida,[b] V. Tomišić[a]

[a] Department of Chemistry, University of Zagreb Faculty of Science, Horvatovac 102a, 10000 Zagreb, Croatia
[b] Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia
* ausenik.chem@pmf.hr

Because the calixarenes are not fluorescent, they cannot be used as luminescent materials without introducing a luminescent center – states the comprehensive monograph *Calixarenes and Beyond*.[1] The luminescence of calix[*n*]arenes, compounds used across a range of areas, including chemical analysis, medicine, and pharmacy,[2] has indeed traditionally been ascribed exclusively to derivatives with additionally introduced fluorophoric moieties. However, we have recently shown that tertiary-amide and ester calix[4]arene derivatives, as well as their monomeric analogue, do fluoresce, with both the intensity and the position of the emission spectral maximum shifting considerably upon binding of alkali and alkaline earth metal cations in several solvents.[3] This property has since been explored for the conformationally more flexible calix[6]arene derivative, which, depending on the cation charge density, can also form ternary complexes.

Changes in fluorescence during the metal-ion binding are highly dependent on the cation size and charge, whereby intensity in some cases substantially increases, whereas in others the emission is quenched. These changes are large enough for quantitative investigations at two to three orders of magnitude lower ligand concentrations compared to those needed for other commonly used experimental methods. Furthermore, large complexation equilibrium constants can be determined by direct fluorimetric titrations, thus avoiding competitive experiments required if using other methods, which are both time and material consuming and add additional uncertainty to the obtained values.

To investigate the origin of the emission and its complexation-induced changes, the structures and stoichiometries of the complex species were addressed experimentally (NMR, MS) and computationally (MD). Time-resolved fluorescence measurements were carried out as well. Kinetic analysis of the emission decay of the ligands and their complexes yielded the corresponding excited-state lifetimes and the fractional contributions of the individual species to the total emission intensity, both governed by the structure of the ligand (complex) and by the solvent. The different fluorimetric response of the monomeric and the cyclotetra- and cyclohexameric compounds on cation binding points to conformational rigidification and/or inclusion of a solvent molecule in the calixarene *basket* as a driving force behind the observed phenomena. In addition, a reduced effect of photoinduced electron transfer in the complexes compared to the free ligands plays an important role. This paves a pathway to using calixarenes with no appended fluorophores for the detection and discrimination of ionic species in solution and for quantitative analysis.

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FROM SUPRAMOLECULAR ANION RECOGNITION TO CO_2 CAPTURE

Angela F. Danil de Namor [a], Nawal Al Hakawati[b]

[a] Laboratory of Thermochemistry, School of Chemistry & Chemical Engineering, University of Surrey, Guildford, Surrey GU2 7XH, UK,[b] Department of Biological Sciences, Faculty of Science, Beirut Arab University, Tripoli P.O. Box 11-5020, Lebanon
*n.elhakawati@bau.edu.lb

A new upper-rim azocalix[4]arene derivative, 5,11,17,23-tetra[(4-ethylacetoxyphenyl)(azo)]calix[4]arene (CA-AZ), was synthesized and characterized as a chromogenic receptor for anion recognition. Among the monovalent anions investigated, CA-AZ exhibited selectivity toward fluoride, producing an immediate visible color change upon complexation, indicative of fast binding kinetics. The receptor–anion interaction was systematically examined, with particular emphasis on the influence of solvent selection on accurately describing the complexation process. UV–Vis spectrophotometry, conductometric analysis, and isothermal titration calorimetry confirmed the formation of a stable 1:1 CA-AZ/F^- complex in DMSO. Thermodynamic parameters associated with the complexation process were also determined.

The isolated fluoride complex was subsequently evaluated as a probe for atmospheric CO_2 detection and capture. Exposure to carbon dioxide induced a distinct color change visible to the naked eye, providing a simple and effective sensing approach while simultaneously enabling CO_2 sequestration. Unlike many conventional carbon capture materials that require elevated temperatures for regeneration, the captured CO_2 could be readily released under mild conditions, allowing efficient recycling and repeated use of the probe. The combination of highly selective fluoride recognition with reversible CO_2 sensing and capture highlights the potential of the CA-AZ/F^- system as a multifunctional platform for environmental monitoring.

ACKNOWLEDGEMENTS N.A. is thankful to the late Melhem Namor for the support provided to the project. The authors would like to dedicate it to his memory. The authors thank John Watts and his staff for invaluable assistance in the use of the SEM equipment available in the Micro Structural Unit and Surface Analysis Laboratory (University of Surrey).

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TWO-ELECTRON MULTICENTRE BONDING (*PANCAKE BONDING*) IN TWO NOVEL SALTS OF TCNQ RADICAL ANION WITH LOW PARTIAL CHARGES

Krešimir Molčanov,[a] Nikola Jakupec,[a] Petra Stanić[a,b]

[a] Ruđer Bošković Institute, Bijenička 54, HR-10000 Zagreb, Croatia, [b] Istrian University of Applied Science, Preradovićeva 9D, HR-52100 Pula, Croatia
* kmolcano@irb.hr

7,7,8,8-Tetracyanoquinodimethane (TCNQ) is a well-known electron acceptor which readily reduces to a semiquinoid radical anion. However, in majority of its radical salts, it has only a partial charge. The most common formal charges are −1/2 and −2/3.[1,2] Full negative charge (−1) is less common. However, in some rare examples, it has other charges. Recently we described a compound in which formal charge of TCNQ moieties is −4/5.[3] In this work we present two novel salts of TCNQ with tetrabutylammonium cation and stoichiometries of 3:1 and 5:2 and respective partial charges of TCNQ moieties of −1/3 and −2/5. In both salts TCNQ moieties form infinite stacks bound by two-electron multicentre bonds (*pancake bonds*).

The 1:3 salt, although comprised of achiral moieties, crystallises in an unusual space group, *P*1. Attempted solution in $P\bar{1}$, results in a positional disorder of tetrabutylammonium cations and high values of *R*. Therefore, chiral crystal packing arises from a chiral arrangement of achiral moieties. The TCNQ moieties form 1D stacks of pancake-bonded trimers (short interplanar distances of <3.3 Å) separated by non-bonding stacking interactions (interplanar separations of 3.40 Å).

Packing of 5:2 salt is similar, but TCNQ moieties stack with longer interplanar separations (3.33 – 3.43 Å). This type of stacking implies long-range 1D antiferromagnetic ordering.

Geometry of TCNQ moieties in both salts is closer to quinoid (neutral) than to semiquinoid (radical) structure, and geometric correlations indicate that the charges of the moieties are indeed close to −1/3 and −2/5, respectively. Therefore, the structures were refined by Hirshfeld atom model (HAR) to reveal more accurate bond lengths as well as additional details of molecular structures, charges and pancake bonding.

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BIOCATALYTIC SYNTHESIS OF CHIRAL PROPARGYLIC ALCOHOLS THROUGH HHDH-CATALYZED CASCADE REACTIONS

Irena Dokli, Danijel Glavač, Petra Švaco, Doroteja Mutak, Maja Majerić Elenkov

Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička 54, 10000 Zagreb, Croatia

* irena.dokli@irb.hr

Chiral propargylic alcohols are versatile synthetic intermediates for the preparation of pharmaceuticals, agrochemicals, natural products and functional materials.[1] Herein, we report a biocatalytic approach to enantioenriched propargylic building blocks through halohydrin dehalogenase (HHDH)-catalyzed cascade reactions. The natural function of HHDHs is the dehalogenation of vicinal haloalcohols (halohydrins) followed by formation of epoxides.[2] Their chemoenzymatic potential extends further due to their ability to catalyze a wide range of bond-forming reactions, including carbon–carbon, carbon–halogen, carbon–nitrogen, carbon–oxygen, and carbon–sulfur bond formation via epoxide ring opening with various negatively charged, non-natural nucleophiles.[3,4] Starting from racemic propargylic chlorohydrins, the enzyme catalyzes an intramolecular dehalogenation to generate the corresponding epoxide intermediate, followed by regioselective azidolysis in the presence of sodium azide. This cascade process enables the kinetic resolution of racemic substrates, affording enantiopure β-azido alcohols and unreacted chlorohydrins (Figure 1). The desired azido alcohols were obtained with enantiomeric excess exceeding 99%, while the recovered chlorohydrins were isolated in similarly high optical purity (>99% ee). The methodology proceeds under mild aqueous conditions and provides a sustainable and efficient route to valuable chiral propargylic synthons. This work expands the synthetic utility of HHDHs in asymmetric synthesis highlighting their potential for the development of cascade processes for the preparation of highly functionalized chiral molecules.

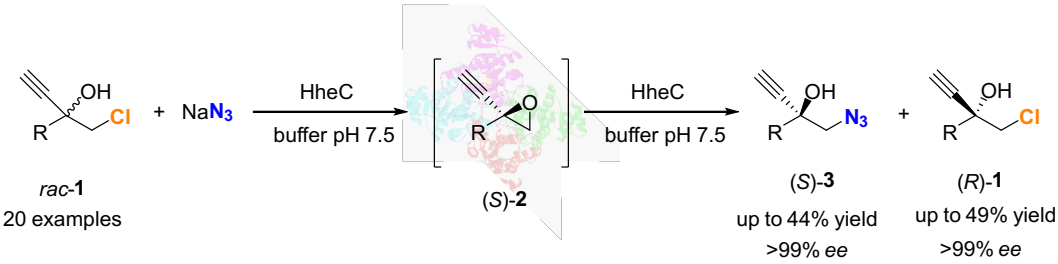


Figure 1. HheC catalyzed cascade reaction in the synthesis of chiral azido alcohols and chlorohydrins.

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NEXT-GENERATION FORMULATIONS FOR IMPROVED PHYTOPHARMACEUTICAL EFFICACY

Donna Danijela Dragun[a], Martina Jović[a], Tihana Mlinarić[a], Iva Rezić Meštrović[b], Ernest Meštrović[a]

[a]University of Zagreb, Faculty of Chemical Engineering and Technology, Trg Marka Marulića 19, 10000 Zagreb, Croatia, [b]University of Zagreb, Faculty of Textile Technology, Prilaz baruna Filipovića 28a, 10000 Zagreb, Croatia

*ddragun@fkit.hr

Despite ongoing progress in medicine, human health faces growing challenges. New diseases are emerging every year, yet many long-known conditions still lack truly effective treatments. The need for safer and more effective therapies has never been greater as microbes constantly evolve and develop resistance. One of the compelling directions is the revival of plant-based medicine – not in its traditional form, but as precisely engineered phytopharmaceuticals. Phytopharmaceuticals are plant-based drugs developed from naturally occurring phytochemicals that show significant therapeutic potential. Polyphenols such as morin, quercetin, coumarin, ferulic acid, rosmarinic acid and gallic acid, which were used in this research, are examples that demonstrate anti-inflammatory effects, the ability to modulate cytokine networks, antioxidant protection, and even potential anticancer activity. However, one of their main weaknesses is poor solubility and, as a result, low bioavailability. Their limitations have kept many promising compounds out of clinical relevance. Our research targets that problem by turning to next-generation formulation technologies. Supramolecular chemistry, particularly cyclodextrin inclusion complexes, offer a way of improving solubility and stabilizing sensitive polyphenols. In parallel, electrospinning enables the incorporation of polyphenols into polymeric nanofibers, creating highly tunable systems with controlled release and enhanced dissolution.[1] When combined, these two approaches could open the door to entirely new, more effective and improved phytopharmaceutical formulations with genuine therapeutic potential. To evaluate these systems, fiber morphology and molecular incorporation were examined using SEM and Raman microscopy, while release kinetics were measured for each new system. By combining advanced formulation strategies, phytochemicals that were once limited by poor solubility and stability could be transformed into innovative phytopharmaceuticals with improved dissolution, enhanced stability, and controlled release, opening the door for the development of new therapies.

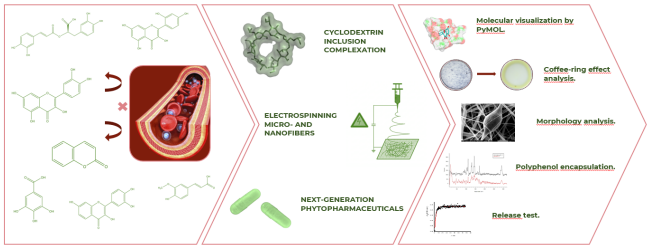


Figure 1. Schematic workflow of motivation, fabrication, and characterization of next-generation phytopharmaceuticals.

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WHEN DIVERSITY BECOMES A SOLUTION: MORIN AND GALLIC ACID IN NEXT-GENERATION PCL NANOFIBERS

Martina Jović, Donna Danijela Dragun, Ernest Meštrović

Department of General and Inorganic Chemistry, Faculty of Chemical Engineering and Technology, Trg Marka Marulića 19, HR-10000 Zagreb, Croatia
*mjovic@fkit.hr

Phytopharmaceuticals represent a valuable source of natural bioactive compounds with pronounced antioxidant, anti-inflammatory and antimicrobial properties, yet their therapeutic application is often limited by poor stability, low bioavailability and sensitivity to environmental conditions. Advanced drug-delivery systems are therefore essential to unlock their full therapeutic potential. In this context, electrospun poly(ε-caprolactone) (PCL) nanofibers emerge as a promising platform for protecting and enabling the controlled release of natural bioactive molecules. This work investigates the incorporation of two chemically contrasting phytopharmaceuticals — morin and gallic acid — into PCL nanofibers to evaluate system adaptability across distinct physicochemical profiles. Morin is a hydrophobic flavonoid with limited solubility and high oxidative sensitivity,[1] whereas gallic acid is a hydrophilic phenolic acid with strong antioxidant activity but rapid degradation and poor membrane permeability.[2] Their chemical diversity provides an ideal model for assessing the versatility of PCL nanofibers as a universal delivery system. Special emphasis is placed on the influence of solvent choice, comparing conventional organic solvents like DCM and DMF with more sustainable alternatives (acetic and formic acid) aligned with green-chemistry principles. FTIR confirmed successful incorporation of both compounds without chemical degradation, while XRD showed preserved PCL crystallinity and amorphous dispersion of the phytochemicals. SEM imaging revealed uniform fibers, indicating good compatibility between PCL and both molecules. DPPH assays demonstrated that morin and gallic acid retained their antioxidant activity after encapsulation, with gallic acid exhibiting the highest radical-scavenging efficiency and morin maintaining strong activity despite its oxidative sensitivity. Overall, the results show that PCL nanofibers enable sustained entrapment of both morin and gallic acid within the matrix while maintaining strong ROS-scavenging activity. This confirms that chemical diversity is not a limitation but an advantage in designing next-generation, adaptable nanofiber-based delivery systems for pharmaceutical and biomedical applications.

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THE INFLUENCE OF TRACE WATER ON THE SOLUTION AGGREGATION OF DRUG MOLECULES TOWARDS CRYSTALLISATION

Benjamin Vella,[a] Marin Liović,[b] Nikola Bregović,[b] Katharina Edkins[a]

[a] Strathclyde Institute of Pharmacy and Biomedical Sciences, University of Strathclyde, 166 Cathedral Street, Glasgow G4 0RE, [b] Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, 10000, Zagreb, Croatia
* benjamin.vella@strath.ac.uk

The outcome of crystallisation experiments depends on the experimental conditions, which must be strictly controlled, particularly for active pharmaceutical ingredients (**APIs**) where reliable production of a specific crystal form is crucial.[1] Solution aggregation prior to nucleation and crystal growth has attracted increasing attention, both within non-classical nucleation theory and through the link hypothesis, which proposes a relationship between molecular interactions in solution and those in the resulting crystal. While these approaches have shown system-dependent success,[2–4] the influence of trace water on the solution aggregation remains largely overlooked, despite water being present in most laboratory solvents at atmospheric conditions.

In this work, we have investigated the effect of water on the solution behaviour of two small organic model compounds, paracetamol (**PCM**) and salicylamide (**SAL**), in acetonitrile (**AcN**). These compounds are similar in size, shape, and hydrogen-bonding ability, yet exhibit markedly different solid-state landscapes: PCM displays polymorphism and hydrate formation, whereas only two polymorphs have been reported for SAL. Solution ^{1}H NMR spectroscopy reveals pronounced shifting on the residual water signal as the concentration of both compounds is increased, indicating significant solute-water interactions. Host-guest titrations with water as the guest demonstrate stronger interactions between water and PCM than between water and SAL. These findings are independently confirmed to be solute-water interactions through dissolution calorimetry measurements. Complementary FTIR spectroscopy reveals significant hydrogen bonding between the PCM carbonyl group and water, leading to the formation of a presumed 1:1 PCM-H_2O complex at trace water concentrations, followed by the emergence of higher-order hydrated aggregates as the water concentration increases. SAL exhibits simpler behaviour as water concentration increases, with only two main species observed corresponding to unbound SAL and a hydrated SAL-water aggregate, with slower interconversion between the two.

These results demonstrate that trace water can substantially alter solution speciation, producing stable solute-water hetero-aggregates even at very low water concentrations. Consequently, the aggregates present in solution may differ significantly from those expected when only homomeric solute interactions are considered. Solute-water clustering is thus a very important factor in solution aggregation and crystallisation studies, as well as in broader solution-based methodologies including chemical synthesis, spectroscopic characterisation, and calorimetric measurements.

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STRUCTURE OF WATER-DIMETHYLFORMAMIDE MIXTURES AND POTENTIAL EFFECTS ON CRYSTALLISATION

Abbie O. R. Madden,[a] Thomas F. Headen,[b] Terri-Louise Hughes,[b] Sophie Janbon,[c] Katharina Edkins[a]

[a] Strathclyde Institute of Pharmacy and Biomedical Sciences, University of Strathclyde, 161 Cathedral Street, Glasgow G4 0RE, UK, [b] ISIS Neutron and Muon Source, Science and Technology Facilities Council, Rutherford Appleton Laboratory, Didcot OX11 0QX, UK, [c] Early Chemical Development, Pharmaceutical Sciences, R&D, AstraZeneca, Charter Way, Macclesfield SK10 2NA, UK

*abbie.madden@strath.ac.uk

Hydrate crystal forms of pharmaceutical compounds often have low bioavailability and poor tablettability,[1] it is hence important to control their crystallisation in industry and research. It is common to use binary solvent mixtures to tailor solubilities during crystallisation, however, many of these solvent mixtures have non-ideal behaviour which present through clustering of the individual components on the molecular level called microheterogeneity.[2] One solvent mixture suggested to be microheterogeneous is water-dimethylformamide (DMF), with molecular dynamics simulations indicating clustering over a range of mixing ratios.[3] These clusters may cause solute localisation in specific areas, creating a "templating" effect promoting the formation of specific crystal forms, e.g. hydrates.[4] To fully understand this, we investigate the structure and interactions of the solution state and relate these to those in the crystalline form.

Crystallisation of some pharmaceutical relevant compounds show that their hydrate formation can be inhibited in water/DMF mixtures at much lower DMF fractions (and corresponding higher water activities) than in other aqueous solvent mixtures, e.g. acetonitrile or methanol. We performed neutron total scattering (NTS) experiments to elucidate the structure of mixtures at DMF mole fractions X_{DMF} = 0.15, 0.35, and 0.5. Although there is no clear microheterogeneity, there is indication of self-association. Monte-Carlo / Molecular-dynamics simulations tethered to our NTS data allow us to interrogate specific site-site interactions in our mixtures. We see that, at X_{DMF} = 0.15, water and DMF molecules form a bi-percolating system, while at higher DMF content, water molecules appear to form linear chain-like structures, filling the space between the larger DMF molecules as a continuous matrix. Further NTS experiments on water-DMF mixtures with the addition of guanidine hydrochloride as a highly lipophilic model solute show that DMF-DMF interactions change little accross all mixtures, but water-water and water-DMF interactions are increased at X_{DMF} = 0.15 and decrease with increasing DMF content, relative to the solvent mixtures. The non-ideality of these solvent mixtures is at a maximum around X_{DMF} = 0.30, close to the mole fraction of hydrate crystallisation inhibition, indicating that solvent structure influences crystallisation. This furthers our understanding of how solvents play a role in crystallisation, enabling smarter solvent choices.

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FORMATION OF O···π 'LAMP MOTIFS' IN MODIFIED 2,3-DICHLORO-5,6-DICYANO-*p*-BENZOQUINONE FACILITATED BY PROTONATED POLYCYANOMETALATES: MECHANISM AND STRUCTURE

Nikola Jakupec, Krešimir Molčanov

Department of Physical Chemistry, Ruđer Bošković Institue, Bljenička cesta 54, Zagreb, Croatia
* njakupec@irb.hr

2,3-Dichloro-5,6-dicyano-*p*-benzoquinone (DDQ) is a widely used oxidizing agent in organic synthesis.[1] Radical anions of DDQ, which are easily prepared, have also recently been used for forming multicentric (pancake) bonded stacks.[2,3] Recent studies have also demonstrated nucleophilic addition to the DDQ ring or one of the oxygen atoms using π-nucleophiles.[4] However, no in-depth mechanistic or crystallographic study was undertaken, meaning the mechanism of formation of such products and their exact crystal structure, along with any interaction motifs, remain unexplored.

In this work we have ventured to resolve the mechanism of formation of DDQ modified by nucleophilic addition and substitution using computational simulations. The reactions themselves were facilitated by using a highly acidic medium (protonated polycyanometallates). SCXRD study of the obtained products shows a persistent O···π intra- and intermolecular 'lamp motif' interaction. The nature of this interaction has been investigated using charge density analysis, Hirshfeld atom refinement and analysis of electrostatic potential mapped onto the Hirshfeld surface of the molecule.

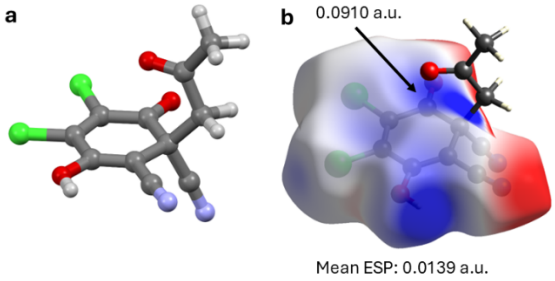


Figure 1. a, structure of a modified DDQ exhibiting a O···π 'lamp motif'; **b**, electrostatic potential mapped onto a Hirshfeld surface of the modified DDQ, mean ESP value is also shown.

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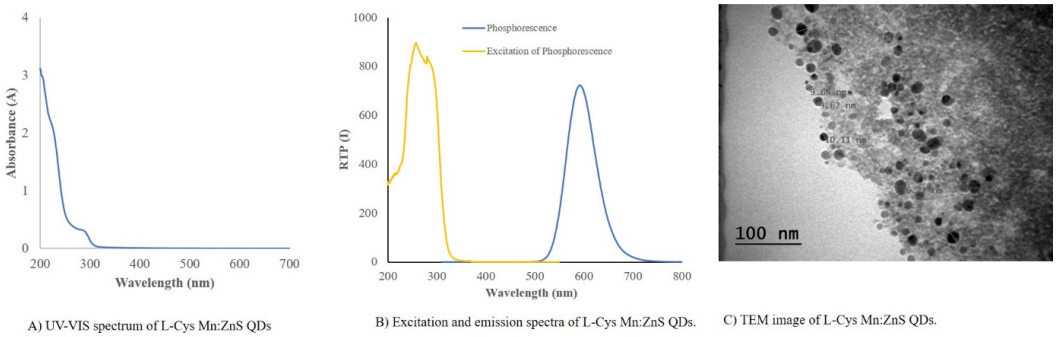
A PHOSPHORESCENT QUANTUM DOT–HYDROGEL HYBRID PLATFORM FOR BIOCOMPATIBLE OPTICAL SENSORS

Huma Yilmaz[a], Iva Karneluti[a], Deepak Joshy[a], Ivana Perković[a], Gerhard J. Mohr[b], Ivana Murković Steinberg[a]

[a] University of Zagreb Faculty of Chemical Engineering and Technology, Trg Marka Marulića 19, 10000 Zagreb, Croatia, [b] Joanneum Research Materials, Franz-Pichler-Straße 30, 8160 Weiz, Austria

* hyilmaz@fkit.hr

Room-temperature phosphorescence (RTP) has emerged as a powerful optical transduction strategy due to its ability to distinguish long-lived phosphorescent signals from short-lived autofluorescence and scattered light, thereby enhancing analytical sensitivity and detection reliability. However, developing RTP materials that simultaneously offer long emission lifetimes, aqueous processability, and mechanical flexibility for wearable sensing applications remains a significant challenge[1]. Herein, we report the fabrication of a phosphorescent sensing platform based on L-cysteine-capped Mn-doped ZnS quantum dots (Mn:ZnS QDs) immobilized within a biocompatible polyurethane hydrogel matrix. The phosphorescent behavior of the Mn:ZnS QDs was systematically investigated in three different configurations: dispersed in aqueous solution, immobilized on a hydrogel-coated substrate, and incorporated into a free-standing hydrogel film. All platforms exhibited stable room-temperature phosphorescence with an emission lifetime of approximately 4 ms, while the hydrogel-based architectures offered enhanced mechanical flexibility and ease of handling, making them particularly suitable for wearable sensing applications. This hybrid material offers a versatile optical sensing platform that combines long-lived emission, excellent processability, and substrate-independent applicability, highlighting its potential for developing next-generation biocompatible phosphorescent sensors.



A) UV-VIS spectrum of L-Cys Mn:ZnS QDs

B) Excitation and emission spectra of L-Cys Mn:ZnS QDs.

C) TEM image of L-Cys Mn:ZnS QDs.

Figure 1. Spectral and morphological characterization of L-Cys Mn:ZnS quantum dots.

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VALIDATION OF WEARABLE OPTICAL BIOCHEMICAL SENSORS USING PHANTOMS REPRESENTING DIVERSE SKIN TONES

Deepak Joshy,[a]* Ivana Perković,[a] Iva Karneluti,[a] Rolf B. Saager,[b] Gerhard J. Mohr,[c] Matthew D. Steinberg,[d] Ivana Murković Steinberg[a]

[a] Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev Trg 19, Zagreb 10000, Croatia, [b] Department of Biomedical Engineering (IMT), Linköping University, Sweden, [c] Joanneum Research Forschungsgesellschaft mbH – Materials, Franz-Pichler-Straße 30, Weiz A-8160, Austria, [d] GoSense Wireless Ltd, Cambridge CB23 6FN, UK

*djoshy@fkit.unizg.hr

Wearable optical sensors are increasingly used for continuous physiological and biochemical monitoring;[1] however, the influence of skin tone on their performance remains a critical challenge. Although skin-tone effects have been extensively investigated for photoplethysmography (PPG) and pulse oximetry,[2,3] their impact on wearable optical biochemical sensors has received little attention. The absence of standardized validation platforms representing diverse skin tones limits the development of accurate and reliable sensing technologies. In this work, PDMS-based tissue-mimicking phantoms were developed with tunable optical scattering and absorption properties corresponding to Fitzpatrick skin types. Phantom optical properties were determined using a Monte Carlo lookup-table-based inverse modelling approach and experimentally characterized using Spatial Frequency Domain Imaging (SFDI) spectroscopy, with SFDI measurements used to optimize and validate the inverse modelling process.[4] To demonstrate the applicability of the phantoms for wearable optical sensor validation, a colorimetric cellulose-based pH sensing foil was employed as a model biochemical sensing platform. Optical responses from the pH sensing foil over a pH range of 4-8 were measured on each skin-tone phantom using both reflectance spectroscopy and a custom-designed colorimeter. For each skin-tone range, pH calibration functions were obtained and analysed using spectrometer and custom-made colorimeter. The proposed phantom platform provides a standardized framework for validating multimodal wearable optical sensors across diverse skin tones and strengthens the development of universal skin-tone-aware calibration strategies.

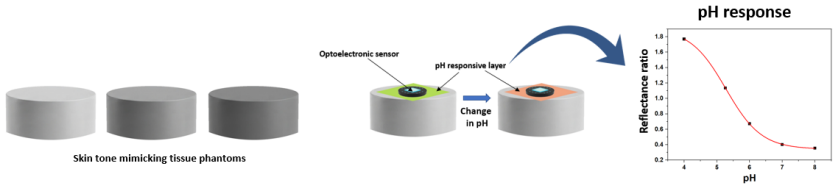


Figure 1. Proposed platform for validating multimodal wearable optical biochemical sensors across diverse skin tones.

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N,O-DONOR MACROCYCLIC LIGANDS AS BUILDING BLOCKS FOR SILVER COORDINATION POLYMERS AND INCLUSION COMPOUNDS

Milenko Korica,[a] Tomislav Balić,[b] Ivica Đilović[c]

[a] Department of Chemistry, Josip Juraj Strossmayer University of Osijek, Ul. cara Hadrijana 8A, Osijek,

[b] Department of Chemistry, Josip Juraj Strossmayer University of Osijek, Ul. cara Hadrijana 8A, Osijek,

[c]Department of Chemistry, Faculty of Science, Horvatovac 102A, 10000 Zagreb

* mkorica@kemija.unios.hr

Macrocyclic Schiff bases represent an important class of ligands owing to their versatile coordination behavior and ability to form host–guest inclusion compounds. This study presents the synthesis, characterization, and structural investigation of a series of novel *N,O*-donor macrocyclic ligands developed within the framework of a doctoral research project.

Nine dialdehyde precursors were synthesized from 2- and 3-hydroxybenzaldehyde and *α,ω*-dibromo alkanes, five of which proved suitable for the preparation of macrocyclic Schiff bases. Three new macrocyclic Schiff bases were successfully synthesized together with three additional macrocyclic derivatives, including one reduced Schiff base (secondary amine) and two pendant macrocycles. The obtained macrocycles exhibited remarkable host–guest properties toward both gaseous (CO_2, H_2S, SO_2, NH_3, and Cl_2) and volatile alcohol molecules. Stable inclusion compounds were obtained without structural degradation of the macrocyclic framework, demonstrating the chemical robustness of the synthesized hosts even in the presence of highly corrosive gases. Furthermore, reactions of the macrocyclic Schiff bases with silver(I) salts afforded one-dimensional coordination polymers. Attention was devoted to evaluating the influence of the counter anion on the resulting coordination architecture and structural features.

Single-crystal X-ray diffraction enabled the structural determination of five dialdehyde precursors, one macrocyclic Schiff base, five inclusion compounds, and four silver coordination polymers, providing detailed insight into their molecular and supramolecular organization. The results demonstrate the potential of these newly synthesized macrocyclic ligands as versatile platforms for crystal engineering, host–guest chemistry, and the design of functional coordination materials.

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DETECTING AND MODULATING PROTEINS WITH MULTIFUNCTIONAL MOLECULAR PROBES

Leila Motiei, David Margulies*

Department of Chemical and Structural Biology, Weizmann Institute of Science, Rehovot, Israel

* leila.motiei@weizmann.ac.il

Protein surfaces play central roles in many biological processes yet effectively targeting them with synthetic agents remains a major challenge. To address this, we have developed multifunctional molecular probes capable of engaging in proximity-induced, nonspecific interactions with protein surfaces. These probes can interact with diverse proteins and can be applied to multiplexed protein sensing as well as to mediate unnatural protein–protein or cell–cell interactions. The first part of the talk will focus on ID-probes, a class of fluorescent probes that mimic the function of the olfactory system.[1-4] Unlike conventional probes designed to detect a single protein, ID-probes generate distinct identification (ID) fingerprints for multiple proteins and their combinations. This capability enables the characterization of protein subpopulations in complex mixtures and in living cells; tasks that are difficult to achieve using conventional chemical “nose/tongue” approaches. In the second part of the presentation, we will describe a strategy for reversibly decorating bacteria with artificial, self-assembled synthetic receptors.[5,6] This supramolecular modification dynamically functionalizes the bacterial surface without genetic manipulation, effectively endowing the cells with new recognition capabilities. By installing synthetic receptor assemblies on bacterial membranes, we created bacterial probes (B-probes) that selectively interact with mammalian cells. These engineered bacteria function as living sensing platforms capable of distinguishing between different cancer cell types, highlighting the potential of combining synthetic chemistry with living systems to develop adaptable and programmable diagnostic tools.

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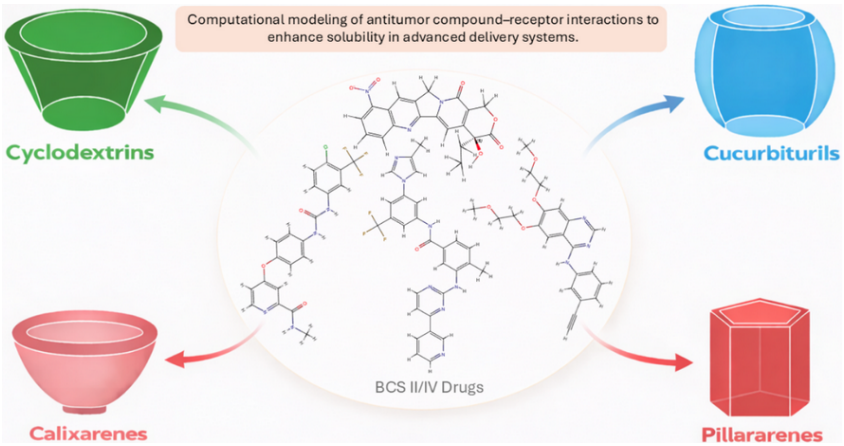
PREDICTIVE ATOMISTIC MODELING OF ANTITUMOR DRUG ENCAPSULATION WITHIN SUPRAMOLECULAR HOSTS

Lucija Vrban Đerek, Robert Vianello

Laboratory for the Computational Design and Synthesis of Functional Materials, Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička cesta 54, 10 000, Zagreb, Croatia

* lucija.vrban@irb.hr

Poor aqueous solubility remains a major limitation in the development of many anticancer drugs, reducing their bioavailability and therapeutic efficacy. Cyclodextrins and cucurbiturils are promising supramolecular drug carriers that enhance drug properties through reversible host–guest complex formation.[1] This study evaluated the ability of selected macrocyclic receptors to encapsulate poorly soluble anticancer drugs (erlotinib, sorafenib, nilotinib, and rubitecan) using a multiscale computational approach combining quantum chemical calculations, molecular docking, all-atom molecular dynamics simulations in explicit solvent, and MM-GBSA binding free energy analysis.[2] The results revealed distinct encapsulation behaviors of the investigated hosts. Cucurbiturils formed highly stable inclusion complexes, whereas cyclodextrins exhibited more dynamic binding, enabling both efficient encapsulation and drug release. These findings demonstrate that successful drug delivery depends not only on strong host–guest interactions but also on controlled guest release, making cyclodextrins promising carriers for poorly soluble anticancer drugs.[3]



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EMPOWERING STUDENTS TO INVESTIGATE SUSTAINABILITY: FROM CHEMISTRY LABORATORIES TO INDOOR AIR QUALITY

Jurica Bauer,[a] Annemarie van Zeijl-Rozema,[b] Gavin Phillips,[c] Katarzyna Dziubińska-Kühn[c], Renaud Jolivet[c]

[a] Faculty of Health, Medicine and Life Sciences, Maastricht University, Universiteitssingel 40, 6229 ER Maastricht, The Netherlands, [b] School of Business and Economics, Maastricht University, Tongersestraat 53, 6211 LM Maastricht, The Netherlands, [c] Faculty of Science and Engineering, Maastricht University, Paul-Henri Spaaklaan 1, 6229 GS Maastricht, The Netherlands
* j.bauer@maastrichtuniversity.nl

How can chemistry education simultaneously develop scientific skills, foster sustainability awareness, and contribute to healthier learning environments? We present the evolution of a student-driven educational initiative that progressed from investigating the environmental impact of chemistry laboratories to indoor air quality (IAQ) in university teaching spaces. Together, these two phases illustrate how sustainability education can evolve from analysing educational practice to becoming an intervention for institutional sustainability.

The first phase engaged a multidisciplinary group of undergraduate students in an extracurricular research project investigating greenhouse gas (GHG) emissions from chemistry-focused practicals. Using commercially available sensors for CO_2, CO, NH_3, total volatile organic compounds (TVOCs), and particulate matter, students measured emissions during laboratory experiments and linked these to specific experimental activities. By quantifying the often-overlooked chemical footprint of routine laboratory teaching, students gained hands-on experience with analytical measurements while developing greater awareness of sustainable laboratory practice.

The second phase expanded beyond laboratories to tutorial rooms and adopted an interdisciplinary approach combining natural and social sciences. A Master's student in Sustainability Science, Policy and Society and a Bachelor's student in Circular Engineering investigated IAQ using continuous environmental monitoring, perception surveys, focus groups, and pre- and post-workshop questionnaires. This mixed-methods approach enabled comparisons between measured and perceived air quality while increasing awareness of greenhouse gases, ventilation, and healthy learning environments. The project also explored relationships between environmental measurements, environmental health literacy, and sustainability awareness.

Compared with the original extracurricular initiative, this phase represents a progression towards a mixed curricular-semicurricular model by embedding the project within a Master's thesis while maintaining extracurricular participation. We present the educational design, emerging correlations and trends, and discuss how integrating chemistry, environmental monitoring, and social science methods creates richer learning experiences and more meaningful sustainability outcomes than either disciplinary perspective alone.

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AN APPROACH FOR STUDENTS WITH A MULTIDISCIPLINARY PROFILE: NANOMATERIALS CHEMISTRY

Catarina de Carvalho Esteves

Coatings, Surfaces & Interfaces, Laboratory of Physical Chemistry, Chemical Engineering and Chemistry Department, Eindhoven University of Technology, Het Kranenveld 14, 5612 AZ Eindhoven, The Netherlands
*a.c.c.esteves@tue.nl

Many of the societal challenges we currently face, for example regarding the materials and energy transition, involve complex problems which require interdisciplinary and multi-perspective approaches. Our students are highly motivated to work in these big challenges and contribute with engineering and scientific solutions to creating alternative and new sustainable and fair pathways. As such, these complex problems require future researchers and engineers to be able to communicate and collaborate across scientific fields while working in mixed environments, where chemists, physicists, (materials) engineers and others (often including biologists and industrial engineers), all contribute with their own expertise.

Nanomaterials (and Nanotechnology) appears as a perfect topic candidate to create such a learning environment, since the field *per se* emerged (and grew) with the contribution of scientists and researchers from different scientific nature, with a great Chemistry footprint.[1] However, from the education point of view, having such a varied student's audience (in discipline and learning level) also creates several chalenges, namely regarding teaching objectives and output - suface *versus* (in-)depth, conceptual *versus* practical learning, integration of knowledge from different disciplines, and assessment methods for a student population with different learning styles, motivational interest and (critical) thinking level.

Taking a wide and conceptual journey through the *Bottom-Up* and *Top-Down* approaches to fabricate Nanomaterials[2] with a Chemistry perspective, we have been teaching a large audience of Bachelor (Engineering) students with a multidisciplinary and multi-level background (Chemistry, Physics, Mechanical, Electrical and Biomedical Eng.) for more than a decade. The large experience with this and other inter-departmental courses at TU/e, under the umbrella of Nanomaterials and Nanotechnology, including now a Challenge Based Learning – practical course running a pilot in 2026/2027, provides us with evidence and key learning points which will be presented and discussed, which expectedly could be taken as inspiration for designing the education of the next generations facing multi- and interdisciplinary challenges.

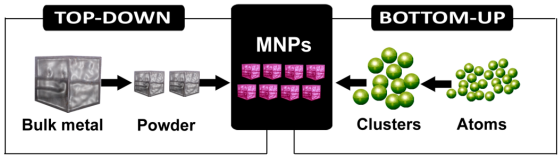


Figure 1. Schematic of *Top-down and Bottom-up* approaches to fabricate nanomaterials.[2]

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TOPOLOGICAL ANALYSIS OF MOLECULAR POTENTIAL ENERGY SURFACES USING SUBLEVEL PERSISTENT HOMOLOGY

Dairo José Hernández Páez

Universidad de La Guajira, Faculty of Engineering, Km 5 Vía a Maicao, Riohacha, La Guajira, Colombia

* djhernandezp@uniguajira.edu.co

Potential energy surfaces (PES) constitute a fundamental framework for understanding molecular stability, conformational transitions, and reaction pathways. However, traditional analyses often focus on local features such as minima and transition states, while the global organization of the energy landscape remains largely unexplored. In this work, we present a topological approach based on sublevel-set persistent homology to characterize the multiscale structure of molecular potential energy surfaces.[1]

The methodology starts with the construction of PES obtained from quantum chemical calculations and systematic conformational sampling over relevant dihedral angles. Energy values are used to generate sublevel filtrations, where each threshold defines a subset of the conformational space. Persistent homology is then computed to identify topological invariants, including connected components, cycles, and higher-dimensional cavities.[2]

Persistence diagrams provide a direct interpretation of molecular energy landscapes. In particular, zero-dimensional births are associated with local minima, while deaths correspond to the merging of energy basins through transition states. Moreover, persistent higher-dimensional features reveal periodicities and cyclic structures arising from the intrinsic topology of conformational spaces.[3,4]

Our results demonstrate that sublevel persistent homology provides a robust and comprehensive description of molecular energy landscapes, complementing conventional computational chemistry approaches. This framework establishes a bridge between algebraic topology and molecular modeling and offers new perspectives for investigating complex molecular systems and their conformational behavior.

ACKNOWLEDGEMENTS

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SUBSTITUENT EFFECTS BIOLOGICAL ACTIVITY AND DRUG-LIKENESS: A MEDICINAL CHEMISTRY BASED STUDY

Deepkumar Joshi

Chemistry Department, Sheth M. N. Science College, Patan-384265, Gujarat, India

* deepkumarsjoshi@yahoo.com

The biological potential of small-molecule drug candidates is profoundly influenced by the nature and position of substituents on the core pharmacophore. In the present study, a comparative medicinal chemistry–oriented evaluation of a series of structurally related compounds bearing electron-donating, electron-withdrawing, and halogen substituents was performed using molecular docking and associated in-silico techniques. Docking studies against a selected biological target were conducted to investigate binding affinity, binding orientation, and key ligand–target interactions governing biological activity. The results indicate that systematic substituent variation markedly affects binding energy, steric fit within the active site, and interaction profiles, including hydrogen bonding, hydrophobic interactions, π–π stacking, and electrostatic contacts. Notably, compounds containing electron-withdrawing and halogen substituents demonstrated improved binding efficiency, attributed to favorable electronic distribution and enhanced active-site complementarity. Furthermore, drug-likeness assessment based on Lipinski's Rule of Five and in-silico bioavailability prediction was performed to evaluate oral drug potential and pharmacokinetic feasibility. The integrated structure–activity relationship (SAR) analysis highlights the critical role of substituent-driven optimization in the rational design of biologically potent and orally bioavailable drug candidates within a medicinal chemistry framework.

HYDROGEL-COATED COLOURIMETRIC FACE SHEET MASK FOR MONITORING SKIN pH

Iva Karneluti,[a] Gerhard J. Mohr,[b] Magdalena Vrđuka,[a] Ivana Perković,[a] Deepak Joshy,[a] Hüma Yilmaz,[a] Ivana Murković Steinberg[a]

[a] Faculty of Chemical Engineering and Technology, University of Zagreb, Trg Marka Marulića 19, 10000 Zagreb, Croatia, [b] Joanneum Research Materials, Franz-Pichler-Straße 30, 8160 Weiz, Austria

* izuvic@fkit.hr

Non-invasive optical platforms that enable visual reporting of pH changes at the skin surface are attracting growing interest as simple analytical tools for assessing physiologically relevant changes in the skin microenvironment.[1] One relevant application is the evaluation of local acidification induced by cosmetic treatments and the subsequent recovery towards physiological skin conditions driven by the skin's natural buffering response. In this work, a commercially available cellulose face sheet mask was transformed into a colourimetric sensing platform by covalent immobilisation of the pH-sensitive azo dye GJM 452 via vinylsulfonyl chemistry.[2] To improve suitability for skin contact, the functionalised substrate was coated with a thin polyurethane hydrogel layer, providing a protective and biocompatible interface while preserving accessibility of the immobilised dye to pH changes. The developed platform exhibited a reversible colour transition from blue through green to yellow-brown over the pH range 3.00-5.50. Colourimetric evaluation was performed using CIELAB colour space analysis, with hue angle selected as the primary parameter for quantifying pH-dependent colour changes. The sensor showed excellent repeatability and reversibility with no detectable dye leaching, confirming the stability of the covalently immobilised sensing layer and its rapid response. Proof-of-concept applicability was assessed using commercially available glycolic acid skincare products capable of inducing local acidification. The functionalised face mask exhibited a clear colourimetric response to pH changes induced by these products, demonstrating the suitability of the developed system for monitoring variations in skin surface pH. Overall, the combination of covalent dye immobilisation, a biocompatible hydrogel coating, reversible colourimetric response, rapid response behaviour and the absence of detectable dye leaching highlights the potential of this cellulose-based platform as an optical sensor for non-invasive skin surface pH monitoring.

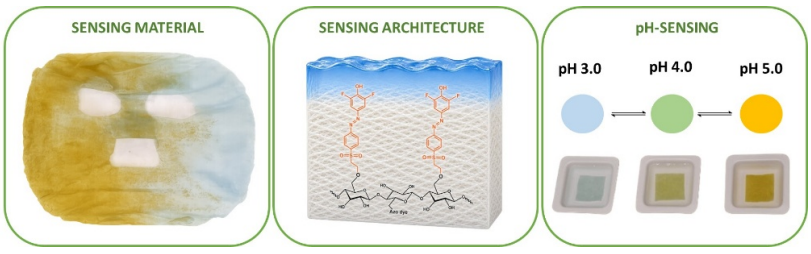


Figure 1. Graphical overview of the hydrogel-coated cellulose face mask developed as a colourimetric platform for monitoring skin surface pH.

ACKNOWLEDGEMENTS This work is supported by the Croatian Science Foundation under the project WearSense HRZZIP-2022-10-2595.

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PRINTED HYDROGEL-BASED SENSING PLATFORMS ON TEXTILE SUBSTRATES FOR DUAL pH AND UREA MONITORING

Ivana Perković,[a] Deepak Joshy,[a] Iva Karneluti,[a] Hüma Yilmaz,[a] Gerhard J. Mohr,[b] Ivana Murković Steinberg[a]

[a] Faculty of Chemical Engineering and Technology University of Zagreb, Trg Marka Marulića 19, 10000 Zagreb, [b] Joanneum Research Materials, Franz-Pichler-Straße 30, 8160 Weiz

iperkovic@fkit.unizg.hr

The development of wearable and non-invasive chemical sensors requires flexible, low-cost, and biocompatible sensing platforms. In this work, cotton and polyester textile substrates are functionalized with printed polyurethane hydrogel layers for dual pH and urea detection. The hydrogel formulation consists of a polyurethane matrix, an ethanol–water solvent system, and the pH-sensitive dye GJM 534,[1] deposited by modified direct ink writing (DIW). Two sensing systems are investigated: pH-responsive hydrogels containing only the indicator dye and urease-functionalized hydrogels for enzymatic urea detection. The pH response exhibits distinct colour changes with increasing pH. Hue angle analysis using a reference optical measurement system is compared with smartphone-based image analysis to evaluate mobile sensor readout. Calibration curves for cotton and polyester substrates enable determination of apparent pK_a values. The sensors show high reversibility and stability during repeated pH switching. Urea detection is based on urease-mediated hydrolysis,[2,3] producing a concentration-dependent colour change. Dye-only systems show no response to urea, confirming the specificity of the enzymatic sensing mechanism. To compensate for variations in the initial sample pH, a reference pH-responsive layer was integrated alongside the urease-functionalized sensing layer to enable differential colourimetric analysis for improved urea quantification. The reversible and specific colourimetric responses of the printed materials highlight their potential for low-cost, flexible, and wearable monitoring of pH and urea in biomedical applications.

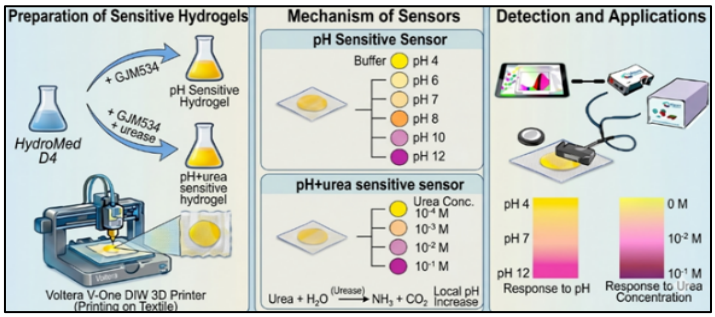


Figure 1. Schematic overview of the printed hydrogel sensors for pH and urea detection.

ACKNOWLEDGEMENTS This work is supported by the Croatian Science Foundation through project WearSense (HRZZ IP-2022-10-2595) and DOK-2025-02-5984 (Young Researchers' Career Development Project–Training of Doctoral Students, doctoral student IP).

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CATALYTIC ZEOLITE 3A AS AN ACTIVE TRANSDUCING INTERFACE FOR NON-ENZYMATIC ELECTROCHEMICAL GLUCOSE SENSING

Laura Manin,[a,b] Elena Stuppia,[a] Filippo Laganà,[a] Srećko Valić,[b,c] Marta Greco,[a] Antonino S. Fiorillo,[a] Salvatore A. Pullano[a,d]

[a] Department of Health Sciences, Magna Graecia University of Catanzaro, 88100 Catanzaro, Italy, [b] Dept. of Medical Chemistry, Biochemistry and Clinical Chemistry, University of Rijeka, 5100 Rijeka, Croatia,

[c] Division of Physical Chemistry, Ruđer Bošković Institute, 10000 Zagreb, Croatia, [d] Department of Electrical Engineering and Computer Science, University of Missouri, Columbia, MO 65211, USA

* laura.manin@studenti.unicz.it

Catalytic nanoporous materials are emerging as multifunctional interfaces for electrochemical sensing owing to their unique ion-exchange capability, structural stability and surface reactivity.[1] However, their potential to operate as active transducing materials, rather than passive supports, remains largely unexplored. Here, Zeolite 3A enables a distinct sensing strategy, in which the electrochemical response originates from a surface-mediated catalytic process instead of the direct electrooxidation of glucose. A flexible sensing platform was fabricated by depositing a Zeolite 3A/soybean oil composite onto a silver-coated Kapton substrate using a scalable preparation procedure. Under alkaline conditions, catalytic basic sites promote the initial stages of glucose-to-fructose isomerization,[2,3] inducing a local redistribution of hydroxyl ions at the electrode/electrolyte interface (Fig. 1). The resulting Ag/AgOx perturbation provides a highly sensitive electrochemical transduction mechanism. The catalytic pathway was investigated by cyclic voltammetry, chronoamperometry and time-dependent FTIR spectroscopy, revealing characteristic glucose- and fructose-related vibrational features. Kinetic analysis using a substrate inhibition model yielded a low apparent K_M of 0.039 mM, supporting strong glucose–interface interactions. The platform enabled glucose detection with a limit of detection of 0.1 µM, two linear concentration ranges spanning 0.1–20 mM, and a maximum sensitivity of 6.68 µA mM^{-1} cm^{-2} at physiologically relevant concentrations. The platform showed high repeatability with negligible interference from fructose, lactose and uric acid, confirming good selectivity.

Beyond glucose monitoring, this work establishes microporous zeolites as multifunctional chemical interfaces capable of coupling heterogeneous catalysis with electrochemical signal generation. The proposed strategy broadens the role of nanoporous aluminosilicates and provides a versatile platform for the development of robust, low-cost electrochemical sensors for non-invasive biofluid analysis and point-of-care diagnostics.[1]

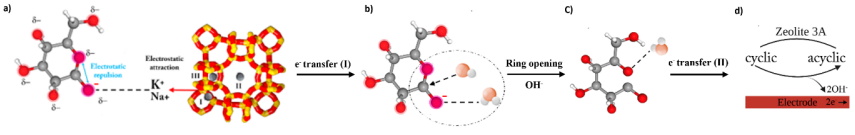


Figure 1. Proposed catalytic pathway for zeolite 3A-assisted electrochemical glucose sensing.

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SILVER SERS SUBSTRATES FOR LABEL-FREE MONITORING OF G-QUADRUPLEX FORMATION: WHICH ONE PERFORMS BEST?

Petra Petrović Popović,[1] Tea Juračić,[1] Nikša Krstulović,[2] Dijana Pavlović Saftić,[3] Snežana Miljanić[1]

[1] Department of Chemistry, University of Zagreb Faculty of Science, Horvatovac 102a, Zagreb, Croatia,

[2] Center for Advanced Laser Techniques, Institute of Physics, Bijenička 46, Zagreb, Croatia, [3] Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička 54, Zagreb, Croatia

* ppetrovic@chem.pmf.hr

Surface-enhanced Raman scattering (SERS) spectroscopy is a promising label-free analytical technique for the structural characterization of biologically relevant molecules.[1] However, its analytical performance strongly depends on the physicochemical properties of the employed plasmonic substrate.[2] In this work, four silver nanoparticle-based SERS substrates were systematically evaluated to identify the most suitable platform for discrimination between the unfolded human telomeric oligonucleotide Tel24 and its G-quadruplex (G4) structure. Citrate- (AgNP_cit) and spermine-stabilized silver nanoparticles (AgNP_sp), citrate-stabilized silver nanostars (AgNS_cit), and silver nanoparticles prepared by pulsed laser ablation in liquid (AgNP_PLAL) were synthesized and characterized using UV/Vis spectroscopy, scanning electron microscopy, dynamic light scattering, zeta potential measurements. The folding of Tel24 into the G4 structure was independently confirmed by circular dichroism (CD) spectroscopy, while SERS spectra were recorded using 785 nm excitation.The investigated substrates (Figure 1) exhibited distinct optical, morphological and surface properties, which were reflected in the quality and spectral features of the acquired SERS spectra. The conformational transition from the unfolded oligonucleotide to the G-quadruplex structure was evidenced by changes in the relative intensities of characteristic adenine- and guanine-associated bands, enabling discrimination between the two structural forms.[3] Among the investigated substrates, citrate-stabilized silver nanoparticles provided the highest spectral quality, allowing the clearest differentiation between the two conformations.The obtained results demonstrate that nanoparticle morphology, synthesis route, and surface chemistry collectively govern the analytical performance of silver SERS substrates and provide practical guidelines for the label-free structural characterization of G-quadruplex-forming oligonucleotides.

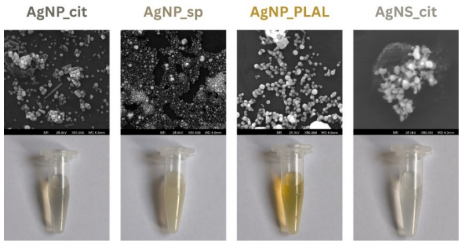


Figure 1. Representative SEM micrographs and photographs of the synthesized silver SERS substrates.

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EVALUATION OF ELECTROSPUN PLGA ULTRAFINE FIBERS FOR CONTROLLED INDOMETHACIN DELIVERY

Ana Jurić, Donna Danijela Dragun, Rafael Anelić, Fabio Faraguna, Ernest Meštrović

Department of General and Inorganic Chemistry, Faculty of Chemical Engineering and Technology, Trg Marka Marulića 19, HR-10000 Zagreb, Croatia
*ajuric@fkit.hr

The development of controlled drug delivery systems is essential for improving the solubility, bioavailability, and therapeutic efficacy of poorly water-soluble drugs while reducing adverse effects. Indomethacin, a nonsteroidal anti-inflammatory drug (NSAID), exhibits low aqueous solubility and may cause gastrointestinal side effects, highlighting the need for prolonged-release formulations.[1,2]

In this study, electrospun PLGA ultrafine fibers were investigated as carriers for controlled indomethacin delivery. Three polymer solutions containing 10% PLGA with different indomethacin loadings (30%, 40%, and 50% relative to the polymer mass) were prepared to evaluate the influence of drug concentration on the morphological, structural, and release properties of the resulting matrices. Electrospinning of these 10% PLGA solutions consistently produced ultrafine fibers embedded with distinct beads. Localized Raman spectroscopy confirmed that these beads function as drug-rich microcapsules, yielding a significantly stronger drug intensity response within the structures compared to the fiber segments.

Fiber morphology was characterized by SEM, drug incorporation and intermolecular interactions by FTIR, crystalline state by XRD, and thermal properties by TGA and DSC. *In vitro* dissolution studies conducted at 37 °C and pH 7.4 demonstrated that the PLGA matrices successfully prolonged indomethacin release. Remarkably, for all evaluated formulations, the time required to release 50% of the loaded drug was 120 hours (5 days), confirming highly sustained release kinetics. The results demonstrate that these electrospun PLGA matrices show considerable potential as prolonged-release carriers for poorly water-soluble therapeutics.

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INDOLE-3-CARBALDEHYDE SCHIFF BASES: FROM SYNTHESIS TO ANTIMICROBIAL ACTIVITY

Katarina Kordej,[a] Dragana Vuk,[a] Vilma Lovrinčević,[a] Marija Vuković Domanovac,[a] Ines Despotović[b]

[a] University of Zagreb Faculty of Chemical Engineering and Technology, Trg Marka Marulića 19, 10000 Zagreb, Croatia, [b] Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia
* kkordej@fkit.hr

Antimicrobial resistance has become one of the most pressing global health challenges, with the WHO reporting that over 1.27 million deaths were directly attributable to resistant bacterial infections in 2019 alone. This urgent need for new antimicrobial agents has directed considerable research interest toward structurally diverse bioactive compounds, among which Schiff bases and indole derivatives occupy a prominent place. Schiff bases, characterized by the azomethine (C=N) functional group, are formed by condensation of primary amines with carbonyl compounds and are well known for their broad spectrum of biological activities, including antibacterial, antifungal, antitumour and antioxidant effects.[1] Indole-3-carbaldehyde represents a particularly versatile starting material for the preparation of Schiff bases, owing to the high reactivity of its aldehyde group at the C-3 position toward nucleophilic addition of primary amines.[2] In this work, a series of new Schiff bases was prepared by classical thermal condensation of indole-3-carbaldehyde with aromatic amines bearing electron-withdrawing and electron-donating substituents in ethanol under reflux. The obtained compounds were fully characterized by ^{1}H NMR and ^{13}C NMR spectroscopy. The antimicrobial activity of all synthesized compounds will be evaluated against selected bacterial and fungal strains in order to assess the influence of substituents on biological activity. This research was conducted within the project OSKomLiMe (112104) financed by the European Union's – NextGenerationEU fund from the source 581 – The recovery and resilience mechanism, in the frame of Programme financing of public higher education institutions and public scientific institutes.

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SYNTHESIS AND BIOLOGICAL ACTIVITY OF NOVEL INDOLE DERIVATIVES

Paula Ćurić,[a] Vilma Lovrinčević,[a] Dragana Vuk,[a] Marija Vuković Domanovac,[a] Ines Despotović[b]

[a] University of Zagreb Faculty of Chemical Engineering and Technology, Trg Marka Marulića 19, 10000 Zagreb, Croatia, [b] Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia
* pcuric@fkit.hr

Heterocyclic compounds occupy a prominent position in the field of organic chemistry, and among them, indoles represent extensively studied systems with a broad range of applications in the treatment and management of various pathophysiological conditions. Indole represents an important bioactive heterocyclic motif that occurs in numerous naturally occurring compounds, such as serotonin, tryptophan and melatonin. The widespread distribution of indole derivatives in nature, together with their broad spectrum of biological activities, has led to significant interest in these compounds within the fields of organic and medicinal chemistry. Consequently, a variety of indole-based compounds are being investigated as potential drug candidates for the treatment of bacterial, fungal, viral, and tubercular infections, HIV, and malaria.[1]

Building upon previous studies and their promising results, this research focuses on the synthesis of novel bisindole derivatives and the evaluation of their biological activity. An efficient and innovative synthetic approach was employed for the preparation of indole derivatives using $Cu(NO_3)_2 \cdot 3H_2O$ as a catalyst. The applied protocol[2] offers several advantages, including the use of a readily available and cost-effective catalyst, mild reaction conditions at room temperature, high selectivity, satisfactory yields, and straightforward experimental procedures. The synthesized indole derivatives were evaluated *in vitro* for their antimicrobial activity against *Aspergillus niger*, *Bacillus subtilis*, *Candida albicans*, and *Pseudomonas aeruginosa* using the agar diffusion method. Furthermore, the potential inhibitory mechanisms underlying their antibacterial and antifungal effects were explored through *in silico* molecular docking studies, providing insight into their potential as novel antimicrobial drug candidates.

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Zr-MEDIATED ALKYNE CYCLIZATION TOWARD CHIRAL MULTISUBSTITUTED CYCLOPENTADIENYL LIGANDS WITH VARIOUS BACKBONE STRUCTURES

Filip Duplić, Marko Purić, Ivana Nikšić-Franjić, Nikola Topolovčan

Department of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička cesta 54, 10000, Zagreb, Croatia
* filip.duplic@irb.hr

Cyclopentadienyl (Cp) ligands have attracted considerable attention in recent years due to their excellent performance in a wide range of catalytic reactions. Despite significant progress, the preparation of structurally diverse Cp ligands remains challenging, with only a limited number of synthetic approaches currently available.[1] One of the strategies for the preparation of such ligands involves zirconocene-mediated intramolecular cyclization of a diyne followed by the insertion of a one-carbon unit building block.[2] Chiral Cp ligands with different backbone structures can be efficiently used in various stereoselective transformations, enabling the synthesis of numerous products with high enantio- and diastereomeric purity. Furthermore, it has been shown that substituents on the Cp ring have a strong influence on the reactivity and catalytic properties of Cp transition metal complexes.[3] Zr-mediated alkyne cyclization was applied in this work for the preparation of four chiral multisubstituted Cp ligands with different backbone structures. This synthetic strategy enabled the preparation of chiral Cp ligands from a chiral primary amine possessing a remote center of chirality and other readily available compounds, such as (*R*)-BINOL, naturally occurring (*L*)-proline and *L*-(+)-tartaric acid. Finally, the tetrasubstituted Cp ligand obtained from *L*-(+)-tartaric acid was successfully transformed into the corresponding chiral cymantrene complex.[4]

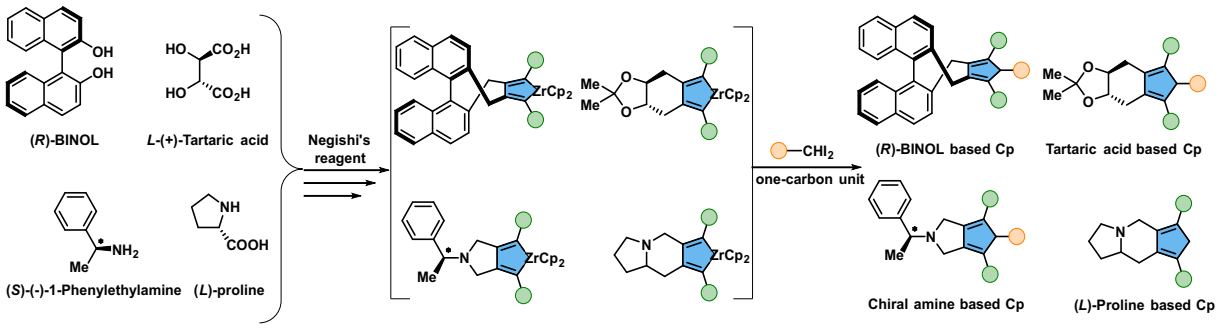


Figure 1. Preparation of multisubstituted Cp ligands with various chiral backbones.

ACKNOWLEDGEMENTS European Union - NextGenerationEU (NPOO.C3.2.R2-I1.06.0022).

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DEGRADATION OF SULFAMETHOXAZOLE AND VENLAFAXINE DURING CHLORINATION

Katarina Marija Drmić, Marina Demut, Angela Dzhasambayeva, Sandra Babić

Department of Analytical Chemistry, University of Zagreb, Faculty of Chemical Engineering and Technology, Trg Marka Marulića 19, 10000 Zagreb, Croatia
* kdrmic@fkit.unizg.hr

Trace pharmaceuticals, including the antibiotic sulfamethoxazole and the antidepressant venlafaxine, are commonly found in aquatic environments. Because these compounds persist in source waters used for drinking water, they reach the chemical disinfection stage. Chlorination effectively eliminates pathogenic microorganisms, but the presence of residual pharmaceuticals leads to undesirable reactions with free chlorine. This triggers chemical transformations that form disinfection byproducts (DBPs), such as trihalomethanes, which are harmful to human health and potentially toxic. This study investigated the degradation of sulfamethoxazole and venlafaxine during chlorination.

Chlorination experiments were performed under controlled conditions to evaluate the effects of pH and initial disinfectant concentrations. Degradation of the parent pharmaceuticals over time were monitored via high-performance liquid chromatography coupled to diode array detector (HPLC-DAD). Identification and quantification of volatile DBPs (trihalomethanes) were conducted using gas chromatography-mass spectrometry (GC-MS).

HPLC-DAD analysis demonstrated that a decrease in the concentration of pharmaceuticals occurs due to the action of the disinfectant, indicating a distinct interaction between the pharmaceuticals and the disinfectant. However, GC-MS analysis revealed that this transformation directly generates harmful halogenated byproducts, with trihalomethanes concentrations increasing over prolonged contact time and higher chlorine doses. Consequently, while chlorination remains vital for pathogen destruction, optimizing operational parameters is essential to minimize the formation of these hazardous disinfection byproducts.

ACKNOWLEDGEMENTS This study was supported by the Croatian Science Foundation under the project number HRZZ-IP-2024-05-7383 titled Innovative approaches for water disinfection byproducts mitigation - new technologies for new challenges (**InWatTechno**).

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LOADING LATANOPROST INTO MICELLES: THE NMR PERSPECTIVE

Ana Čikoš,[a] Maša Safundžić-Kučuk[b]

[a]NMR Centre, Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia, [b]JGL d.d. Jadran Galenski Laboratorij, Svilno 20, 51000 Rijeka, Croatia
*ana.cikos@irb.hr

Latanoprost, a prostaglandin F2α analogue, is widely used in the treatment of glaucoma due to its ability to lower elevated intraocular pressure.[1] However, the development of latanoprost aqueous formulations is challenging because of its very limited aqueous solubility, susceptibility to hydrolysis and tendency to adsorb onto container surfaces, both of which may reduce its concentration in solution.[2–4] To address these limitations, various surfactant-based micellar systems can be employed to improve solubilization and stabilization of poorly water-soluble drugs.

To better understand the molecular interactions underlying latanoprost solubilization in ophthalmic formulations, this study compared the association of latanoprost with benzalkonium chloride, a cationic surfactant, and with three non-ionic surfactants.. Sodium hyaluronate was included because of its relevance as a viscosity-enhancing and ocular surface-protective excipient in ophthalmic formulations and its influence on latanoprost loading into micelles was also evaluated. Results of NMR analysis showed that tested surfactants efficiently incorporate latanoprost, while sodium hyaluronate does not disrupt latanoprost-loaded micellar assemblies, supporting their potential application in the development of stable ophthalmic formulations.[5]

ACKNOWLEDGEMENTS This work has been funded through the project "Collaborative research and development of an innovative product for the treatment of glaucoma and related diseases of the ocular surface - GlauCollab", NPOO. C3.2.R3-I1.04.0013 and Next Generation EU project.

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CERIC-ERIC: A DISTRIBUTED RESEARCH INFRASTRUCTURE FOR MATERIALS CHARACTERISATION

Marcello Turconi

CERIC-ERIC, SS 14, Km 163.5, 34149 Basovizza, Trieste, Italy

marcello.turconi@CERIC-ERIC.EU

CERIC is a European Research Infrastructure Consortium (ERIC) integrating and providing open access to some of the most advanced analytical facilities in Europe to help science and industry advance in all fields of materials, biomaterials and nanotechnology, with a focus on energy materials and life sciences. With a single entry point to some of the leading national research infrastructures in 8 European countries, it enables the delivery of innovative solutions to societal challenges in the fields of energy, health, food, cultural heritage and more.

CERIC's main aim is to contribute to the creation of excellent science, both as in-house activity and as a service to international users. This is achieved mainly by providing open access to its research facilities through two calls for proposals per year, addressing researchers requiring the use of one or more complementary techniques for structural investigation, analysis, synthesis and imaging of materials and biomaterials down to the nano-scale. Between 2014 and 2022, 1956 proposals were received from research groups coming from 59 countries worldwide. 1165 proposals were selected for open access to the CERIC facilities, and the number of publications has significantly increased over the years.

POSTER PRESENTATIONS

BEYOND SINGLE BINDING SCAFFOLDS: COMBINING ADAMANTANE AND DIAMANTANE CAGES

Petr Janovský,[a] Barbora Gřešková,[a] Michal Rouchal,[a] Marija Alešković,[b] Marina Šekutor,[b] Robert Vícha*[a]

[a] Department of Chemistry, Faculty of Technology, Tomas Bata University in Zlín, Vavrečkova 5669, 760 01 Zlín, Czech Republic, [b] Department of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia
* marija.aleskovic@irb.hr

The adamantane (Ada) molecule has long been established as a key cage hydrocarbon in supramolecular chemistry. Owing to its excellent geometric complementarity with the cavities of cucurbit[n]urils (CB[n]s) and cyclodextrins (CDs), Ada derivatives form stable inclusion complexes with widespread applications in molecular recognition, drug delivery, and functional supramolecular systems. Diamantane (Dia), the next hydrocarbon in the diamondoid series,[1] has recently emerged as a promising scaffold for supramolecular host–guest chemistry.[2] Its rigid cage structure, exceptionally high affinity toward CB[n] hosts, and the possibility of regioselective functionalization at distinct apical or medial positions make it particularly attractive for the design of multitopic guests.[3] While Dia ammonium salts form ultra-stable complexes with CB[n]s in the aqueous solution, their complexation with CDs remains largely unexplored, in contrast to the well-known affinity of Ad derivatives for CD cavities. Herein, we report the synthesis of novel tritopic guests based on 4,9- or 1,6-diaminodiamantane cores bearing terminal Ad units connected by linkers of varying length. Their interactions with CB[n]s and CDs were investigated with particular emphasis on host selectivity, binding strength, and, for CDs, host orientation. Mass spectrometry, ^{1}H NMR titrations, ^{1}H–^{1}H NOESY, and computational analysis were used to elucidate the structures of the resulting inclusion complexes. These combined results provide molecular-level insight into the recognition of multitopic diamondoid guests by two complementary classes of macrocyclic hosts.

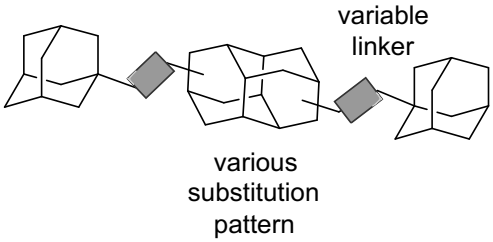


Figure 1. Schematic representation of studied multitopic guests.

ACKNOWLEDGEMENTS This work was supported by the Croatian Science Foundation (HRZZ, grant No. IP-2025-02-9623) and the Czech Science Foundation (GAČR, grant No. 26-20330L) within the framework of the bilateral project "MultiDia".

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SPEEDING UP PHARMACEUTICAL ASSAY: A RAPID AND RELIABLE UPLC METHOD FOR ETRASIMOD QUANTIFICATION

Daniela Amidžić Klarić,[a*] Jelena Kovačić Šantek,[a] Petra Bajt,[a] Nikša Turk,[b] Željko Krznarić,[b,c] Ana Mornar[a]

[a] University of Zagreb Faculty of Pharmacy and Biochemistry, A. Kovačića 1, Zagreb, Croatia, [b] Clinical Hospital Center Zagreb, Kišpatićeva 12, Zagreb, [c] University of Zagreb School of Medicine, Šalata 2, Zagreb

* daniela.amidzic@pharma.unizg.hr

Etrasimod is a selective sphingosine-1-phosphate (S1P) receptor modulator recently approved for the treatment of moderately to severely active ulcerative colitis. Given its potent therapeutic profile and low-dose formulations, the development of rapid, highly selective, and efficient analytical methods for routine quality control and assay testing is critical to ensure patient safety and product uniformity. Building upon our previously published comprehensive characterization of etrasimod stability and behaviour,[1] the objective of this study was to advance this analytical framework by establishing a high-throughput ultra-performance liquid chromatographic (UPLC) platform tailored for rapid pharmaceutical assay screening.

Chromatographic separation was performed using an Agilent 1290 chromatographic system. The optimized separation was achieved on a Poroshell 120 SB-C18 column (2.1 x 50 mm, particle size 1.7 µm) maintained at 30.0 ± 0.1 ºC. The mobile phase consisted of an isocratic mixture of acetonitrile and Milli-Q water (67:33, *v*/*v*) acidified with 0.1% formic acid, delivered at a flow rate of 0.6 mL/min. The injection volume was set to 1 µL, and UV detection to 280 nm. Method validation was thoroughly conducted following ICH Q2(R2) regulatory guidelines.

Etrasimod showed a sharp peak, exhibiting a short retention time of 1.90 min with relative standard deviation of 0.92% (symmetry = 1.1; number of theoretical plates = 5568). System suitability tests verified excellent instrument performance, showing a peak area of 219.1 mAU·s with RSD of 0.28% (n = 10). A working range encompassing 80% to 120% of the target concentration (50 µg/mL) was selected for routine assay validation, demonstrating strong statistical linear compliance (r = 0.997) and homoscedastic residual distribution. Method accuracy was confirmed with excellent recovery percentages across three concentration levels, spanning from 98.3% to 102.0%. Method precision was highly satisfactory, with a repeatability RSD of 1.71% and an intermediate precision RSD of 1.87%. Finally, the method was successfully implemented for the analysis of Velsipity® (2 mg) tablets by Pfizer, yielding an excellent recovery of 98.1% with no interference from excipients.

The developed UPLC method is fast, robust, and fully compliant with ICH validation parameters. By significantly reducing the total runtime to under two minutes while maintaining exceptional peak symmetry and accuracy, this platform provides an excellent high-throughput analytical solution for industrial quality control, stability monitoring, and routine assay testing of etrasimod formulations.

ACKNOWLEDGEMENTS The research is funded by the Croatian Science Foundation grant (IP-2025-02-2541, SMART-IBD) and the National Recovery and Resilience Plan, funded by the European Union – NextGenerationEU (grant 2025-203, GreenLab).

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

Jakov Babić, Dalibor Tatar, Jelena Kojčinović, Stjepan Šarić, Petra Šušak, Igor Djerdj

Department of Chemistry, Josip Juraj Strossmayer University of Osijek, Cara Hadrijana 8/A, HR-31000 Osijek, Croatia
* jakovbabic32@gmail.com

A family of materials known as high-entropy oxides (HEOs) is associated with a wide range of potential applications due to their unique compositions and crystal structures. Exceptional stability is exhibited by these single-phase solid solutions containing five or more principal metal cations in equiatomic proportions, owing to the random distribution of cations within the crystal lattice.[1] In the present study, Ce–Zr–Pr–Sm–Eu-based high-entropy oxides with systematically varied Pr content were synthesized via a modified sol-gel citrate method to investigate the influence of Pr incorporation on lattice structure, defect formation, and photocatalytic performance.[2] A single-phase cubic fluorite structure was maintained across all synthesized compositions, while gradual lattice expansion and increased microstrain were detected with increasing Pr concentration as a result of substitution by larger Pr^{3+} ions. Morphological and surface characterization revealed the formation of porous nanostructures at intermediate Pr levels, whereas excessive Pr incorporation led to densification and reduced surface accessibility. The presence of Pr^{3+}/Pr^{4+} and Ce^{3+}/Ce^{4+} redox pairs, pronounced 4f–2p orbital hybridization, and enhanced defect-related electronic states contributing to bandgap reduction were confirmed through spectroscopic analysis. Under UV irradiation, the optimized Pr-containing composition achieved almost complete degradation of methylene blue within 30 minutes. This behavior in semiconductors with a narrowed bandgap is attributed to enhanced charge separation efficiency, together with redox cycling between Ce and Pr centers.

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NITRATE ANION AS A HALOGEN BOND ACCEPTOR IN METAL-ORGANIC IONIC COCRYSTALS

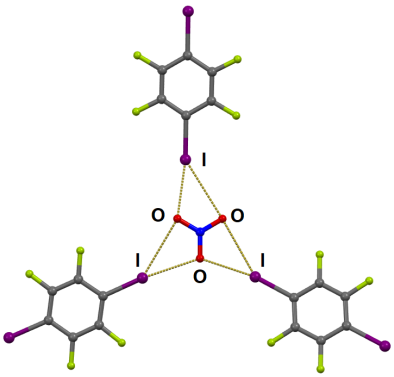
Nikola Bedeković, Tea Maršić, Dominik Cinčić

Department of Chemistry, Faculty of Science, Horvatovac 102a, 10000 Zagreb

* nbedekovic@chem.pmf.hr

The use of halogen bonds in metal-organic multi-component crystals[1] is a common strategy in solid-state supramolecular chemistry aimed at developing new materials where the properties are primarily attributed to the metal centers. This strategy relies on the interaction between a donor molecule and a Lewis base, which is either coordinated to the metal center or exists as a non-coordinated anionic species. Oxoanions (nitrate, sulfate, phosphate) just like (pseudo)halides[2] often appear as counterions in transition metal salts, yet they are significantly less represented as acceptor species in halogen-bonded materials. Due to their structural characteristics they are potentially interesting acceptor groups, as they can engage in a greater number of interactions (due to the higher number of oxygen atoms) and serve as nods for halogen bonds within crystal structures.[3-5]

Herein we have synthesized four new halogen-bonded cocrystals starting from the tris(1,10-phenanthroline)nickel(II) nitrate, tris(2,2'-bipyridine)nickel(II) nitrate and perhalogenated donors, through mechanochemical and solution methods. The successes of the syntheses were monitored via powder X-ray diffraction, thermogravimetric analysis, and differential scanning calorimetry. The molecular and crystal structures of the resulting compounds were elucidated using single crystal X-ray diffraction. Structural analysis revealed that the dominant interaction is the halogen bond I···ONO_2^-, with the nitrate anion acting as a polytopic halogen bond acceptor. The supramolecular architecture varies from discrete motifs to two-dimensional anion-donor halogen-bonded networks, with cations occupy the voids in corresponding crystal structure.



ACKNOWLEDGEMENTS This work has been supported by the Croatian Science Foundation under the project IP-2025-02-6539 and the European Union – NextGenerationEU through the National Recovery and Resilience Plan 2021–2026 via Institutional grants of the University of Zagreb Faculty of Science (NextGenChem and CryoLab).

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BILE ACID–DERIVED COMPOUNDS AS MODULATORS OF STEROID RECEPTORS AND AKR1C ENZYMES

Sofija Bekić,[a] Maja Marinović,[b] Dimitar Jakimov,[c] Andrea Nikolić,[a] Anđelka Ćelić,[b] Edward Petri,[b] Ksenija Pavlović[a]

[a] Department of Chemistry, Biochemistry and Environmental Protection, Faculty of Sciences, University of Novi Sad, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia, [b] Department of Biology and Ecology, Faculty of Sciences, University of Novi Sad, Trg Dositeja Obradovića 2, 21000 Novi Sad, Serbia, [c] Oncology Institute of Vojvodina, Faculty of Medicine, University of Novi Sad, Put Dr Goldmana 4, 21204 Sremska Kamenica, Serbia

* sofija.bekic@dh.uns.ac.rs

Hormone-dependent malignancies represent a major global health problem and remain a significant cause of cancer-related mortality. Therapeutic strategies targeting steroid hormone signaling pathways, including inhibition of steroid-converting enzymes such as aldo-keto reductases (AKRs), as well as modulation of steroid receptor activity, are of considerable interest in anticancer drug discovery. Bile acids are attractive scaffolds in medicinal chemistry due to their availability and structural versatility, enabling the design of biologically active derivatives. In this study, we evaluated biological activity of bile acid derivatives synthesized via microwave-assisted green chemistry approaches or conventional synthetic routes. The compounds were evaluated for cytotoxic activity against a panel of human cancer cell lines and a healthy cell line using MTT assay. Several derivatives showed strong and selective antiproliferative effects against cancer cells, with low toxicity toward normal fibroblasts. Interactions with ligand-binding domains (LBDs) of estrogen receptor α (ERα), estrogen receptor β (ERβ), androgen receptor (AR) and glucocorticoid receptor (GR) were evaluated using a yeast-based fluorescent biosensor. Furthermore, inhibitory activity toward recombinant human AKR1C3 and AKR1C4 was measured through spectroscopic monitoring of NADPH consumption, identifying several inhibitors. Finally, molecular docking was performed to provide structural insights into the observed protein-ligand interactions. Overall, bile acid derivatives represent promising scaffolds for the development of multitarget agents against hormone-dependent cancers.

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STREPTOCOCCUS GORDONII MANGANESE METALLOSENSOR

Branimir Bertoša,[a] Katarina Radman,[a] Ivana Leščić

[a] University of Zagreb Faculty of Science, Department of Chemistry, Horvatovac 102a, Zagreb, Croatia,
[b] Division of Physical Chemistry, Ruđer Bošković Institute, Bijenička cesta 54, Zagreb, Croatia
* bbertosa@chem.pmf.hr; branimir.bertosa@chem.pmf.unizg.hr

Manganese metallosensors are that regulate Manganese homeostasis in bacteria is controlled by transcription of proteins involved in transport and storage of Mn^{2+} ions by transcriptional factors called manganese metallosensors.[1,2] Manganese ions (Mn^{2+}) are necessary for essential processes in bacterium cell, such as DNA replication and resistance to oxidative stress, but could be also toxic if are present in too large cellular concentration. Therefore, their intracellular concentration must be carefully regulated which is achieved by manganese metallosensor. Protein Scar is manganese metallosensor of bacterium *Streptococcus gordonii* which is oral bacteria that grow as a plaque biofilm on the tooth surface. Structural and dynamical changes of Scar protein caused by Mn^{2+} ions binding was investigated computationally (molecular dynamics (MD) simulations) and experimentally (circular dichroism (CD), differential scanning calorimetry (DSC), isothermal titration calorimetry, electronic paramagnetic resonance (EPR), etc.). Obtained results show that Mn^{2+} ions binding induces significant conformational changes, which primarily affects positioning of DNA binding domains (DBD) increasing the affinity of protein for DNA binding. The allosteric mechanism that initiates conformational change of the protein Scar due to Mn^{2+} binding was identified. Key amino acid residues of that allosteric mechanism were mutated in order to confirm the importance of allosteric mechanism and mutants were investigated computationally and experimentally. Further, Scar-DNA complex was studied and the most important interactions were identified.

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INNOVATIVE 3D-PRINTED FLOW CELL DESIGN ENABLING *IN OPERANDO* PRINTED ELECTROCHEMICAL SENSOR REPLACEMENT

Željka Boček, Elizabeta Forjan, Andrej Molnar, Marijan-Pere Marković, Domagoj Vrsaljko, Petar Kassal

University of Zagreb Faculty of Chemical Engineering and Technology, Trg Marka Marulića 19, 10000 Zagreb
* zbocek@fkit.unizg.hr

Technological advancements in additive manufacturing have allowed fabrication of modular, adjustable microfluidic cells that can be readily tailored to specific analytical applications. Conventional microfluidic flow cells used for electrochemical detection employ different fastening mechanisms with magnets or screws to enable printed sensor replacement. However, such systems also require partial or complete disassembly of the flow system and disruption of the monitored flow process.

In this work, a 3D-printed modular flow cell was assembled with a mobile sensor holder comprised of two materials – a rigid polyacrylate cover which maintains sealing of the sample chamber and enables uninterrupted flow during sensor exchange, and a flexible holder made of thermoplastic polyurethane that holds the sensor in place during operation, but allows replacement when the mask is ejected. This novel design allows semicontinuous monitoring of analytes whose sensing is hindered by electrode surface fouling during operation without flow cell disassembly or flow process interruption. The performance and functionality of the flow cell were systematically evaluated using Methylene blue as a model analyte.

Methylene blue was selected due to its strong adsorption onto carbon electrode surfaces, which prevents reliable repeated measurements using a single electrode. Direct electrochemical detection was performed using unmodified carbon screen-printed electrodes and square wave voltammetry method. Optimized flow measurements yielded a linear response within a concentration range of 0.01–0.07 μM, a sensitivity of 65.59 μA/μM, a calculated detection limit of 7.75 nM, and an interelectrode relative standard deviation of 1.87 %, demonstrating the suitability of the proposed platform for semicontinuous electrochemical monitoring.[1]

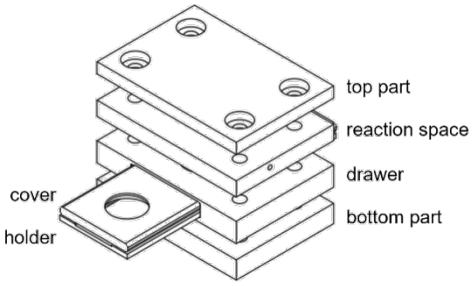


Figure 1. Schematic of the 3D-printed flow cell for *in operando* printed sensor replacement.

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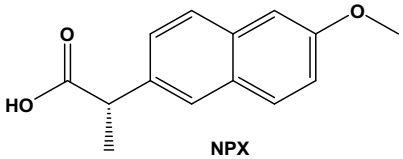
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INFLUENCE OF BUFFER SPECIES AND ADDED SALT ON THE BINDING OF NABUMETONE AND NAPROXEN TO β-CYCLODEXTRINS

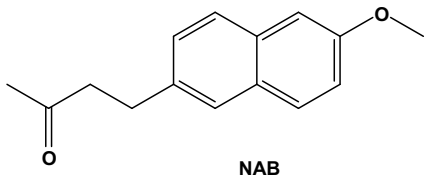
Ana Budimir,[a] Robert Kerep,[b] David Klarić,[b] Nives Galić[b]

[a] University of Zagreb Faculty of Pharmacy and Biochemistry, Ante Kovačića 1, 10000 Zagreb, Croatia,
[b] Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, 10000 Zagreb, Croatia
* ana.budimir@unizg.pharma.hr

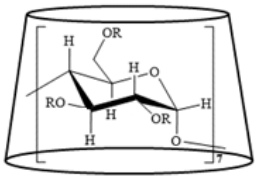
β-Cyclodextrins (β-CDs) are cyclic oligosaccharides widely used in pharmaceutical formulations because of their ability to form inclusion complexes with hydrophobic drug molecules. The stability of these complexes, expressed by the complex formation constant (*K*), is influenced by the physicochemical properties of the system. This study investigated the effects of buffer composition and added NaCl on the complexation of two nonsteroidal anti-inflammatory drugs (NSAIDs), naproxen (NPX) and nabumetone (NAB), used in the treatment of osteoarthritis and rheumatoid arthritis, with β-cyclodextrin (β-CD) and its derivatives: hydroxypropyl-β-CD (HP-β-CD), randomly methylated β-CD (RM-β-CD), and sulfobutylether-β-CD (SBE-β-CD). Naproxen, a weak acid (pK_a ≈ 4.2), is predominantly present in its anionic form at pH 6.8, whereas nabumetone is a neutral compound that does not undergo acid-base ionization. Binding constants and thermodynamic parameters were determined by isothermal titration calorimetry (ITC) at 25 °C and pH 6.8 in phosphate and PIPES buffers. The effect of increasing NaCl concentration in phosphate buffer on complex stability was also evaluated. The results provide insight into the influence of buffer species, ionic strength, and drug ionization on β-CD–drug interactions and enhance the understanding of the factors governing the stability of cyclodextrin inclusion complexes.



NPX



NAB



β-CD: R = H_{21}

HP-β-CD: R = H_{21-n} or $(–CH_2CH(OH)CH_3)_n$, n = 2–8; DS = 4.5

RM-β-CD: R = H_{21-n} or $(–CH_3)_n$, n = 9–15; DS = 12

SBE-β-CD: R = H_{21-n} or $(–(CH_2)_4SO_3Na)_n$, n = 3–7; DS = 6.

Figure 1. Structures of naproxen, nabumetone and β–cyclodextrins.

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DYNAMIC BOND POSITION IN pH-RESPONSIVE NONIONIC SUPRAMOLECULAR ASSEMBLIES

Roko Budiselić,[a,b] Aleks Logožar,[b] Anamarija Knežević[b]

[a] Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, 10000 Zagreb,

[b] Laboratory for Stereoselective Synthesis and Biocatalysis, Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia

* rbudiselic.chem@pmf.hr

Nonionic supramolecular assemblies formed from amphiphilic molecules represent a promising class of nanostructured materials. In water, these molecules spontaneously organize as the hydrophobic segments minimize contact with water while the hydrophilic segments remain solvated, thereby forming different aggregate morphologies such as micelles, vesicles, fibers, worms and others.[1] The position of a dynamic bond within the molecular structure of an amphiphile is important in the design of dynamic supramolecular systems., it defines the "breaking point" of the molecule and determines its disassembly products.[2] Its proximity to either the aqueous layer or the hydrophobic core can also strongly influence dynamicity, structural stability, and pH-dependent behavior in solution. This work investigates pH-responsive nonionic supramolecular aggregates by comparing two amphiphilic structural isomers containing dynamic covalent bonds at different positions within their molecular frameworks. Positions of dynamic covalent bonds in these two structural isomers were selected to understand how structural variations affect self-assembly and aggregate responsiveness under different pH values. To obtain and study these architectures, novel designer amphiphiles were synthesized with two key functional motifs: naphthalene subunits, which promote linear organization through π–π stacking interactions, and dynamic covalent imine bonds, which enable controlled assembly and disassembly under specific aqueous conditions. The volume ratio of hydrophilic and hydrophobic moieties was also considered during molecular design. The resulting insight into temperature-induced transformations and pH-triggered assembly and disassembly provides a deeper understanding of these systems and supports the future development of advanced supramolecular environments.

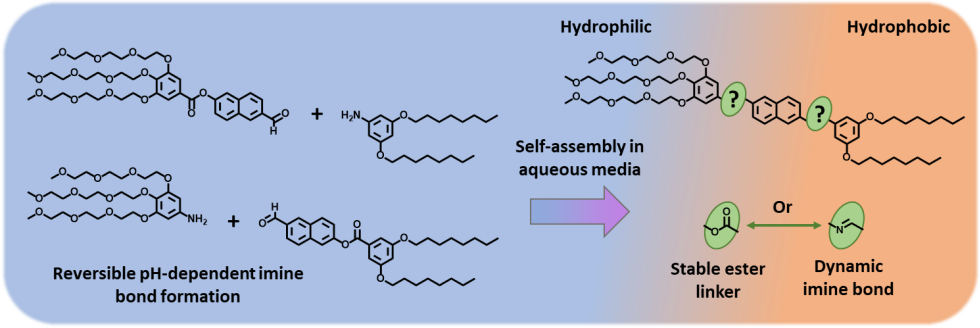


Figure 1. Nonionic pH-dependent supramolecular assemblies in aqueous media.

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REACTIVITY OF METHYLSULFINATE IN ETHANOL AND AQUEOUS ETHANOL

Mia Bušljeta,* Bernard Denegri, Mirela Matić

University of Zagreb, Faculty of Pharmacy and Biochemistry, A. Kovačića 1, Zagreb, Croatia
* mia.busljeta@pharma.unizg.hr

Knowing the heterolytic reactivity of leaving groups is essential for understanding reaction mechanisms and predicting the stability of organic compounds. Furthermore, knowledge of solvolytic reactivity is crucial for the correct handling and successful performance of synthetic procedures involving potentially labile sulfinic esters.[1] In this work, the nucleofugality of the methylsulfinate leaving group was measured in ethanol and ethanol–water mixtures. A series of differently substituted benzhydryl methylsulfinates were synthesized, and their first-order solvolysis rate constants were measured in neat ethanol and in 80 % and 60 % ethanol–water mixtures at 25 °C using the conductometric method (Figure 1). The leaving group ability of methylsulfinate was quantified in terms of the nucleofugality parameter N_f according to the Mayr equation.[2]

$$\log k = s_f(E_f + N_f) \quad (1)$$

In equation (1), E_f denotes the electrofugality parameter of the benzhydryl reference electrofuges, while s_f and N_f represent nucleofuge-specific parameters. The obtained N_f and s_f values describe the heterolytic reactivity of methylsulfinate in different solvents and enable its comparison with other leaving groups on the nucleofugality scale.[1-3] Furthermore, by combining the nucleofuge parameters of methylsulfinate with known E_f values of reference electrofuges, rate constants and half-lives for solvolytic decomposition of methylsulfinate derivatives in ethanol and aqueous ethanol at 25 °C can be predicted. These results contribute to a better understanding of the structure-reactivity relationships governing the stability and solvolytic behavior of sulfinic esters.

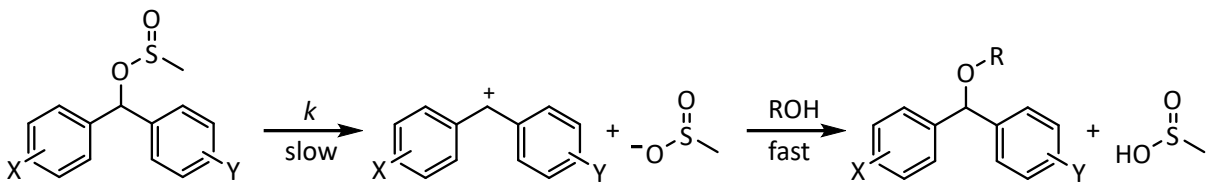


Figure 1. Solvolysis of substituted benzhydryl methylsulfinates in ethanol solutions.

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SELECTIVE SYNTHESIS OF SULFINATES AND SULFONES: CHALLENGES AND STRATEGIES

Mia Bušljeta,* Mirela Matić, Bernard Denegri

University of Zagreb, Faculty of Pharmacy and Biochemistry, A. Kovačića 1, Zagreb, Croatia
* mia.busljeta@pharma.unizg.hr

Sulfones and sulfinates are important classes of organosulfur compounds with diverse applications in organic synthesis. Sulfone-containing molecules exhibit a wide range of biological activities and are frequently found in pharmaceuticals and agrochemicals. In contrast, sulfinates are widely used as versatile synthetic intermediates and leaving groups in various chemical transformations.[1,2]

Because the sulfinate anion is negatively charged, its reaction with alkyl electrophiles via nucleophilic substitution represents a straightforward synthetic approach. However, the ambident nature of the sulfinate anion allows nucleophilic attack at either the sulfur or the oxygen atom (Figure 1). Since S-alkylation is generally favored, the selective synthesis of sulfinates remains a significant synthetic challenge. This challenge is further complicated by the tendency of sulfinates to undergo further transformation into sulfones under certain reaction conditions.[3,4] To overcome these issues, various synthetic strategies and reaction conditions have been investigated to identify suitable methods for the selective preparation of sulfinates and sulfones.

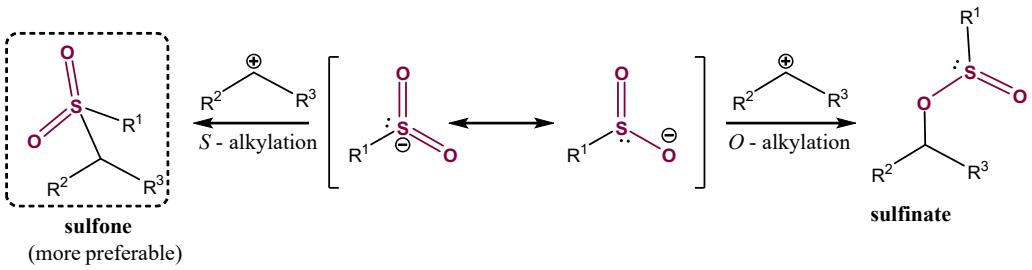


Figure 1. Ambident behaviour of sulfinate anion.

ACKNOWLEDGEMENTS This paper has been funded by the European Union (NextGenerationEU) under the National Recovery and Resilience Plan 2021–2026 (NRRP), through the UNIZG Faculty of Pharmacy and Biochemistry institutional project "OPAREA; NPOO25-FBF-11", approved by the Republic of Croatia Ministry of Science, Education and Youth (component C3.2, source 581).

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ANALYSIS OF CROATIAN SPARKLING WINES BY NMR SPECTROSCOPY

Karla Čargonja,[a] Ana-Marija Jagatić Korenika,[b] Tomislav Jednačak, Franka Sunjka,[a] Tomica Hrenar,[a] Jakov Borovec,[a] Jelena Parlov Vuković,[c] Predrag Novak[a]

[a] University of Zagreb, Faculty of Science, Department of Chemistry, Horvatovac 102a, HR-10000 Zagreb, Croatia, [b] University of Zagreb, Faculty of Agriculture, Department of Viticulture and Enology, Svetošimunska cesta 25, HR-10000 Zagreb, Croatia, [c] Ruđer Bošković Institute, Bijenička cesta 54, HR-10000 Zagreb, Croatia
* karla.cargonja@student.pmf.hr

Understanding the chemical composition of wine is essential for identifying the compounds that influence its quality, stability, and commercial value. Sparkling wines represent a distinct category of wines, characterized by the release of CO_2 upon opening, which produces a more or less persistent effervescence. Considering the current positive market trends, sparkling wine production is expected to gain increasing importance within both the total wine production and the global wine market, emphasizing the need for further research in this area. 132 Croatian sparkling wine samples were analysed using various NMR techniques, including ^{1}H NMR with NOSEY solvent suppression for water and ethanol signals, quantitative ^{13}C NMR and diffusion-ordered NMR spectroscopy (DOSY NMR). Interpretation of NMR spectra provides insight into various metabolites present, serving as a wine fingerprint.

A major potential in wine analysis lies in combining the information obtained by NMR with multivariate statistical analyses for processing experimental data, such as deep reinforcement learning. This approach can provide reliable models for wine classification based on different attributes including age, geographical origin, authenticity and physio – chemical properties.

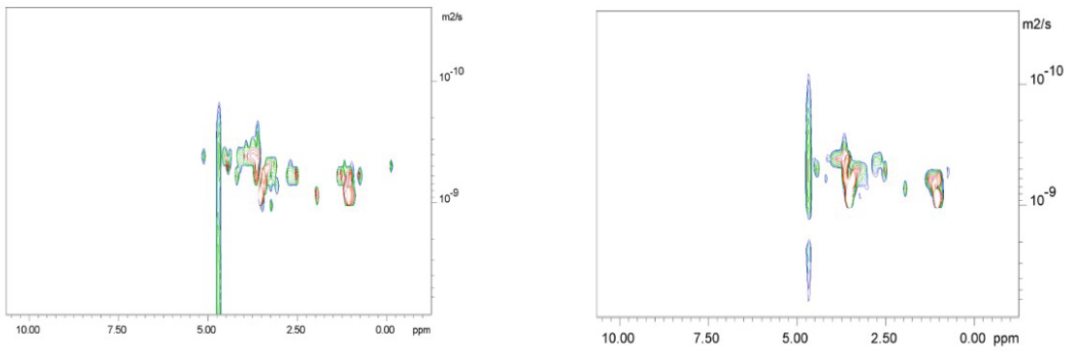


Figure 1. a) Representative DOSY NMR spectra of 2 Pinot samples from different geographical regions

ACKNOWLEDGEMENTS. This research has been supported by NPOO.C3.2.R3-I1.06.0211.

CALIXARENE HETEROASSEMBLIES IN SOLUTION BASED ON THIOUREA–CARBOXYLATE INTERACTIONS

Marija Cvetnić, Nikola Bregović, Vladislav Tomišić

Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, Zagreb, Croatia

* marija.cvetnic@chem.pmf.unizg.hr

Stimuli-responsive supramolecular assemblies have attracted increasing attention in modern supramolecular chemistry.[1] The reversible nature and directional character of non-covalent interactions, particularly hydrogen bonding, enables the construction of adaptive molecular systems with controllable structures and functions. Thiourea and carboxylate groups exhibit complementary hydrogen-bonding capabilities, yet their use in macrocyclic heteroassemblies remains underexplored. We recently demonstrated that the thiourea-functionalized calix[4]arene **TU** (Figure 1a) efficiently binds a range of anions with affinities comparable to, or higher than, those of its urea analogue **U**.[2] Furthermore, the urea-functionalized calix[4]arene, was shown to form reversible, acid/base-controlled formation of molecular heterodimers with the bis-acetate calixarenes **BA** and **BABA** (Figure 1a).[3] Herein, we resynthesized **TU**, **BA**, and **BABA** to investigate the thermodynamics of heterodimer formation in acetonitrile and to compare the stability of the resulting assemblies with those of the calixarene **U**. A combination of UV–Vis spectroscopy, ^{1}H NMR spectroscopy, isothermal titration calorimetry (ITC), and DOSY NMR spectroscopy revealed the formation of highly stable heteroassemblies. **TU** showed comparable or higher heterodimer stability than **U** with **BA** and **BABA**, respectively. Notably, interaction with **BABA** revealed a unique behavior of **TU**, not observed for **U**, namely the formation of three distinct heteroassemblies. DOSY NMR spectroscopy was particularly valuable for elucidating this complex binding behavior and distinguishing between the different assembled species (Figure 1b).

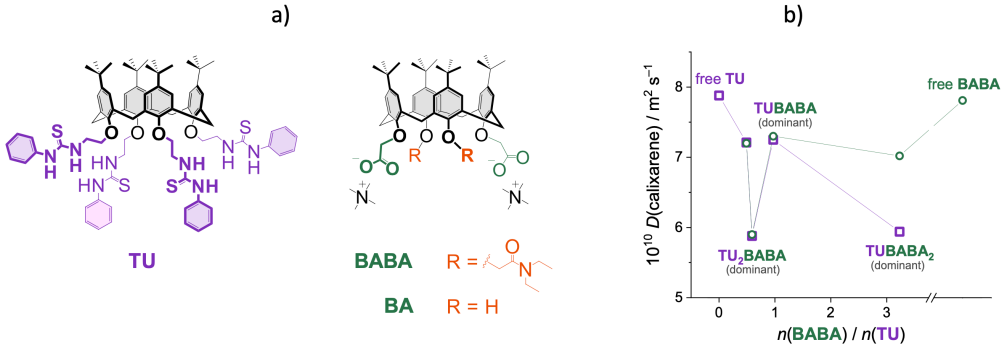


Figure 1. a) Calixarenes used for the formation of heteroassemblies. b) The results of DOSY NMR study on **TU**+**BABA** system where 3 different types of assemblies were detected in MeCN at 25 °C.

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

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MECHANOCHEMICAL SYNTHESIS OF Co(III)-AMMINE HETEROPOLYOXOMOLYBDATES INCORPORATING SELECTED d-BLOCK ELEMENTS

Vladimir Damjanović,[a] Dino Kuzman,[b] Marina Cindrić,[b] Višnja Vrdoljak[b]

[a] Department of Chemistry and Biochemistry, School of Medicine, University of Zagreb, Šalata 3, Zagreb, Croatia, [b] Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, Zagreb, Croatia

* vladimir.damjanovic@mef.hr

Polyoxometalates (POMs) represent a structurally diverse class of metal–oxo clusters renowned for their rich topologies and versatile physical and chemical properties. Owing to their tunable sizes, structures, and redox behaviors, these materials are highly promising candidates for applications in catalysis, biomedicine, and materials science. A prominent subclass, the polyoxomolybdates (POMos), comprises anionic molybdenum oxoclusters, $[Mo_mO_y]^{n-}$, formed *via* the condensation of $\{MoO_4\}$ units. Species containing additional p-, d- or f-block heteroatom (X) are termed heteropolyoxomolybdates, $[X_xMo_mO_y]^{n-}$. The formation of higher-nuclearity clusters and their eventual crystallization are primarily governed by hydrogen bonding and electrostatic interactions. Complex cations play a pivotal role in POMo synthesis: beyond providing charge compensation, they engage in supramolecular interactions that direct the condensation of $\{Mo_mO_y\}$ units through labile coordination or hydrogen bonding, thereby dictating the templating effects, stabilization, reactivity, and structural diversity of the resulting products. Building upon our previous research into heteropolyoxomolybdates obtained mechanochemically in the presence of selected p-block elements[1], in this work, mechanochemical synthesis combining liquid-assisted ball milling and vapor-assisted aging was used to prepare heteropolyoxomolybdates with copper, chromium, cobalt, and iron as heteroatoms. The reaction systems comprised molybdate ion, malonic acid, various cobalt(III) complex cations ($[Co(en)_3]^{3+}$, $[Co(C_2O_4)(en)_2]^{+}$, $[Co(NH_3)_6]^{3+}$ or $[Co(C_2O_4)(NH_3)_4]^{+}$), and selected d-block metal ions (Cu^{2+}, Cr^{3+}, Co^{2+} or Fe^{3+}). By systematically varying both the Co(III)-ammine complexes and the heterometal ions under solid-state conditions, several novel $[X_xMo_mO_y]^{n-}$ species were successfully isolated. All synthesized products were structurally characterized using single-crystal X-ray diffraction.

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DISTINGUISHING DIFFUSION DOMAINS IN A WEAKLY SUPPORTED ELECTROLYTE: A NOVEL ELECTROCHEMICAL CRITERION

Josipa Dugeč,[a] Jure Krolo,[b] Mauricia Bolfek,[a] Nives Vladislavić,[a] Marijo Buzuk[a]

[a] Department of General and Inorganic Chemistry, Faculty of Chemistry and Technology, University of Split, Ruđera Boškovića 35, 21000 Split, Croatia, [b] Department of Production Engineering, Faculty of Electrical Engineering, Mechanical Engineering and Naval Architecture, University of Split, Ruđera Boškovića 32, 21000 Split, Croatia
* josipa.dugec@ktf-split.hr

A new approach is presented to elucidate the phenomena occurring within a porous single-walled carbon nanotubes (SWCNTs) modified glassy carbon electrode (GCE) that impact its electrochemical behavior. Data obtained *via* electrochemically *"in-situ"* generated $[Fe(CN)_6]^{3-}$ by cyclic voltammetry, reverse pulse voltammetry, and double potential step chronoamperometry revealed that the interplay of the mass transport regimes within the porous SWCNT layer is responsible for behavior often misinterpreted as an apparent electrocatalytic effect.

Based on analysis of the results, a novel and simple criterion is proposed for distinguishing different diffusion domains, enabling estimation of the transition points between them. The results demonstrate that the porous SWCNT layer suppresses expansion of the double layer and contributes to ion condensation within the Gouy–Chapman layer, leading to improved electrochemical response. Relaying on this knowledge, optimization of pulse and interval times can yield a significantly improved cathodic response using reverse pulse voltammetry. An unexpectedly improved cathodic response was obtained at lower ionic strengths of the electrolyte, with negligible shifts in potential relative to fully supported conditions. Additionally, counterintuitive voltammetric behaviors were observed, including the independence of peak currents from the ionic strength of the supporting electrolyte, a parabolic dependence of peak potentials on scan rate, and the appearance of steady-state currents.[1]

The presented findings provide new insight into the role of porous carbon nanomaterials in electrochemical systems and may contribute to improved modeling and optimization of devices based on porous conductive and non-conductive materials. Beyond electrochemical sensing, the proposed analysis and criteria may also be relevant for energy-storage technologies, including EDLCs, pseudocapacitive systems, and related electrochemical devices. Furthermore, the presented approach may serve as an alternative to reported single-entity methodologies[2] for clarifying the role of carbon nanotubes and other porous materials, such as metal-organic frameworks and modified CNT-based systems, in a broad range of electrochemical applications.

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SYNTHESIS OF PROPARGYLIC CHLOROHYDRINS VIA ORGANOMETALLIC ADDITION TO α-CHLOROKETONES

Petar Fičko, Danijel Glavač, Irena Dokli

Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička 54, 10000 Zagreb, Croatia

* petar.ficko@student.pmf.hr

Propargylic chlorohydrins are valuable synthetic intermediates due to the presence of alkyne, hydroxyl, and chloride functionalities, which enable a wide range of subsequent selective transformations.[1] In addition, they represent promising substrates for halohydrin dehalogenase (HHDH)-catalyzed cascade reactions, providing access to optically active compounds under mild and sustainable reaction conditions.[2] Consequently, the efficient synthesis of structurally diverse propargylic chlorohydrins is of considerable interest for both synthetic organic chemistry and biocatalysis. In this work, an efficient method for their synthesis was developed through the nucleophilic addition of ethynylmagnesium bromide to α-chloroketones in tetrahydrofuran (THF).

A broad range of substrates with diverse electronic and steric properties was investigated, and the influence of the Lewis acids $CeCl_3$ and $LaCl_3$/LiCl on the reaction efficiency was evaluated. Comparison of the reaction conditions revealed that the addition of Lewis acids generally improved the product yields compared to reactions performed without additives. $CeCl_3$ proved particularly effective for several substrates, providing isolated yields of up to 74%, while the $LaCl_3$/LiCl system also enhanced the yields for selected substrates. The developed protocol exhibited good functional-group tolerance toward aliphatic, aromatic, cyclic, and heterocyclic substituents, although limited reactivity was observed for certain substrates.

These results demonstrate that the use of appropriate Lewis acids is an effective strategy for optimizing the synthesis of propargylic chlorohydrins and expands the scope of accessible substrates. The obtained compounds represent versatile building blocks for the preparation of structurally diverse and functionally enriched organic molecules.

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YEAST ALCOHOL DEHYDROGENASE KINETICS: A STUDENT PROGRESS CURVE EXERCISE

Blaženka Foretić,[a]* Boštjan Petrič,[b]* Igor Picek,[a] Željka Vukelić[a]

[a] Department of Chemistry and Biochemistry, School of Medicine, University of Zagreb, Šalata 2, 10000 Zagreb, Croatia, [b] Institute of Biochemistry and Molecular Genetics, Faculty of Medicine, University of Ljubljana, Vrazov trg 2, 1000 Ljubljana, Slovenia
* blazenka.foretic@mef.hr; bostjan.petric@mf.uni-lj.si

Alcohol dehydrogenase (ADH) is a key zinc(II) metalloenzyme that catalyzes the reversible oxidation of primary and secondary alcohols to their corresponding aldehydes and ketones, coupled with the reduction of the NAD^+ cofactor to NADH. It is one of the most commonly used enzymes in enzymatics practical courses. However, in a teaching context, the kinetics of ADH are almost always determined via initial velocities, despite past attempts to popularize determining them from entire progress curves.[1]

The objective of this student exercise is to determine the key kinetic parameters of yeast ADH (K_m and V_{max}) for the NAD^+ co-substrate using the progress curve method. While the traditional initial velocity approach requires several measurements to acquire a single set of kinetic parameters, the progress curve method enables parameter calculation from a single, continuous reaction run. The assay (1 mL reaction mixture) was optimized at ambient temperature in a pH 8.5 buffer with ethanol in excess (50 mM) and NAD^+ (0.5 mM), and initiated with ADH (20 nM). The reaction progress was monitored spectrophotometrically by measuring NADH absorbance at 340 nm for 600 seconds, with 15-second intervals until a plateau was reached.

Non-linear regression was performed by applying the integrated form of the Michaelis-Menten equation:

$$\int_0^t dt = \int_{c(S)_0}^{c(S)_t} \frac{K_m + c(S)}{V_{max} \cdot c(S)}\, dc(S) \;\Rightarrow\; t = \frac{1}{V_{max}} \left(K_m * ln \frac{c(S)_0}{c(S)_0 - c(P)} + c(P)\right)$$

through an iterative curve-fitting model. A web-based software (www.curve.fit) was utilized to analyze the time-course data (c(P) as a function of t) and optimize the kinetic constants (K_m and V_{max}), alongside operational parameters: initial substrate concentration c_0(S) and baseline absorbance (bl). Determining K_m and V_{max} allowed students to calculate the enzyme's turnover number (k_{cat}) and specificity constant (k_{cat}/K_m), which describes catalytic efficiency and substrate preference.

This exercise successfully demonstrates the application of progress curve kinetics in analyzing enzymatic reactions. The progress curve method provides students with deeper conceptual insight into the mathematical modeling of biochemical processes, significantly reduces reagent consumption, and shortens experimental time compared to traditional initial velocity methods, making it a highly sustainable and effective educational tool.

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FACTORS DETERMINING MECHANICAL RESPONSE IN ORGANIC MOLECULAR CRYSTALS: A COMPUTATIONAL INVESTIGATION

Tea Frey, Ivan Kodrin

University of Zagreb, Faculty of Science, Department of Chemistry, Horvatovac 102a, Zagreb, Croatia
* tfrey@chem.pmf.hr

A wide range of physical properties makes organic molecular crystals promising materials for use in advanced technologies such as organic electronics, molecular actuators, nanomachinery, pharmaceuticals, etc. However, a major limitation of molecular crystals is their inherent brittleness. By understanding the relationship between crystal structure and mechanical response, it is possible to design molecular crystals that are elastic or plastic, making them much more applicable for everyday use.[1] In this work, we use a series of p-halogenated benzene-based esters to computationally explore how molecular structure, intermolecular interactions and crystal packing influence crystal flexibility. The bromine derivatives, whose polymorphs are reported as either elastic or brittle,[2] allow us to directly correlate crystal packing with mechanical properties. We extend previous research by varying para-substituted halogens (chlorine, bromine and iodine) to see how small molecular changes impact both crystal packing and the mechanical flexibility of the resulting materials. To rationalize experimental findings, we use periodic DFT methods implemented in CRYSTAL23 program. Crystal structures are optimized, and various mechanical properties evaluated with the PBE-D3 functional and pob-TZVP-rev2 basis set. We apply a series of virtual tensile tests, where crystal structures are deformed along specific directions orthogonal to crystallographic planes to simulate deformation under applied stress. Additionally, QTAIM analysis provides deeper insight into how intermolecular interactions transform during the simulated crystal deformations. We compare the computed and experimental Raman spectra of both relaxed and deformed crystals. Our work is further complemented experimentally by the discovery of new crystal structures and polymorphs of the studied compounds, exhibiting different mechanical properties. Through this combined computational and experimental approach, we hope to establish a computational framework that can be used to analyse the impact of weak intermolecular interactions and crystal packing on the mechanical properties of similar organic molecular crystals.

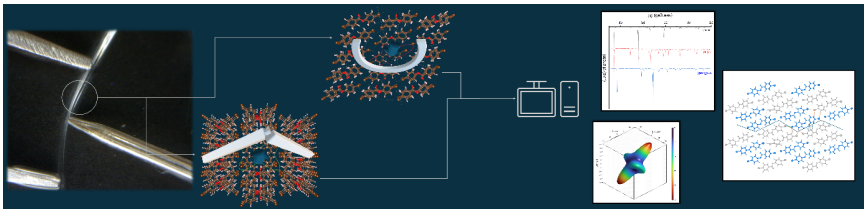


Figure 1. Computational modeling of mechanical properties in organic molecular crystals.

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SYNTHETIC DIVERSIFICATION OF ENANTIOENRICHED PROPARGYLIC ALCOHOLS TOWARD STRUCTURALLY DIVERSE CHIRAL SCAFFOLDS AND BIOISOSTERIC REMODELING TO α-CHIRAL BCPs

Danijel Glavač, Irena Dokli, Maja Majerić Elenkov

Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička 54, 10000 Zagreb, Croatia

* danijel.glavac@irb.hr

Chiral propargylic alcohols have emerged as privileged synthetic intermediates in modern organic chemistry. The coexistence of a carbon–carbon triple bond and a hydroxyl group provides numerous opportunities for selective functionalization, enabling the rapid generation of molecular complexity. Through carefully designed transformations, these compounds can be converted into a wide variety of valuable chiral scaffolds commonly found in pharmaceuticals, natural products, and biologically active molecules. [1]

An efficient HHDH-catalyzed cascade kinetic resolution protocol was developed, enabled the synthesis of enantiopure propargylic β-azido alcohols and chlorohydrins with excellent enantiopurities (>99% ee). These compounds serve as versatile chiral building blocks for subsequent synthetic elaboration. A series of selective post-transformations was employed to access structurally diverse molecular architectures from common propargylic alcohol intermediates. Functional-group manipulations afforded cyclic carbonates, isocoumarins, phosphoramidates, and vicinal amino alcohols, while ring-closing metathesis provided access to bicyclic frameworks.

Motivated by the increasing importance of sp^3-rich bioisosteres in medicinal chemistry, the platform was extended to α-chiral bicyclo[1.1.1]pentane (BCP) derivatives via bioisosteric replacement of para-substituted aryl groups and carbon–carbon triple bonds.[2-4] The resulting enantiopure BCP alcohols were accessed through HHDH-catalyzed cascade reactions and kinetic resolution with excellent enantioselectivities (>99% ee), providing a complementary class of conformationally rigid and medicinally relevant chiral building blocks. Collectively, these results establish enantioenriched propargylic alcohols as versatile platforms for scaffold diversification and bioisosteric design, enabling the synthesis of structurally diverse, medicinally relevant chiral architectures.

ACKNOWLEDGEMENTS This work was supported by the Croatian Science Foundation under the project number [HRZZ-IP-2024-05-1376] and funded by the European Union – NextGenerationEU (IRB - MZ3-25a)

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3D-LC-MS/MS PLATFORM FOR CYCLIC PEPTIDE SEQUENCE CHARACTERIZATION: A CASE STUDY ON VASOPRESSIN IMPURITIES

Saša Grubešić, Edvin Brusač

Research and Development, Analytical Development, Hikma Pharmaceuticals, Slavonska avenija 24/6

* sgrubesic@hikma.com

Therapeutic peptides are increasingly used in modern medicine, from intensive care to chronic therapies. The analysis of such species, however, is often challenging due to their structure and physicochemical properties. Moreover, regulatory requirements demand each impurity found in such a product to be structurally characterized. Identification, in terms of peptide sequence, can easily be done „*online*“ for small linear peptides using conventional LC-MS/MS with collision induced dissociation considering the characteristic fragmentation patterns of peptide bonds. Cyclic peptides containing disulfide bonds, however, first have to be converted to their linear form and the cysteine residues capped,[1] which, if done as an *offline* sample pretreatment, changes the chromatographic profile and complicates method development. An automated approach is therefore desirable to reduce sample preparation and preserve chromatographic profile integrity.

In this work, a 3D-LC-MS/MS approach is presented, consisting of 2D-LC chromatography to capture the peak of interest, dithiothreitol (DTT) derivatization to linearize the cyclic peptide and MS/MS analysis for structural characterization, using Vasopressin as a model cyclic peptide. Using a validated first-dimension method, three major degradation products were separated, captured, and transferred to a second-dimension column for DTT derivatization via a 3D complex consisting of a pump and switching valve. Following reagent washout from the column, MS and MS/MS analyses were conducted for the three impurities, which were shown to be deamidations at different amino acid residues having the same molecular weight and thus could not be differentiated without linearization. MS/MS spectra enabled assignment of the exact peptide sequences.

The developed approach proved viable for *online* structural characterization of Vasopressin impurities. The 2D-LC aspect allows for methods with non-MS compatible mobile phases to be used, making it possible to characterize unknown impurities in already validated or compendial methods. In addition, immediate analysis after derivatization minimizes the risk of disulfide-scrambling artefacts in peptides containing multiple disulfide bonds. This approach can be used for other cyclic peptides containing disulfide bridges, simplifying method development and identification challenges.

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SOLUTION AND DFT STUDIES OF Co- AND Mn-PORPHYRIN NITRITE REACTIONS WITH ORGANIC DISULFIDE AND TRISULFIDE

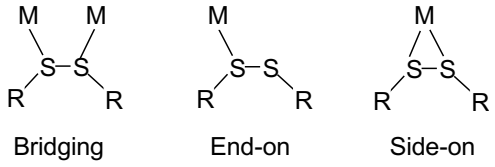
Gurgen Gulyan, Astghik Hovhannisyan, Ashkharuhi Aleksanyan, Hayk Aghekyan, Garik Martirosyan

The Scientific and Technological Centre of Organic and Pharmaceutical Chemistry NAS, Azatutyan 26, Yerevan 0014, Armenia
* g.m.gurgen58@gmail.com

Nitro derivatives of cobalt and manganese porphyrins have been widely studied as the bioinspired models of hemoproteins and for catalytic applications.[1–3]

The results presented here originate from the observations in the course of our recent studies on the reactions cobalt and manganese porphyrin nitrites with ethanethiol in the solid sublimed films.[4] We found that ethanethiol reduce nitro Co(TTP)(NO_2) and nitrito Mn(TTP)(ONO) to the Co(TTP)(NO) and Mn(TTP)(NO) to generate simultaneously diethyl disulfide and water. Some IR spectroscopic features were detected, allowing to suggest that produced diethyl disulfide may act as a ligand for both Co(TTP)(NO_2) and Mn(TTP)(ONO) to form six-coordinate complexes. Possibility of the further disulfide oxidation to the thiosulfinates by the nitroporphyrin complexes was also of interest because oxidation of diethyl disulfide to the thiosulfinates in an oxygen medium on the metal oxides and by singlet oxygen have been earlier reported.

Here we present the results of the reactions of cobalt and manganese porphyrin nitrites with organic disulfide and trisulfide in CCl_4 solution followed by Uv-Vis spectroscopy. The optical changes suggest formation of the novel six-coordinate complexes with disulfide and trisulfide ligands. Density functional theory calculations were applied to explore availability of the proposed adducts. Transition metal complexes possessing organic disulfides RSSR may coordinate the ligand in three different ways (Scheme 1). The possible structures of complexes are discussed.



Scheme 1. Most common coordination modes of organic disulfide RSSR ligands.

ACKNOWLEDGEMENTS The financial support from SCS RA (Project 21AG-1D040) is gratefully acknowledged.

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CLASSICAL VS. DFTB QM/MM MOLECULAR DYNAMICS SIMULATIONS OF CYCLOPENTALEUCINE-ANION COMPLEXES

Gordan Horvat,[a] Antonija Tomić[b]

[a] Department of Chemistry, Faculty of Science, Horvatovac 102a, Zagreb, Croatia, [b] Department of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička cesta 54, Zagreb, Croatia
* ghorvat@chem.pmf.hr

Cyclopentapeptides can serve as reliable hosts for the recognition and binding of anions,[1–3] with their macrocyclic structure and hydrogen-bonding interactions playing a key role in complex formation. In this work, we compare the results of molecular dynamics (MD) simulations of cyclopentapeptide–anion complexes performed using two computational approaches: classical MD with the OPLS-AA force field in GROMACS and QM/MM MD based on density-functional tight-binding (DFTB) methods as implemented in AMBER. The simulations were used to assess the ability of the two approaches to describe peptide–anion interactions. Despite the different levels of theory and simulation frameworks, both approaches yield comparable structural characteristics and similar complex geometries. The good agreement between the two methodologies supports the reliability of the classical OPLS-AA simulations for describing the investigated systems, while the QM/MM results provide an independent, higher-level validation of the predicted structures and interactions.

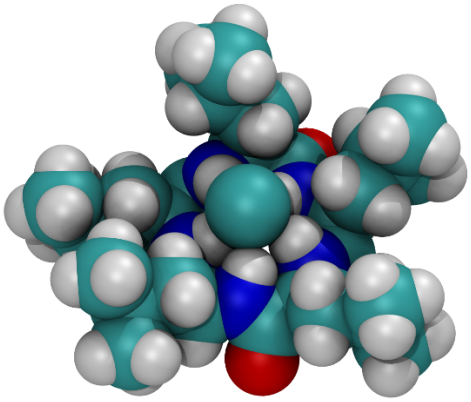


Figure 1. Chloride complex of cyclopentaleucine.

ACKNOWLEDGEMENTS: This work was supported by the Croatian Science Foundation under project IP-2025-02-8238 (CPepFunxIon), European Union – NextGenerationEU through the National Recovery and Resilience Plan 2021-2026. via Institutional grants of the University of Zagreb Faculty of Science *(NextGenChem and CryoLab),* European Regional Development Fund (project CluK, KK.01.1.1.02.0016) and HR-ZOO project of the University of Zagreb University Computing Centre (SRCE).

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IMPACT OF STERILIZATION METHODS ON THE CRITICAL QUALITY ATTRIBUTES OF A CARBOMER-BASED GEL FORMULATION

Patrizia Janković Bevandić,* Ivana Poropat, Antonela Baćac, Tajana Ibriks Glavan, Karla Dubaić, Laura Gubić, Lucija Ažić, Tea Kukić, Lela Munjas Jurkić, Leo Štefan

Research and Development, Jadran-Galenski Laboratorij d.d., Svilno 20, 51000 Rijeka
*patrizia.jankovicbevandic@jglpharma.com

Sterilization is a critical requirement in pharmaceutical manufacturing, ensuring product safety and preventing microbial contamination. Regulatory guidelines recommend terminal sterilization (e.g., steam, dry heat, ionizing radiation, or gas sterilization) whenever feasible, as it is considered the most reliable approach for guaranteeing the sterility of the final product.[1] However, selecting an appropriate sterilization method can be challenging, particularly for semi-solid dosage forms such as gels, since sterilization processes may alter structural integrity, physicochemical characteristics, and functional performance. Carbomer-based gels are widely used in pharmaceutical and medical applications due to their favorable rheological characteristics and formulation versatility. Nevertheless, sterilization may affect both the carbomer matrix and the active pharmaceutical ingredient (API), potentially impacting formulation properties, product quality, and performance.[2,3]

The aim of this study was to evaluate the impact of different sterilization methods on the physicochemical properties of a carbomer-containing gel and to identify sterilization-induced changes that could affect product development and manufacturing. The effect of the sterilization methods on the formulation was evaluated through pH determination, viscosity measurements, and rheological characterization, while the stability of the active pharmaceutical ingredient after sterilization was assessed by high-performance liquid chromatography (HPLC).

These results provide insight into how different sterilization approaches influence the properties of carbomer-based gel formulations. Understanding these effects supports the selection of appropriate sterilization strategies during the development of sterile semi-solid pharmaceutical products and contributes to the improved control of product quality and robustness through manufacturing.

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DEVELOPMENT OF A COARSE-GRAINED MODEL OF THE *ESCHERICHIA COLI* CELL ENVELOPE FOR LARGE-SCALE MOLECULAR DYNAMICS SIMULATIONS

Mario Jurada, Matej Kožić, Boris Gomaz, Branimir Bertoša

Department of Chemistry, University of Zagreb, Faculty of Science, Horvatovac 102a, Zagreb, Croatia

* mjurada.chem@pmf.hr

The Gram-negative cell envelope is a structurally complex biological assembly central to cellular function and interactions with the surrounding environment. Molecular dynamics (MD) simulations provide detailed insight into these processes. However, atomistic approaches are limited by accessible time and length of scales. Coarse-grained (CG) molecular dynamics offers an efficient alternative, enabling simulations of larger systems over extended timescales while retaining most of the essential physicochemical features. Therefore, we focused on the development of a CG model of the *Escherichia coli* cell envelope, comprising the inner membrane (IM), peptidoglycan layer (PG), and outer membrane (OM). Models were subjected to MD simulations. Simulations were performed using the GROMACS package and the MARTINI 3.0 coarse-grained force field. The model was constructed by integrating established, literature-based representations of each component, with emphasis on experimentally informed and previously validated lipid and membrane models.[1-3] These components are combined in a physically consistent manner to reproduce the asymmetric architecture of the bacterial envelope. An iterative model-building strategy was employed, in which individual subsystems were assembled, evaluated, and refined prior to full integration. The resulting framework was designed to enable the investigation of structural and dynamical properties of the bacterial cell envelope at large scale, while maintaining physical consistency and stability under long-timescale molecular dynamics conditions.

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FROM SOLUTION CHEMISTRY TO FORMULATION DESIGN: TEMPERATURE-DEPENDENT β-CYCLODEXTRINS COMPLEXATION OF NABUMETONE AND NAPROXEN

Robert Kerep,[a] David Klarić,[a] Ana Budimir,[b] Nives Galić[a]

[a] Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, 10000 Zagreb, Croatia, [b] Department of General and Inorganic Chemistry, Faculty of Pharmacy and Biochemistry, University of Zagreb, Ante Kovačića 1, 10000 Zagreb, Croatia
* robert.kerep@chem.pmf.hr

Cyclodextrins (CDs) are widely used pharmaceutical excipients that enhance the solubility, stability, and bioavailability of poorly water-soluble drugs by forming inclusion complexes. Because the stability of these complexes is temperature dependent, understanding how temperature affects host–guest interactions is important for pharmaceutical formulation development.[1]

To investigate the effects of temperature and guest ionization on cyclodextrin complexation, two structurally related, poorly water-soluble nonsteroidal anti-inflammatory drugs (NSAIDs) were selected: naproxen (NPX), a weakly acidic drug predominantly present in its anionic form at physiological pH ($pK_a \approx 4.2$), and nabumetone (NAB), a neutral prodrug metabolized to 6-methoxy-2-naphthylacetic acid (6-MNA). Their binding to native β-cyclodextrin (β-CD) and its derivatives, hydroxypropyl-β-CD (HP-β-CD), randomly methylated β-CD (RM-β-CD), and sulfobutylether-β-CD (SBE-β-CD), was investigated by isothermal titration calorimetry in 0.20 mol L^{-1} phosphate buffer (pH 6.8) over the temperature range (293 – 313) K.

NAB consistently exhibited higher binding affinities than NPX with all cyclodextrins studied. SBE-β-CD showed the strongest binding toward NAB, whereas β-CD displayed the highest affinity for NPX. The results indicate that both temperature and ionization state of the guest molecule influence cyclodextrin complexation. These findings provide further insight into the thermodynamics of CD–drug interactions and may support the rational selection of cyclodextrins and formulation conditions for the development of stable pharmaceutical products.

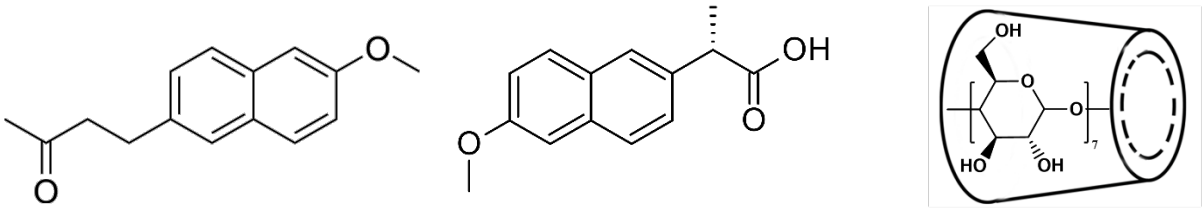


Figure 1. Chemical structures of nabumetone, naproxen and β–CD, respectively.

ACKNOWLEDGEMENTS

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SOLUTION- AND VAPOR-PHASE SYNTHETIC APPROACHES TO IMMOBILIZED METAL-ORGANIC FRAMEWORKS (MOFs)

Maria Kolympadi Markovic,*[a] Karlo Veličan,[a] Iva Šarić Janković,[a] Ivna Kavre Piltaver,[a] Robert Peter,[a] Ivana Jelovica Badovinac,[a] Dean Marković,[b] Gabriela Ambrožić[a]

[a] Faculty of Physics, and Centre for Micro- and Nanosciences and Technologies (NANORI), University of Rijeka, Rijeka, Croatia, [b] Faculty of Biotechnology and Drug Development, University of Rijeka, Rijeka, Croatia

* maria.kolympadi@uniri.hr

Metal–organic frameworks (MOFs) are porous materials composed of metal ion clusters interconnected by organic linkers, forming crystallline or amorphous networks with high surface areas, tunable pore structures and chemical functionalities. These characteristics have made MOFs attractive candidates for gas storage and separation, catalysis, sensing, and energy-related applications.[1] While MOFs are traditionally synthesized as powders, their immobilization on solid substrates has become a key step toward these applications. Surface-immobilized MOFs (SURMOFs) in the form of thin films combine the advantages of porous frameworks with improved stability and handling, in devices such as membranes, electrodes, sensors, and catalytic reactors etc.[2] Among the numerous MOF families, zinc-based MOFs (Zn-SURMOFs) have been extensively studied due to their low cost, low toxicity, stability, and large potential in applications where the surface area is crucial, such as CO_2 capture and utilization.[3] Vapor-phase processing techniques, including atomic and molecular layer deposition (ALD/MLD) have emerged as scalable and sustainable fabrication routes alternative to conventional solution-based synthesis, such as solvothermal growth methods. These methods that utilize precursors from the vapor phase provide superior control over film uniformity and conformality, and facilitate the integration of MOFs in advanced devices.[4] Despite the progress in the direct vapor-phase synthesis of MOFs thin films from vapor-phase precursors, the resulting films often require elevated processing temperatures while still leading to poorly crystalline products. The combination of ALD grown ZnO thin films as templates and sacrificial layers in solvothermal methods has been proven an efficient and fast route to the synthesis of surface-mounted highly crystalline MOFs.[4] Here, we present our efforts toward the growth of MOF thin films on ALD-deposited ZnO using various dicarboxylic acid linkers under solution-phase conditions. In parallel, building on our previous work on the ALD synthesis of metal oxide thin films and the MLD-based stepwise deposition of organic monolayers with terminal carboxylic acid groups,[5] we are developing fully vapor-phase ALD/MLD processes for the fabrication of MOF thin films. Both of these two approaches we aim to optimize in view of developing MOF-coated surfaces for applications in carbon dioxide adsorption.

ACKNOWLEDGEMENTS: Financed by the European Union- NextGenerationEU: (UNIRI PU 2025) uniri-iz-25-236, by the University of Rijeka: uniri-mladi-prirod-22-71, uniri-iskusni-prirod-23-22, uniri-iskusni-prirod-23-235, and by the Croatian Science Foundation: WATPUR (IP-2016-06-3568, G. Ambrožić).

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INTERACTION OF ANOPLIN-COATED GOLD NANOPARTICLES WITH MODEL BACTERIAL MEMBRANES

Vedrana Krajnović,[a] Emanuele Bosurgi,[b] Matthieu Edely,[c] Marc Lamy de la Chapelle,[c] Andreja Jakas,[a] Danijela Bakarić[a]

[a] Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, [b] Department of applied science and technology, Politecnico di Torino, Corso Duca degli Abruzzi, 24, 10129 Torino, Italy, [c] The Institute of Molecules and Materials of Le Mans, University of Le Mans, Avenue Olivier Messiaen 72085, Le Mans cedex 9, France
* vedrana.krajnovic@irb.hr

Anoplin (ANP), a natural decapeptide found in the venom of solitary wasps[1], is considered as promising alternative to conventional antibiotics because it permeabilizes bacterial membranes. However, its more extensive biomedical application is limited by poor stability and susceptibility to proteolytic degradation as well as the need for high local concentration[2]. In parallel, gold nanoparticles (Au NPs) have gained considerable attention in modern biomedicine[3] due to their potential as drug delivery platforms, offering improved tissue penetration, enhanced loading capacity, and protection of sensitive biomolecules from degradation[4]. Thus, this work aimed to characterize the interactions between ANP and ANP-functionalized Au NPs with model bacterial membranes composed of phosphoethanolamine (PE) and phosphatidylglycerol (PG) in a 3:1 ratio. Accordingly, lipid membranes in the presence of ANP and Au NPs (coated with ANP) were explored spectroscopically, microscopically (Figure 1) and calorimetrically. Besides identifying a parameter that the most faithful depicts lipid membrane disorder, we found that the disorder introduced by ANP-coated Au NPs exceeds that introduced by individual components.

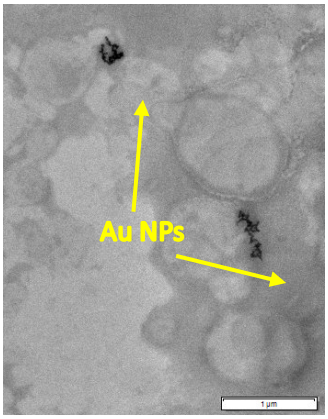


Figure 1. Au NPs on model bacterial membranes imaged by TEM.

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NEXT-GENERATION OPEN-HARDWARE ELECTROSPINNING FOR ADVANCED BIOMATERIALS

Karlo Krhlanko,[a] Donna Danijela Dragun,[a] Iva Rezić Meštrović,[b] Ernest Meštrović[a]

[a] University of Zagreb, Faculty of Chemical Engineering and Technology, Trg Marka Marulića 19, 10000 Zagreb, Croatia, [b] University of Zagreb, Faculty of Textile Technology, Prilaz baruna Filipovića 28, 10000, Zagreb, Croatia
* kkrhlanko@fkit.hr

Electrospinning is a cornerstone technology in advanced nanomedicine, uniquely capable of transforming polymeric solutions into biomimetic matrices that significantly enhance drug stability and bioavailability.[1] This study unveils a next-generation, open-hardware electrospinning platform engineered to bypass the prohibitive costs and rigid "black-box" limitations of commercial equipment. Built for approximately 6,000 €, an order of magnitude more cost-effective than commercial alternatives, this fully functional prototype provides precise process control up to 30 kV. Its modular architecture features interchangeable targets, allowing researchers to seamlessly transition from single fibers to large-surface membranes. Safe operation with volatile solvents (DCM/DMF) is managed via real-time microclimate and VOC tracking using a Bosch BME680 sensor paired with an integrated three-stage HEPA filtration system, while its data-logging capability ensures the platform is inherently AI-ready. To prove its high fidelity, the system was validated through a rigorous 22-run Design of Experiments framework. Comprehensive characterization via SEM, FTIR, XRD, TGA, and DSC confirmed the production of ~500 nm poly(ε-caprolactone) nanofibers. The model drug used in this work, indomethacin, was successfully encapsulated inside the fibers and stabilized in its amorphous state to enhance potential bioavailability. This robust, adaptable system offers a highly flexible and intelligent tool to accelerate breakthroughs in biomaterials and targeted drug delivery.[2]

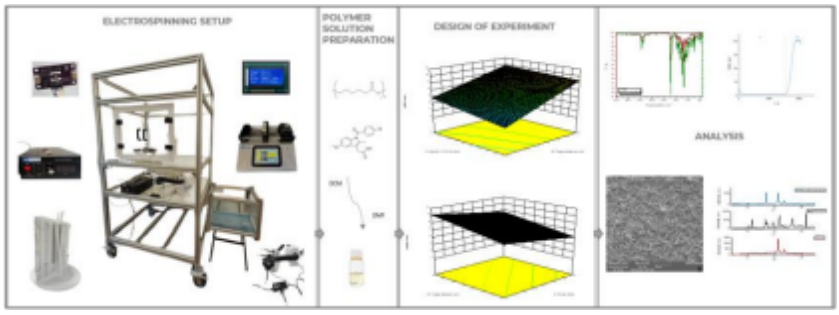


Figure 1. Workflow from custom electrospinning hardware design to DoE-optimized advanced biomaterials.

ACKNOWLEDGEMENTS This work was funded by the Croatian Science Foundation under the project IP-2024-05-4339 entitled “The ‘Coffee Ring’ Effect in a Lab on a Chip Environment for the Development of Novel Drug Formulations” (project leader: Prof. Ernest Meštrović), as well as by the University of Zagreb through the institutional research project “Advanced Technologies for the Fabrication of (Bio)chemical Sensors and Lab on a Chip Devices” (112103).

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POROUS ORGANIC POLYMERS BASED ON CALIX[4]RESORCINARENES FOR ADSORPTION AND CATALYTIC CONVERSION OF CARBON DIOXIDE

Filip Kučas, Mladen Borovina, Ivana Biljan
University of Zagreb, Faculty of Science, Department of Chemistry, Horvatovac 102a, Zagreb, Croatia
* fkucas@chem.pmf.hr

Porous organic polymers (POPs) represent a class of materials characterized by high porosity and chemical stability. Through the incorporation of diverse organic building blocks, their properties can be tuned to obtain novel functionalized materials.[1] As a result of their simple functionalization and ease of synthesis, POPs have become highly attractive for applications in selective gas adsorption and storage. Various POPs based on porphyrins, triazines, tetraphenylmethanes, and other functional organic building blocks have been extensively studied for carbon dioxide (CO_2) capture and catalytic conversion.[2] However, calixarene-based POPs have received limited attention, particularly regarding their potential for CO_2 adsorption and catalytic cycloaddition reactions with epoxides.

In this work, azo-linked porous organic polymers (CalPOFs) based on C-alkylcalix[4]resorcinarene monomers were synthesized via the diazocoupling reaction of 4,4'-biphenyldiamine with C-alkylcalix[4]resorcinarenes. The influence of the alkyl chain length of the C-alkylcalix[4]resorcinarene building blocks (methyl, ethyl, and propyl) on the CO_2 adsorption and catalytic performance of the synthesized CalPOFs was investigated. The CO_2 adsorption capacities, determined by thermogravimetric (TGA) measurements, decreased with increasing alkyl chain length. Furthermore, the synthesized CalPOFs were evaluated for their catalytic activity in the presence of a cocatalyst in the thermal cycloaddition of CO_2 to phenyl glycidyl ether and the photocatalytic cycloaddition of CO_2 to styrene oxide. In both catalytic systems, the conversion increased with increasing alkyl chain length, with a more pronounced increase observed under photocatalytic conditions.

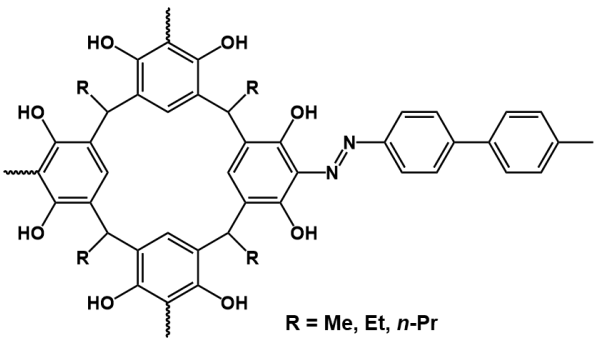


Figure 1. Structure of herein prepared CalPOFs.

ACKNOWLEDGEMENTS This work was supported by the European Union—*NextGenerationEU* through the National Recovery and Resilience Plan 2021–2026 via Institutional grants of the University of Zagreb Faculty of Science (*NextGenChem*).

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INTERACTIONS OF TRIMERIC AND TETRAMERIC STYRYL DERIVATIVES WITH G-QUADRUPLEX DNA STRUCTURES

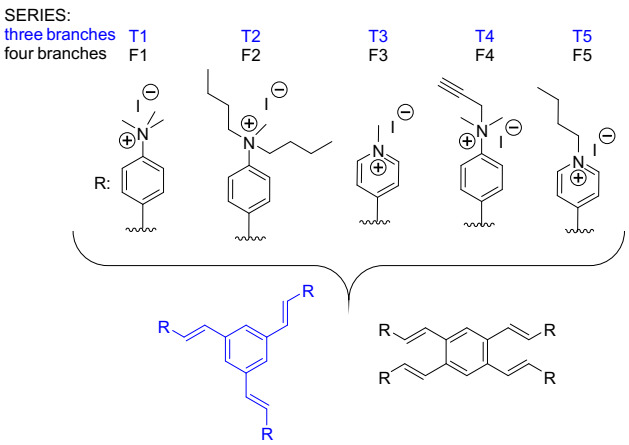
Bojan Kuridža,[a] Željka Ban,[a] Joaquín Calixto García Martínez,[b,c] Ivo Piantanida[a]

[a] Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia, [b] Department of Inorganic and Organic Chemistry and Biochemistry, Faculty of Pharmacy, Universidad de Castilla-La Mancha, C/José María Sánchez Ibáñez s/n, 02008 Albacete, Spain, [c] Regional Center for Biomedical Research (CRIB), Universidad de Castilla-La Mancha, C/Almansa 13, 02008 Albacete, Spain
* bkuridza@irb.hr

G-quadruplexes (G4) are non-canonical nucleic acid structures involved in the regulation of key cellular processes and represent attractive targets for anticancer drug development.[1,2] Building upon a recently reported series of trimeric and tetrameric cationic styryl derivatives,[3] we investigated their interactions with structurally distinct DNA targets, including human telomeric G-quadruplexes folded in potassium- and sodium-containing media (hTelo-K and hTelo-Na), the promoter G-quadruplex c-MYC, and the duplex DNA model ds26.

The binding affinity, selectivity, and effects of five trimeric and five tetrameric styryl ligands on G-quadruplex conformation were investigated by fluorescence and circular dichroism (CD) titrations. Thermal denaturation experiments further evaluated ligand-induced changes in G-quadruplex stability. In addition, interactions with folded and unfolded oligonucleotide forms were assessed by gel electrophoresis.

The results demonstrate that the investigated styryl ligands interact with G-quadruplex structures, producing diverse spectroscopic responses that depend on both ligand structure and G-quadruplex topology. These findings provide a basis for understanding the interactions of multivalent styryl ligands with different DNA secondary structures and for guiding the design of G-quadruplex-targeting ligands.



Scheme 1. Structures of the investigated compounds. The trimeric (T) and tetrameric (F) cores were functionalized with different substituents (R), yielding two series of five analogues each.

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COMPARATIVE INHIBITION OF BUTYRYLCHOLINESTERASE BY CHIRAL AND RACEMIC QUATERNARY QUINUCLIDINE PEPTIDOMIMETICS

Matea Laučan, Alma Ramić, Ines Primožič

Department of Chemistry, Faculty of Science University of Zagreb, Horvatovac 102a, Zagreb, Croatia

* mlaucan@chem.pmf.hr

Bioactive chemical compounds, such as quinuclidine derivatives, are recognized as compounds with a broad spectrum of biological activities, including applications in the field of neurodegenerative diseases. Accordingly, they are used in the treatment of Alzheimer's disease.[1-3] The treatment of Alzheimer's disease is based mainly on increasing the level of the neurotransmitter ACh by inhibiting enzymes that hydrolyze them, which is the most common approach in treatment.[4] In this work, novel racemic and chiral (*R*)- and (*S*)-quinuclidine peptidomimetics were synthesized using a microwave-assisted Ugi multicomponent reaction.[5] The (±)-, (*R*)-, or (*S*)-3-aminoquinuclidine was used as the amino component, benzyl isocyanide as the isocyanide component, paraformaldehyde as the carbonyl component and benzoic acid as the acid component. A series of new quaternary derivatives was prepared by quaternization of the quinuclidine nitrogen atom with selected, variously substituted alkyl halides. The selected compounds have different modifications in the structure to define the structural parameters important for achieving improved biological activity in the interaction with cholinesterases. The melting points and optical rotations of the prepared compounds were determined, and their structures were confirmed by infrared spectroscopy, mass spectrometry and 1D and 2D nuclear magnetic resonance spectroscopy. Finally, the inhibitory potential of all prepared quaternary quinuclidine peptidomimetics toward the enzyme butyrylcholinesterase from horse serum (EC 3.1.1.8) was evaluated using the Ellman method for the colorimetric determination of cholinesterase activity.[6]

ACKNOWLEDGEMENTS This work was supported by The Croatian Science Foundation under the project numbers HRZZ-IP-2022-10-9525 and HRZZ-DOK-NPOO-2023-10-1323, and by European Union - NextGenerationEU through the National Recovery and Resilience Plan 2021-2026 via Institutional grant NextGenChem of the University of Zagreb Faculty of Science.

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FROM OXYGEN TO SULFUR: A COMPARATIVE STUDY ON THE CATION BINDING OF AMIDE AND THIOAMIDE CALIX[4]ARENES BEARING PHENANTHRIDINE SUBUNITS

Katarina Leko, Dajana Barišić, Vladislav Tomišić

University of Zagreb Faculty of Science, Department of Chemistry, Horvatovac 102A, 10000 Zagreb, Croatia

* katarina.leko@chem.pmf.unizg.hr, dbarisic@chem.pmf.unizg.hr

Calixarenes are macrocyclic oligomers composed of phenolic residues linked by methylene bridges in the *ortho* position.[1] Depending on the size and functionalization of upper and/or lower rim, these compounds can be very efficient or even selective receptors for various ionic and neutral chemical species.[1,2] Among them, calixarenes with sulfur-containing functional groups form stabile complexes with low-charge-density and soft metal cations.[3] Moreover, those bearing fluorescent moieties can be considered as potentially very sensitive fluorimetric ion sensors due to the high sensitivity of fluorescence spectroscopy and high affinity of these macrocyclic ligands towards cations.[4] In the scope of this work, novel phenanthridine-based thioamide calix[4]arene derivative **L2** (Figure 1) was synthesized. The binding affinities of ligands **L1** and **L2** (Figure 1) towards selected metal cations in acetonitrile/dichloromethane mixture (ϕ = 0.5) were investigated by spectrophotometry, fluorimetry, isothermal titration calorimetry, and NMR spectroscopy.

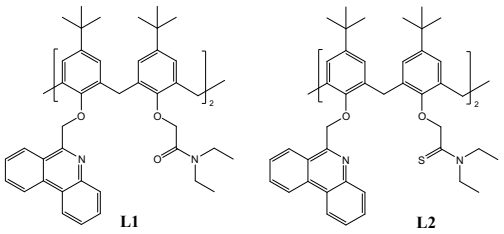


Figure 1. Molecular structure of calix[4]arene derivatives **L1** and **L2**.

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

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PREPARATION, SCALE-UP, AND DISSOLUTION: INDOMETHACIN SALTS/COCRYSTALS WITH IMIDAZOLE AND ISONICOTINAMIDE

Marin Liović,[a] Donna Danijela Dragun,[a] Nika Rimaj,[a] Rafael Anelić,[a] Lea Čolakić,[c] Fabio Faraguna,[a] Edi Topić,[b] Ivan Halasz,[c] Ernest Meštrović[a]

[a] Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, Zagreb, [b] Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, Zagreb, [c] Ruđer Bošković Institute, Bijenička cesta 54, Zagreb

* mliovic@fkit.unizg.hr

Cocrystallization and salt formation are powerful crystal-engineering strategies for modifying drug properties while preserving the molecular scaffold of the drug molecule.[1] Indomethacin (**INDO**H), a non-steroidal anti-inflammatory drug (NSAID)[2], was selected as a candidate for such modification given its poor aqueous solubility at physiological pH which limits its oral bioavailability and therapeutic efficacy.[3] In this work, three previously unreported multicomponent crystal phases were prepared by liquid-assisted grinding (LAG) of **INDO**H with two pharmaceutically acceptable coformers: a 1:1 INDOH-isonicotinamide phase and two **INDO**H-imidazole phases with 2:1 and 1:2 stoichiometries. Single crystals of the 2:1 **INDO**H-imidazole salt were prepared from ethanol solution and characterized by single-crystal X-ray diffraction. The mechanochemical formation of the **INDO**H-imidazole phases was investigated by *in situ* Raman monitoring during LAG experiments in a modified vibratory mill. The scalability of the phase preparation was evaluated using both vibratory milling and a co-rotating twin-screw extruder used as a continuous mechanochemical reactor. Dissolution behaviour was examined in several solvents, and drug release from hypromellose capsules containing either 1:1 **INDO**H-isonicotinamide or 2:1 **INDO**H-imidazole phase was monitored in phosphate buffer at pH 6.15 and 37 °C.

coformer (X)	reactant ratio *n*(INDOH) : *n*(X)	vibratory mill: NG	vibratory mill: LAG H_2O	vibratory mill: LAG EtOH	vibratory mill: LAG EtOH (1g scaleup)	mortar/pestle: LAG EtOH	mortar/pestle: LAG IPA	crystallization experiments
imidazole (im)	2:1	×	2:1+**INDO**H	2:1	2:1	/	/	2:1 or **INDO**H or **im**
	1:1	×	2:1+1:2	2:1	/	2:1+1:2	1:2+2:1 or 2:1	
	1:2	×[a]	1:2	1:2+2:1	/	/	/	
isonicotinamide (inicam)	1:1	×	1:1	1:1	1:1	/	/	1:1+**inicam**+?[b]

[a] initially a liquid which spontaneously crystallizes
[b] "?" represents an unknown phase

phases identified in **product mixtures** obtained by cocrystal/salt screening

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DYNAMIC COVALENT AMPHIPHILES: SELF-ASSEMBLY AND HYDROLYTIC STABILITY IN AQUEOUS MEDIA

Ivan Lisjak,[a] Marc C. A. Stuart,[b] Anamarija Knežević[a]

[a] Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička cesta 54, Zagreb, Croatia, [b] Stratingh Institute for Chemistry, University of Groningen, Nijenborgh 7, 9747AG Groningen, The Netherlands

* ilisjak@irb.hr

Stimuli-responsive supramolecular systems have attracted considerable interest in the development of adaptive materials, particularly those capable of responding to pH changes in aqueous environment. In these systems, amphiphilic molecules self-assemble into dynamic structures whose behavior can be regulated by external stimuli. The structural diversity of amphiphiles is a key factor governing their self-assembly behavior and the resulting material properties.[1–3] In this work, a series of nine amphiphilic molecules has been synthesized (Fig. 1). Three pH-responsive dynamic covalent linkages (imine, salicylimine, and acylhydrazone) were incorporated to investigate their influence on hydrolytic stability. Within each subgroup, the hydrophobic alkyl chain length was systematically varied to evaluate its influence on self-assembly and the resulting supramolecular structures in water. The compounds were assessed for their water solubility and the thermal behavior of the resulting solutions was investigated, revealing distinct trends depending on both the type of the dynamic bond and the alkyl chain length. Transmission electron microscopy confirmed the formation of nanoscale aggregates in aqueous media, with morphologies dictated by molecular structure. The hydrolytic stability and pH-responsiveness of these systems will be presented, providing insight into the role of supramolecular organization in controlling dynamic covalent behavior in aqueous media. Their resistance to hydrolysis is being evaluated both in the self-assembled and in the disassembled state to determine the influence of supramolecular organization on hydrolytic stability. Overall, this study provides a comparative framework for understanding how the type of the dynamic covalent linkage, hydrophobic chain length, and self-assembly affect the behavior of these supramolecular systems in aqueous environments.

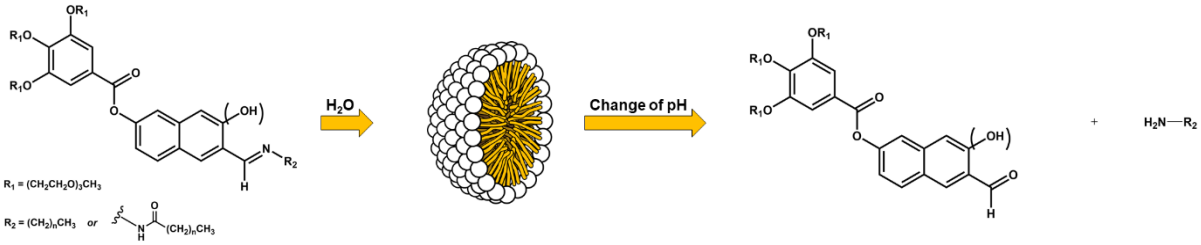


Figure 1. Self-assembly and pH-influenced disassembly of the amphiphiles.

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EXPLICIT WATER MOLECULES IN THE CHLORINATION TRANSITION STATES OF OXAZAPHOSPHORINE DRUGS

Antonio Ljulj, Anamarija Jurjević, Elena Erlić, Valerije Vrček

Faculty of Pharmacy and Biochemistry, University of Zagreb, Ulica Ante Kovačića 1, 10 000 Zagreb, Croatia

* aljulj@pharma.hr

Oxazaphosphorine anticancer drugs cyclophosphamide and ifosfamide are found in waste waters where they are commonly subjected to chlorination during the treatment process. Under these conditions, the amine moieties of these compounds undergo electrophilic chlorination.

In this DFT study we investigated the role of explicit solvent (water) molecules, combined with implicit solvation in stabilising the transition states of electrophilic chlorination using hypochlorous acid (HOCl) as a chlorinating agent. Using a stochastic method, we identified the most stable transition states containing between zero and five explicit water molecules involved in the reaction site, then we performed DFT calculations and observed their effect.

The addition of explicit water molecules had a notable stabilizing effect on the transition states, with the activation energies being greatly reduced at first, then settling around a minimum as additional waters were added. In the reaction site the explicit waters either directly participated in a cyclic transition state by facilitating proton transfers, or acted as observers, forming hydrogen bonds with the reacting species. Since there are multiple forms of the molecules that could be involved in the reaction, this procedure was repeated for both the tautomer and the anionic forms, giving similar results for both cases. When the barriers are compared to the results obtained by NMR experiments it becomes clear that to reproduce the experimental results, explicit solvent molecules are necessary.

These findings demonstrate the necessity of including explicit water molecules alongside continuous solvation models to accurately describe the thermodynamics of chlorination reactions involving oxazaphosphorines.

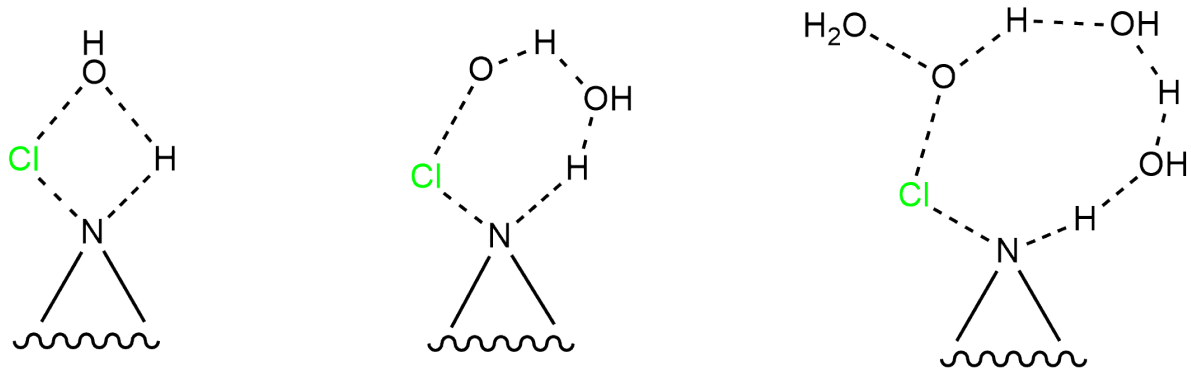


Figure 1. Chlorination transition states with n=0,1,3 explicit water molecules.

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TUNING THE PROPERTIES OF NDI AGGREGATES IN WATER BY STERICALLY HINDERING SURFACTANT π-π INTERACTIONS

Aleks Logožar, Anamarija Knežević

Laboratory for Stereoselective Synthesis and Biocatalysis, Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia

* Aleks.Logozar@irb.hr

Amphiphilic molecules self-assemble in water, yielding an array of nanostructures, such as micelles, vesicles, bilayers, rods, tubes, toroids, and others.[1] Their self-assembly is driven by favorable non-covalent interactions between hydrophobic moieties, while hydrophilic ones remain oriented towards aqueous environment, enabling the solubility of newly formed nanostructures. Multiple structural factors and experimental conditions directly influence the morphology of an aggregate. The volumes of the hydrophilic and hydrophobic moieties of a surfactant, charge, presence of specific functional groups (directional hydrogen or π-π bonding), as well as concentration, temperature and ionic strength are of the most important ones.[2] For simple amphiphiles the geometric models are used for the prediction of aggregate morphology, the most notable being the critical packing parameter (the *CPP*).[3] However, for designer nonionic amphiphiles bearing additional functional groups that form strong non-covalent interactions, such models are insufficient.

In our work, we are oriented on the synthesis of novel nonionic designer amphiphiles with propensity for linear self-assembly and growth, as well as on studying the properties of those aggregates. The targeted formation of linear anisotropic assemblies is enabled by the naphthalene diimide (NDI) subunit in surfactant structure (Figure 1). The volume ratios and structures of hydrophilic and hydrophobic moieties have been optimized to obtain the amphiphilic self-assembly and their desired properties, such as solubility in water. The strongly directing π-π interactions of the NDI unit, as well as the overall two-dimensional planarity of prepared amphiphiles, yield stable and highly ordered aggregates. In order to obtain aggregates with desired properties for future utilization, different alkyl substituents with defined stereochemistry were introduced at a strategic linker position close to the NDI subunit. These groups hinder the close packing of the NDI molecules in water, yielding chiral aggregates of different morphologies and distinct thermal and spectroscopic properties.

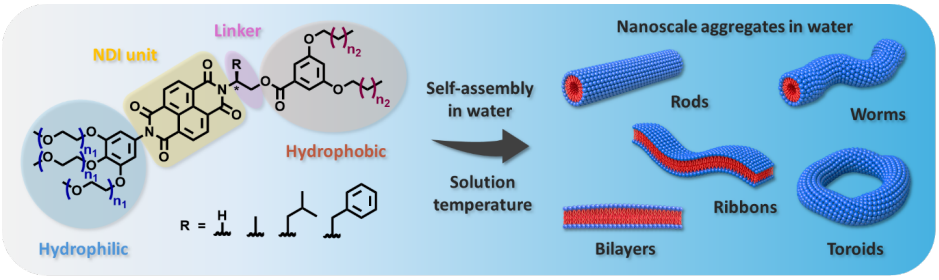


Figure 1. Morphology changes in amphiphilic NDI aggregates in water upon the introduction of simple sterically hindering functional groups in linker position.

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STRUCTURE OF WATER-DIMETHYLFORMAMIDE MIXTURES AND POTENTIAL EFFECTS ON CRYSTALLISATION

Abbie O. R. Madden,[a] Thomas F. Headen,[b] Terri-Louise Hughes,[b] Sophie Janbon,[c] Katharina Edkins[a]

[a] Strathclyde Institute of Pharmacy and Biomedical Sciences, University of Strathclyde, 161 Cathedral Street, Glasgow G4 0RE, UK, [b] ISIS Neutron and Muon Source, Science and Technology Facilities Council, Rutherford Appleton Laboratory, Didcot OX11 0QX, UK, [c] Early Chemical Development, Pharmaceutical Sciences, R&D, AstraZeneca, Charter Way, Macclesfield SK10 2NA, UK

*abbie.madden@strath.ac.uk

Hydrate crystal forms of pharmaceutical compounds often have low bioavailability and poor tablettability,[1] it is hence important to control their crystallisation in industry and research. It is common to use binary solvent mixtures to tailor solubilities during crystallisation, however, many of these solvent mixtures have non-ideal behaviour which present through clustering of the individual components on the molecular level called microheterogeneity.[2] One solvent mixture suggested to be microheterogeneous is water-dimethylformamide (DMF), with molecular dynamics simulations indicating clustering over a range of mixing ratios.[3] These clusters may cause solute localisation in specific areas, creating a "templating" effect promoting the formation of specific crystal forms, e.g. hydrates.[4] To fully understand this, we investigate the structure and interactions of the solution state and relate these to those in the crystalline form.

Crystallisation of some pharmaceutical relevant compounds show that their hydrate formation can be inhibited in water/DMF mixtures at much lower DMF fractions (and corresponding higher water activities) than in other aqueous solvent mixtures, e.g. acetonitrile or methanol. We performed neutron total scattering (NTS) experiments to elucidate the structure of mixtures at DMF mole fractions X_{DMF} = 0.15, 0.35, and 0.5. Although there is no clear microheterogeneity, there is indication of self-association. Monte-Carlo / Molecular-dynamics simulations tethered to our NTS data allow us to interrogate specific site-site interactions in our mixtures. We see that, at X_{DMF} = 0.15, water and DMF molecules form a bi-percolating system, while at higher DMF content, water molecules appear to form linear chain-like structures, filling the space between the larger DMF molecules as a continuous matrix. Further NTS experiments on water-DMF mixtures with the addition of guanidine hydrochloride as a highly lipophilic model solute show that DMF-DMF interactions change little accross all mixtures, but water-water and water-DMF interactions are increased at X_{DMF} = 0.15 and decrease with increasing DMF content, relative to the solvent mixtures. The non-ideality of these solvent mixtures is at a maximum around X_{DMF} = 0.30, close to the mole fraction of hydrate crystallisation inhibition, indicating that solvent structure influences crystallisation. This furthers our understanding of how solvents play a role in crystallisation, enabling smarter solvent choices.

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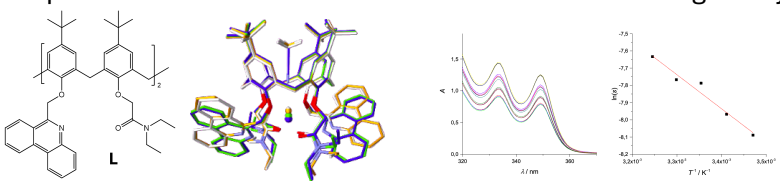
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THERMODYNAMIC AND STRUCTURAL STUDIES OF SOLVENT INCLUSION IN THE HYDROPHOBIC CAVITY OF A CALIX[4]ARENE BEARING PHENANTHRIDINE AND AMIDE SUBSTITUENTS

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

Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102A, 10000 Zagreb
* smarinac.chem@pmf.hr

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



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ENGINEERING A THERMOSTABLE METAGENOMIC POLYESTERASE FOR PLASTIC DEGRADATION

Aleksandra Maršavelski,[a]* Ivana Kekez,[a] Lucija Brtan,[a] Želimira Filić,[b] Margaux Aubel,[c] Erich Bornberg-Bauer[c]

[a] University of Zagreb, Faculty of Science, Horvatovac 102a Zagreb, Croatia, [b] Ruđer Bošković Institute, Bijenička cesta 54, Zagreb, Croatia, [c] Molecular Evolution and Bioinformatics, Institute for Evolution and Biodiversity, University of Münster Münster, Hüfferstraße 1, 48149 Münster, Germany

*amarsavelski.chem@pmf.hr

Plastic pollution represents a growing environmental challenge, driving the need for efficient and sustainable biocatalysts capable of degrading synthetic polymers, particularly polyesters.[1] In this study, we report the engineering of a novel metagenome-derived polyesterase, MGY, exhibiting poly(lactic acid) (PLA)-degrading activity. Although MGY showed promising catalytic potential, its practical applicability was limited by low solubility, poor expression yield, and insufficient thermostability. To overcome these limitations, ancestral sequence reconstruction (ASR)[2] was employed to generate thermostable ancestral variants of MGY. All reconstructed enzymes retained substantial PLA-degrading activity, while one variant additionally exhibited activity toward polycaprolactone (PCL). Notably, the most thermostable variant displayed a melting temperature (T_m) of 84 °C, representing the highest thermostability reported to date for a PLA-degrading enzyme.

To enable accurate assessment of polyester hydrolysis, we developed a high-performance liquid chromatography (HPLC)-based assay for the quantification of total lactate released following enzymatic PLA degradation. Thermal characterization of PLA and PCL substrates further enabled identification of optimal temperature windows for enzymatic hydrolysis. Structural and computational analyses revealed that enhanced thermostability primarily arises from loop rigidification,[3] achieved through both direct stabilization of a short surface loop and remote core mutations that stabilize a longer loop–helix motif proximal to the active site. Despite an unchanged primary sequence within this flexible region, remote mutations increased the number of simultaneous hydrophobic contacts, significantly reducing structural mobility. These findings demonstrate the effectiveness of ancestral sequence reconstruction for engineering robust polyester-degrading enzymes and provide mechanistic insight into the molecular basis of enzyme thermostability, supporting the development of sustainable biocatalysts for bioplastic recycling.

ACKNOWLEDGEMENTS This research was funded through National Recovery and Resilience Plan, The Development Research Support (NextGenerationEU) for the project Enzyme engineering for sustainable recycling of bioplastics (NPOO.C3.2.R2-I1.06.0041) and through Woman in Research (WiRe) Postdoc Fellowship granted by University of Münster in Germany. In addition, this research was supported by the European Union – NextGenerationEU through the National Recovery and Resilience Plan 2021-2026. via Institutional grants (**NextGenChem**, **CryoLab**, **PMF-CROFUND** and **PMF-INDIPRO**) of the University of Zagreb Faculty of Science.

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THIOL ASSISTED NITRITE REDUCTION AT MANGANESE PORPHYRIN. SOLUTION AND DFT STUDIES

Garik Martirosyan, Gurgen Gulyan, Armenuhi Mnatsakanyan, Ashkharuhi Aleksanyan, Hayk Aghekyan

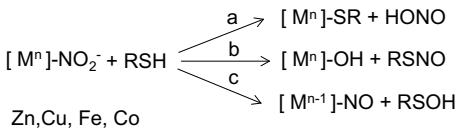
The Scientific and Technological Centre of Organic and Pharmaceutical Chemistry NAS, Azatutyan 26, Yerevan 0014, Armenia

* g.g.martirosyan@gmail.com

In both the global geochemical nitrogen cycle and mammalian biology nitrite (NO_2^-) and nitric oxide (NO) are widely recognizedas as the key actors. In the nitrogen cycle NO_2^- to the NO reduction is an important step in nitrate (NO_3^-) to the nitrogen denitrification pathway.[1] In mammalian biology NO_2^- to NO interconvertions are involved to the complex biological signaling processes. Numerous studies have proved that nitrite can be reduced *in vivo* by the variety of heme-iron containing proteins.[2] At the same time, due to the availability of biological thiols in mammalian tissue nitrite reduction assisted by these endogenous reducing agents is of potential biological relevance. Several pathways for transition metal involving model compounds capable of thiol assisted reduction of nitrite to nitrosyl have been proposed, such as nucleophilic attack, acid-base exchange, and the oxygen atom transfer (OAT) mechanism (Scheme 1).

Recently we reported ethantehiol assisted nitrite to nitrosyl reduction at the biologically relevant manganese porphyrin in the sublimated porphyrin solids.[3] It was proposed that reaction pathway proceed via the OAT pathway involving an elusive sulfenic acid intermediate, which, however has not been detected IR spectroscopically.

Here we report the results of reactions of manganese porphyrin nitrite with a set of aliphatic thiols in toluene solution followed by UV-Vis spectroscopy. We also demonstrate formation of the respective disulfide products identified by ESI-MS analysis of reaction mixture of Mn(TPP)(ONO) and thiols. Density functional theory calculations were applied to compare the energetic costs needed for each of possible pathways the Mn(TPP)(ONO) to Mn(TPP)(NO) conversion. The most plausible reaction mechanism is discussed.



Scheme 1. a - acid-base exchange; b - nucleophilic attack, c - oxygen atom transfer.

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COUPLED NAVIER–STOKES AND MASS TRANSPORT ANALYSIS OF COFFEE-RING PATTERN

Donna Danijela Dragun,[a] Marin Liović,[a] Nika Šajković,[a] Iva Rezić Meštrović,[b] Ernest Meštrović[a]*

[a] University of Zagreb Faculty of Chemical Engenering and Technology, Trg Marka Marulića 19, HR 10000 Zagreb Croatia, [b] University of Zagreb Faculty of Textile Technology, Prilaz baruna Filipovića 28, Zagreb, Croatia

* ernest.mestrovic@fkit.unizg.hr

When a sessile droplet containing a non-volatile solute dries with a pinned contact line, the solute is deposited as a ring along the droplet perimeter – the "coffee-ring" effect:[1] evaporation is strongest at the droplet edge, and the replenishing outward capillary flow convects the solute towards the rim. Control of this phenomenon is important for inkjet printing, biosensing and the development of new drug formulations in "Lab on a Chip" environments.

A time-dependent, two-dimensional axisymmetric model of an evaporating water droplet (contact radius R_0 = 1 mm, initial apex height h_0 = 0.5 mm, 293.15 K) was developed in COMSOL Multiphysics 6.4, coupling Laminar Flow (incompressible Navier–Stokes equations), Transport of Diluted Species (diffusion coefficient $D = 5{\cdot}10^{-10}$ m^2 s^{-1}, initial concentration c_0 = 20 mol m^{-3}) and Deformed Geometry, in which the free surface recedes with the local evaporation velocity $J(r) = J_0/(1 - (r/R_0)^2 + \varepsilon)^{1/2}$, $J_0 = 10^{-7}$ m s^{-1}, reproducing the divergence of the evaporative flux at the pinned contact line[1,2] (ε and a ramp function ensure numerical stability). The mesh of 2608 triangular elements (Figure 1a) allowed the 5 s drying interval to be solved in just 15 s.

The simulation captures the key features of the early drying stage. The contact line remains pinned at $r = R_0$ while the free surface recedes (Figure 1b); in the accelerated-drying scenario the computed apex height decreases from $5.0{\cdot}10^{-4}$ m to $2.7{\cdot}10^{-4}$ m after 2.4 s of drying. The non-uniform evaporation flux drives an outward flow in the thin wedge near the rim, convecting the solute towards the edge, in agreement with the coffee-ring mechanism.[1] Ongoing work addresses solute deposition kinetics, Marangoni stresses[3] and validation against "Lab on a Chip" experiments with model drug formulations.

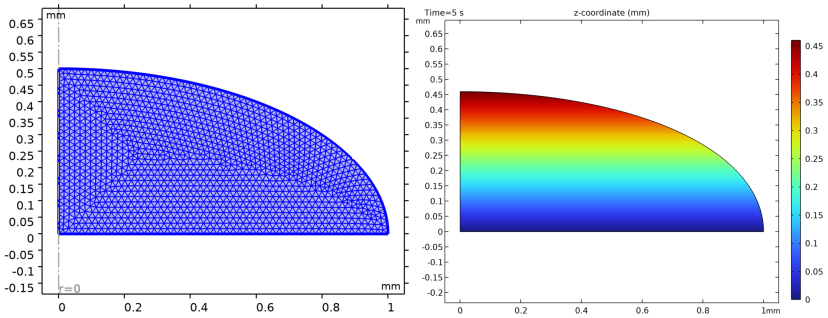


Figure 1. (a) Computational mesh of the axisymmetric droplet model; (b) position of the droplet free surface at the end of the simulated drying interval (t = 5 s), coloured by the z-coordinate.

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SILVER AND GOLD NANOSTARS AS SERS SUBSTRATES FOR STRUCTURAL ANALYSIS OF G-QUADRUPLEX DNA

Snežana Miljanić,[a] Petra Petrović Popović,[a] Adriana Kenđel,[a] Tea Juračić,[a] Dijana Pavlović Saftić[b]

[a] University of Zagreb Faculty of Science, Department of Chemistry, Horvatovac 102A, 10000 Zagreb, Croatia, [b] Ruđer Bošković Institute, Division of Organic Chemistry and Biochemistry, Bijenička cesta 54, 10000 Zagreb, Croatia
* snezana.miljanic@chem.pmf.unizg.hr

It is well known that the metal type, morphology (size and shape), and surface properties of nanoparticles (NPs) strongly affect the magnitude of the surface-enhanced Raman scattering (SERS).[1] Among the various NP morphologies, metallic nanostars (NSs) are particularly attractive due to their multiple intrinsic electromagnetic "hotspots" generated by their sharp tips and edges, which produce strong local field enhancement compared to nanospheres. To evaluate the suitability of metallic nanostars as SERS substrates for detecting DNA structural forms, silver (AgNS) and gold (AuNS) nanostars were synthesized by chemical reduction and thoroughly characterized. For testing SERS efficiency of the prepared NSs, a human telomeric DNA oligonucleotide d[$(TTAGGG)_4$] (Tel24) was employed as a model system. Owing to its repetitive guanine-rich sequence, it is capable of folding into an antiparallel G-quadruplex (G4) form stabilized by sodium ions.[2]

SERS spectra of the unfolded and G4 structure in AgNS and AuNS colloids were acquired using 532 nm and 785 nm excitation. Circular dichroism (CD) spectroscopy was used to confirm the presence of the corresponding Tel24 structural forms in the colloidal samples. Due to the anionic species remaining after synthesis on the AgNS and AuNS surface, the prepared nanostars carried a negative charge. Given a highly negatively charged phosphate backbone of Tel24, SERS spectra of the unfolded oligonucleotide were observed only after addition of the aggregating agent (0.1 $MgSO_4$) into the colloidal sample, whereas 0.1 M Na^+, required for G4 formation, simultaneously reduced electrostatic repulsion and promoted interaction with the NS surface. While SERS bands originating from the AuNS surface layer interfered with Tel24 bands, AgNS enabled clear discrimination between unfolded and G4 conformations. The spectral differences included shifts of guanine bands associated with Hoogsteen hydrogen bonding, the appearance of marker bands assigned to G-tetrads and d(TTA) loops, and pronounced changes in the relative intensities of adenine and guanine ring breathing modes. These results indicated that Ag nanostars are promising SERS substrates for structural studies of G-quadruplex DNA.

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BINDING OF ANIONIC FLUORESCENT DYES TO LEUCINE AND PHENYLALANINE CYCLOPENTAPEPTIDES

Matija Modrušan,[a] Lucija Otmačić,[a] Klara Šimunić,[a] Nikola Cindro,[a] Nikolina Vidović,[b] Giovanna Speranza,[c] Vladislav Tomišić,[a] Gordan Horvat[a]

[a] Department of Chemistry, University of Zagreb Faculty of Science, Horvatovac 102a, 10000 Zagreb, Croatia, [b] University of Rijeka, Faculty of Biotechnology and Drug Development, Radmile Matejčić 2, 51000 Rijeka, Croatia, [c] Department of Chemistry, University of Milan, Via Golgi 19, 20122 Milan, Italy
* mmodrusan@chem.pmf.hr

During the past few decades there has been a growing interest in research of cyclopeptides as anion receptors. These investigations showed that small cyclopeptides have high affinities towards anionic species in organic and aqueous media.[1–3] Cyclopentapeptides exhibit superior anion binding ability compared to the cyclopeptides comprised of four or six amino acid residues towards halide anions.[4] In this work the binding affinity of cyclopentapeptides comprised of leucine and phenylalanine residues towards several fluorescent anionic dyes (ANS, TNS, *N*-Ac-Phe, *N*-Ac-Trp) in acetonitrile was studied by spectrofluorimetric and ^{1}H NMR titrations (Figure 1). Additionally, the insight into the structural properties of the formed complexes was investigated by MD simulations with explicit solvent molecules. The obtained results were used to elucidate the effect of amino acid residue type on the stability of the cyclopeptide-dye complexes.

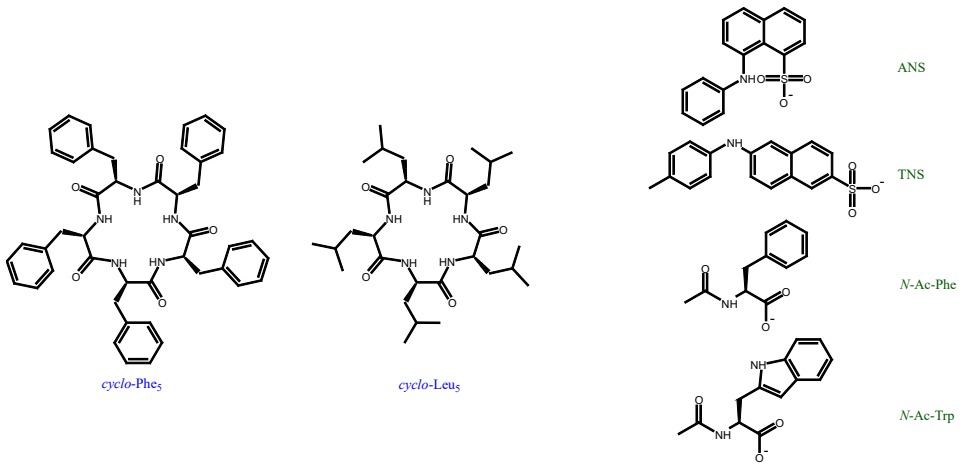


Figure 1. Structures of ligands (blue) and dyes (green) used in this work.

ACKNOWLEDGEMENTS This work was supported by the Croatian Science Foundation under project IP-2025-02-8238 (*CPepFunxIon*), IP-2024-05-2012 (*CalixCORE*), European Regional Development Fund (*CIuK*, KK.01.1.1.02.0016) and European Union – NextGenerationEU through the National Recovery and Resilience Plan 2021-2026 via Institutional grants of the University of Zagreb Faculty of Science *(NextGenChem)*.

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OXIDOVANADIUM(V) HYDRAZONE COMPLEXES: CONNECTING SOLID-STATE STRUCTURE AND SOLUTION PROPERTIES

Danijela Musija,[a] Dino Kuzman,[b] Juraj Toplak,[b] Višnja Vrdoljak[b]

[a] Department of Chemistry and Biochemistry, School of Medicine, University of Zagreb, Šalata 3, Zagreb, Croatia, [b] Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, Zagreb, Croatia

* danijela.musija@mef.hr

Vanadium complexes with hydrazone ligands continue to attract significant interest due to their structural diversity and wide range of applications.[1] Driven by the remarkable coordination versatility of the vanadium center and the prominent pharmaceutical potential of its compounds,[1,2] these systems remain at the forefront of bioinorganic and materials research. Here, we report the synthesis and comprehensive characterization of a series of oxidovanadium(V) complexes with 4-substituted salicylaldehyde (iso)nicotinoyl hydrazone ligands bearing various peripheral groups (R = H, OMe, NMe_2, NEt_2), aiming to offer new insights into ligand-field effects and solute–solvent interactions.

The synthesized complexes were structurally characterized in the solid state using infrared spectroscopy and single-crystal X-ray diffraction, confirming a polymeric architecture maintained by intermolecular coordination. To systematically evaluate how these solid-state networks behave in different liquid environments, UV–visible spectrophotometric studies were conducted in organic media of varying polarities and coordination abilities, namely hexane, chloroform, isopropanol, and acetonitrile.

Rather than exhibiting uniform dissolution behavior, the complexes demonstrated a strong dependence on both the nature of the solvent and the ligand substituent. The observed variations in dissolution kinetics and spectroscopic profiles raise fundamental questions regarding how specific 4-substituents and the position of the pyridine nitrogen modulate intermolecular forces, thereby dictating the ease of dissolution in non-polar media. Furthermore, shifting from non-coordinating environments to coordinating media highlights the extent to which the chosen solvent influences the coordination sphere, prompting distinct spectroscopic features that range from sharp solubility thresholds to considerably broadened band profiles. By correlating solid-state structural findings with solution-state data, this work offers a rational interpretation of these phenomena, providing solutions for the future design of smart materials and metallodrugs.

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HALOHYDRIN DEHALOGENASES AS BIOCATALYSTS FOR THE ENANTIOSELECTIVE DESYMMETRIZATION OF DICHLOROALCOHOLS

Doroteja Mutak, Maja Majerić Elenkov, Irena Dokli

Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Hrvatska

* dmutak@irb.hr

Halohydrin dehalogenases (HHDHs) are enzymes used in biocatalysis that catalyze the intramolecular conversion of alcohols into epoxides.[1] These epoxides can then react in ring-opening reactions with different nucleophiles, which allows the formation of a wide range of chiral products.[2] The discovery of new substrates compatible with the active site of HHDHs broadens the scope of accessible biocatalytic transformations.[3,4]

In this study, we explore the enzymatic conversion of synthetically prepared dichloroalcohols through a two-step cascade desymmetrization reaction. In the first step, HHDHs catalyze the formation of epoxides from prochiral dihaloalcohols. The resulting epoxides are then opened in situ by selected nucleophiles to afford chiral alcohols (Figure 1). A diverse set of substrates and nucleophiles was synthesized and evaluated in screening experiments to assess enzyme activity, substrate acceptance, and stereoselectivity.

The strategy provides access to enantioenriched substituted alcohols in good yields and high enantioselectivities. Overall, the results demonstrate the potential of HHDHs as valuable tools for the development of new asymmetric biocatalytic transformations through systematic variation of substrates and nucleophiles.

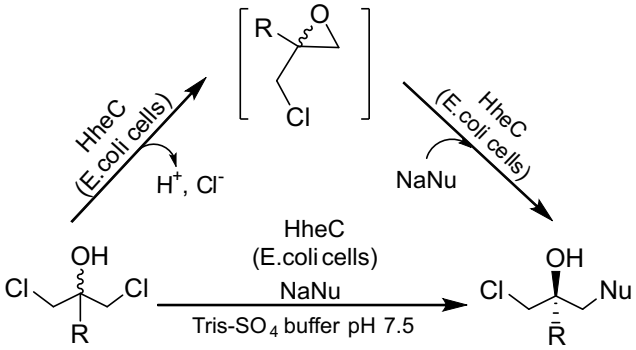


Figure 1. Chemoenzymatic cascade reaction catalyzed by HheC.

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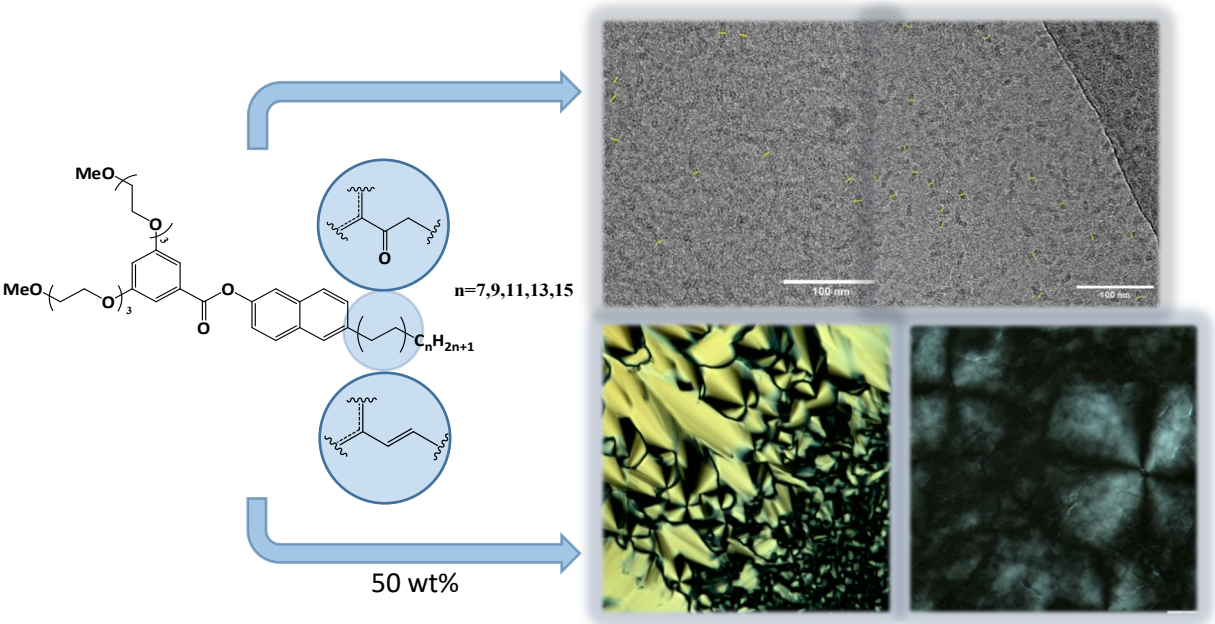
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ETHYLENE GLYCOL NONIONIC AMPHIPHILES FOR THE CONTROL OF SUPRAMOLECULAR ORGANISATION IN WATER

Karlo Petrić,[a] Anamarija Knežević

Department of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb,
* kpetric@irb.hr

In an effort to make industrial-scale synthesis greener and less polluting, solvent selection has increasingly shifted toward water as one of the most prominent reaction media. However, the use of water still presents significant limitations.[1,2] Micellar systems offer a promising solution to some of these limitations, but their application is constrained by their relatively narrow effective concentration range. Lyotropic liquid crystalline (LLC) phases are anisotropic, self-assembled structures formed by amphiphilic molecules in solution, typically in water. LLC phases can form at higher amphiphile concentrations but have so far been largely overlooked because of their increased structural complexity.[3] In our view, this field holds considerable promise and merits further investigation. This research focuses on the design of an ethylene glycol-based nonionic amphiphilic molecule that self-assembles in aqueous media to form nanotubules at low concentrations[4] while also being capable of forming LLC phases at higher concentrations. A series of such amphiphilic compounds has been synthesised, and several have been shown to form micelles at low concentrations and LLC phases at high concentrations, as expected. Following the comprehensive characterisation of these systems, the next step will be to develop their application in specific organic reactions carried out in water.



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HARNESSING LIGHT: UNLOCKING SINGLET OXYGEN GENERATION THROUGH PORPHYRIN-BASED POROUS POLYMERS

Matija Popović, Ivana Biljan

University of Zagreb Faculty of Science, Department of Chemistry, Horvatovac 102a, HR 10000 Zagreb
* mpopovic1@chem.pmf.hr

Porous organic polymers (POPs) with a central porphyrin subunit represent promising materials for heterogeneous photocatalysis. Such systems combine chemical stability and a large specific surface area with the ability of the macrocycle to act as a photoreactive center, which, by absorbing light, initiates energy or electron transfer to adjacent molecules.[1–3] In this study, a series of novel porphyrin-containing POPs were synthesized. The polymer networks were constructed by connecting the core units with aromatic linkers, utilizing three different linkages (N=N, CH=N and C≡C). The obtained polymers were characterized using infrared spectroscopy (IR) and powder X-ray diffraction (PXRD). Additionally, their optical band gaps were determined via diffuse reflectance spectroscopy (UV-Vis DRS) to investigate their semiconducting properties. Finally, the ability of the prepared polymers to act as photosensitizers for singlet oxygen ($^1O_2$) generation was investigated. Their photocatalytic activity was monitored in a solution of 9,10-diphenylanthracene (DPA) in toluene under white-light irradiation, where DPA was used as a selective trap for the generated $^1O_2$. The results demonstrate the potential of porphyrin-based POPs for applications requiring efficient conversion of light energy.

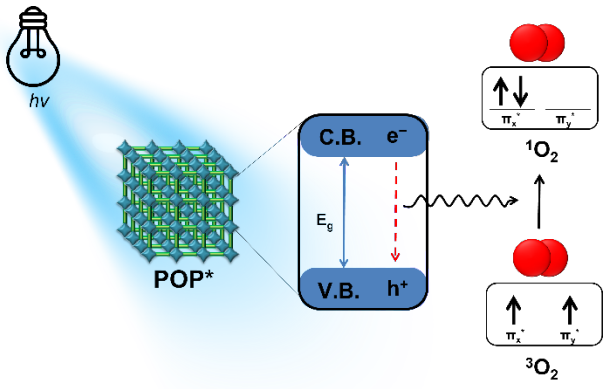


Figure 1. Mechanism of the photocatalytic oxygen activation and singlet oxygen generation using porous organic polymers (POPs).

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NEW BENZYLIDENEMALONONITRILES AS FLUORESCENT SENSORS FOR METAL IONS — SYNTHESIS, SPECTROMETRIC CHARACTERIZATION AND ACID-BASE PROPERTIES

Temenuzhka Radoykova,[a] Stela Georgieva,[a] Meglena Kandinska[b]

[a] Department of Analytical Chemistry, University of Chemical Technology and Metallurgy, 8 "St. Kl. Ohridski blvd, 1756 Sofia, Bulgaria, [b] Department of Organic Chemistry and Pharmacognosy, Faculty of Chemistry and Pharmacy, Sofia University "St. Kl. Ohridski", 1 J. Bourchier Ave., 1164 Sofia, Bulgaria

* nusha_v@uctm.edu

The present study aims to synthesize, characterize, and evaluate the analytical potential of six new derivatives of benzylidenemalononitrile containing different nucleophiles in their structures. The compounds were synthesized by Knoevenagel reaction and isolated in high yield, and their structure and analytical purity were proven by ^{1}H- and ^{13}C-NMR spectroscopy and melting temperatures. The spectral properties were investigated by UV-Vis molecular absorption and fluorescence spectroscopy in organic and aqueous media, with the analysis of the physicochemical parameters showing a significant influence of the polarity of the solvent on the fluorescence intensity and absorption. The acid-base constants (p*K*a, p*K*b) were determined by three independent spectral methods, with the obtained values showing good agreement.

The sensing properties of three of the compounds with introduced BOC-piperazine, 3-methylpiperidine, or thiomorpholine rings in their structure were evaluated by fluorescence and UV-VIS spectrometry at different pH values and metal: ligand molar ratios in aqueous and organic media (acetonitrile) towards Cu^{2+}, Cd^{2+}, and Hg^{2+} ions. The observed changes in the intensity of the fluorescence signals were interpreted as a result of complexation, and the resulting chelates exhibit high complex stability. The compound 2-(4-(3-methylpiperidin-1-yl) benzylidenene) malononitrile at pH 12 exhibits the most pronounced fluorescence quenching in the presence of Cu^{2+} and Cd^{2+}, highlighting it as the most promising sensor for the analytical detection of metal ions in aqueous media.

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TARGETING Aβ OLIGOMERS FOR EARLY THERANOSTICS OF ALZHEIMER'S DISEASE

Shai Rahimipour,[a] M. Habashi,[a] K. Tripathi,[a] S. Senapati,[a] A. Haviv-Chesner,[a] M. Richman,[a] R. Mulamreddy,[b] S-A. Mohand,[c] V. Dumulon-Perreault,[c] B. Guérin,[c,d] W.L. Lubell[b]

[a] Department of Chemistry, Bar-Ilan University, Ramat-Gan, Israel, [b] Département de Chimie, Université de Montréal, Complexe des Sciences, B-3015 1375 Avenue Thérèse-Lavoie-Roux Montréal, Québec H2V 0B3 Canada, [d] Department of Nuclear Medicine and Radiobiology, Université de Sherbrooke 3001, 12th Avenue North, Sherbrooke, QC, J1H 5N4, Canada, [d] Sherbrooke Molecular Imaging Center (CIMS), Research centre of the CHUS (CRCHUS) 3001, 12th Avenue North, Sherbrooke, QC, J1H 5N4, Canada

* shai.rahimipour@biu.ac.il

Alzheimer's disease (AD) is an incurable neurodegenerative disease characterized by cognitive impairment, progressive synaptic dysfunction, and neuronal loss. The misfolding, aggregation, and accumulation of Aβ and tau proteins are the main hallmarks of AD. Recognizing the critical need for early detection and treatment of AD, innovative diagnostic and therapeutic strategies have been developed using self-assembled cyclic D,L-α-peptides. These abiotic cyclic peptides, composed of an even number of alternating D- and L-α-amino acids, self-assemble into peptide nanotubes that replicate the intermolecular hydrogen-bonding pattern of amyloid cross-β-sheets and mimic the structural and functional features of amyloid proteins. The discovered cyclic D,L-α-peptide hexamers exhibit cross-reactivity with Aβ, α-synuclein, and tau, inhibiting their aggregation and toxicity, as shown by various biophysical and biochemical approaches, including thioflavin T assays, transmission electron microscopy, circular dichroism, photoinduced cross-linking of unmodified proteins, and immunochemical methods. In a transgenic AD mouse model, brain PET imaging using stable cyclic D,L-α-peptide radiotracers enabled unprecedented early oligomer detection in pre-symptomatic transgenic 5xFAD mice, outperforming the clinically used 11C-PIB. No tracer accumulation was detected in the cortex and hippocampus of imaged AD mice; instead, intense PET signals were observed in the thalamus, from where Aβ oligomers may spread to other brain regions during disease progression. Early AD diagnosis was also demonstrated when AD mice were treated with the lead cyclic D,L-α-peptide conjugated to biocompatible liposomes or gold nanoparticles and subsequently imaged by fluorescence imaging or computed tomography (CT), respectively. Effectively crossing the blood–brain barrier, the lead cyclic D,L-α-peptides and their liposome/gold nanoparticle conjugates prolonged the lifespan of transgenic AD *Caenorhabditis elegans* and ameliorated memory and behavioral deficits in AD mice by reducing Aβ oligomer levels. This presentation highlights the versatility of self-assembled cyclic D,L-α-peptides and their nanoparticle conjugates as novel tools for studying β-sheet assembly and disruption, holding promise for the early detection and treatment of amyloid diseases.

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COMMERCIAL *GANODERMA LUCIDUM* PRODUCTS AS A SOURCE OF BIOACTIVE POLYPHENOLS: INFLUENCE OF EXTRACTION STRATEGY ON AKR1C3 INHIBITORY POTENTIAL

Milena Rašeta,* Sofija Bekić, Ljiljana Milovanović, Ivana Beara

Department of Chemistry, Biochemistry and Environmental Protection, Faculty of Sciences, University of Novi Sad, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia
* milena.raseta@dh.uns.ac.rs

Ganoderma lucidum (Curtis) P. Karst. 1881 is one of the most extensively consumed medicinal mushrooms worldwide, yet the influence of extraction strategy on its phenolic composition and aldo-keto reductase 1C3 (AKR1C3) inhibitory activity remains poorly understood. This study compared hot-water (WGL1–WGL3) and hydroethanolic (EGL1–EGL3) extracts prepared from three commercially available *G. lucidum* products marketed in Serbia. Total phenolic content (TPC), total flavonoid content (TFC), phenolic profiles determined by LC–MS/MS, and *in vitro* AKR1C3 inhibitory activity were evaluated. Hydroethanolic extraction yielded significantly higher amounts of phenolics and flavonoids than hot-water extraction, with EGL1 exhibiting the highest TPC (67.40 ± 1.05 mg GAE/g d.w.) and TFC (16.81 ± 4.24 mg QE/g d.w.), whereas hot-water extracts contained 11.02–15.34 mg GAE/g d.w. and 1.27–1.70 mg QE/g d.w., respectively. LC–MS/MS analysis identified phenolic acids as the dominant constituents, with 2,5-dihydroxybenzoic, protocatechuic, *p*-hydroxybenzoic, hydroxyphenylacetic, vanillic, syringic, quinic, gallic, caffeic, cinnamic, and ellagic acids representing the principal metabolites. WGL1 generally exhibited the highest concentrations of most detected phenolic compounds, although marked compositional differences were observed among commercial products and extraction solvents. In contrast to the phenolic profiles, hot-water extracts displayed substantially stronger AKR1C3 inhibition than hydroethanolic extracts. WGL2 showed the highest inhibitory activity (45.23%), closely matching the reference inhibitor ibuprofen (46.52%), followed by WGL3 (38.64%), whereas hydroethanolic extracts exhibited only negligible inhibition (0–3.51%). These findings demonstrate that phenolic abundance alone does not explain AKR1C3 inhibition and suggest that highly polar, water-soluble constituents, potentially including polysaccharides and glycoproteins, may contribute substantially to the observed activity. To the best of our knowledge, this is the first report describing AKR1C3 inhibition by *G. lucidum* extracts, highlighting commercially available *G. lucidum* products as promising sources of bioactive metabolites with potential relevance for hormone-dependent disorders and reproductive health.

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AROMATIC BIOBASED TEXTILES AS SUSTAINABLE ALTERNATIVE TO RAW MATERIALS

Iva Rezić Meštrović,[a] Marie Natalie Drobac,[a] Darinka Cvetković,[b] Maja Somogyi Škoc[b]

[a] Department of Applied Chemistry, University of Zagreb Faculty of Textile Technology, Prilaz baruna Filipovića 28a, 10000 Zagreb, Croatia, [b] Department of Materials Testing, University of Zagreb Faculty of Textile Technology, Prilaz baruna Filipovića 28a, 10000 Zagreb, Croatia
* iva.rezic@ttf.unizg.hr

The replacement of petroleum-derived materials with renewable aromatic biobased resources has become a key objective in the development of sustainable functional textiles. Plant-derived polymers and bioactive compounds, including vegetable oils and natural polyphenols, offer renewable, biocompatible, and environmentally friendly alternatives with antioxidant activity and high chemical reactivity. In particular, plant polyphenols have emerged as promising substitutes for fossil-derived aromatic monomers in advanced polymeric materials. In this study, biobased textile coatings containing olive oil were developed and characterized for potential application in cosmetic facial masks. Four formulations were prepared by combining olive oil with glycerol, chitosan, and essential fatty acid-rich oils (rosehip and evening primrose oils). Prior to application onto a biodegradable viscose substrate by dip coating methodology, the formulations were analyzed by UV–VIS spectrophotometry and high-performance liquid chromatography (HPLC) to confirm the presence of bioactive compounds. The textiles after modification were subsequently characterized using FTIR–ATR, scanning electron microscopy (SEM/SEM–EDX), and physicochemical testing, including coating uniformity, softness, hydrophilicity, and recovery angle. All formulations exhibited pH values compatible with human skin, supporting their suitability for cosmetic applications. Drop tests confirmed the hydrophilic nature of the coated textiles, while recovery angle measurements demonstrated preserved elastic behavior. FTIR and SEM analyses verified the successful deposition of the biobased coatings without compromising the inherent properties of the cellulose substrate. These results demonstrate that biodegradable polymers combined with natural vegetable oils provide an effective platform for developing sustainable cosmetic textiles, supporting the replacement of petroleum-based materials with renewable aromatic biobased alternatives for future healthcare and cosmetic applications.

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OPTIMIZATION OF GREEN ENZYMATIC SYNTHESIS OF Au, Ag AND ZnO NANOPARTICLES BY DESIGN OF EXPERIMENT

Iva Rezić Meštrović,[a] Lela Martinaga,[a] Ana Vrsalović Presečki[b]

[a] Department of Applied Chemistry, University of Zagreb Faculty of Textile Technology, Prilaz baruna Filipovića 28a, 10000 Zagreb, Croatia, [b] Department of Reaction Engineering and Catalysis, University of Zagreb, Faculty of Chemical Engineering and Technology, Marulićev Trg 19, 10000 Zagreb, Croatia

* iva.rezic@ttf.unizg.hr

The growing application of gold (Au), silver (Ag), and zinc oxide (ZnO) nanoparticles in advanced textile materials has created a demand for sustainable synthesis routes that minimize energy consumption and the use of hazardous chemicals.[1] In this study, an environmentally friendly enzymatic approach was employed for the synthesis of Au, Ag, and ZnO nanoparticles using three biocatalysts: cellobiose dehydrogenase (MtCDH), glucose dehydrogenase (GcGDH), and urease. The influence of key process parameters, including temperature and stirring rate, was systematically investigated and optimized using Design of Experiment (DoE) methodology, combining Central Composite Design (CCD) for process modelling with Response Surface Methodology (RSM) for optimization. The synthesis process and the obtained nanomaterials were comprehensively characterized by UV–VIS spectroscopy, scanning and transmission electron microscopy (SEM, TEM), atomic force microscopy (AFM), SEM–EDX, Fourier-transform infrared spectroscopy (FTIR), differential scanning calorimetry (DSC), high-performance liquid chromatography (HPLC), and nanoparticle tracking analysis (NTA). The developed statistical models successfully described the influence of synthesis parameters on nanoparticle formation and enabled prediction of optimal operating conditions. The optimized enzymatic synthesis produced nanoparticles with controlled size, morphology, and structural characteristics, including spherical Au and Ag nanoparticles and core–shell ZnO nanostructures. The results demonstrate that the integration of green biocatalytic synthesis with statistical optimization represents an efficient strategy for the controlled production of metal and metal oxide nanoparticles suitable for advanced textile applications, including antimicrobial, UV-protective, flame-retardant, and hydrophobic functional materials.

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DNA/HSA BINDING, IONIC LIQUID-MEDIATED INTERACTIONS, AND ANTICANCER PROPERTIES OF NOVEL PYRROLYL-TERPYRIDINE Ru(II) COMPLEXES

Ana Rilak Simović,[a] Milica Međedović Stefanović,[b] Nevenka Gligorijević,[c] Milan Vraneš,[d] Nenad Janković[a]

[a]Department of Natural Sciences, University of Kragujevac, Institute for Information Technologies Kragujevac, Kragujevac, Serbia, [b]Faculty of Science, University of Kragujevac, Kragujevac, Serbia, [c]Department of Experimental Oncology, Institute of Oncology and Radiology of Serbia, Belgrade, Serbia, [d]Faculty of Science, Trg Dositeja Obradovića, University of Novi Sad, Novi Sad, Serbia
*anarilak@kg.ac.rs

We described the synthesis and characterization of two new mononuclear Ru(II) polypyridyl complexes of the general formula *mer*-[Ru(pyrrolyl-tpy)(*N*-*N*)Cl]Cl, where pyrrolyl-tpy is 4'-(2-pyrrolyl)-2,2':6',2"-terpyridine and *N*-*N* is 2,2'-bipyridine (bpy, **1**) or phenanthroline (phen, **2**). The complexes were characterized by elemental analysis and various spectroscopic techniques, such as UV-Vis, IR, $^{1}H/^{13}C$ NMR, and ESI-MS.[1] Kinetic data for the reactions of compounds **1** and **2** clearly showed that complex **2** (phen) is more reactive toward biologically relevant ligands, 50-GMP and L-cysteine (L-Cys). This increased reactivity is attributed to the p-acceptor character of the phenanthroline ligand, which lowers the electron density at the Ru(II) center, enhancing its ability to accommodate incoming electron density. The data also confirmed the known dependence of substitution rates on the nature of the entering nucleophile. DNA-binding studies using calf thymus DNA indicated a mixed binding mode partial intercalation and minor groove binding, with complex **2** showing higher affinity. Both complexes also exhibited strong binding to human serum albumin (HSA) without site selectivity, supported by experiments in PBS (pH 7.4) and biocompatible ionic liquids (Bio-ILs), where increased solvent polarity enhanced binding efficiency. Molecular docking corroborated the experimental findings. Complex **2** demonstrated greater cytotoxicity and selectivity toward HeLa cells compared to other cancer and normal cell lines (MRC-5). It induced cell cycle arrest at the G2 phase and showed a concentration-dependent ability to trigger apoptosis, although less pronounced than classical agents like cisplatin. These findings highlight complex **2** as a promising candidate for further investigation, particularly regarding alternative mechanisms of cell death beyond apoptosis.

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TOWARDS IMPROVED RIPK2 INHIBITORS: A COMPUTATIONAL STUDY

Tamara Rinkovec,[a] Marina Galić,[b] Rosana Ribić,[c] Leentje Persoons,[d] Dirk Daelemans,[d] Marijana Hranjec,[b] and Robert Vianello[a]

[a] Laboratory for the Computational Design and Synthesis of Functional Materials, Ruđer Bošković Institute, Bijenička cesta 54, Zagreb, Croatia, [b] Department of Organic Chemistry, University of Zagreb, Faculty of Chemical Engineering and Technology, Marulićev trg 19, Zagreb, Croatia, [c] Department of Nursing, University North, 104. brigade 3, 42000 Varaždin, Croatia,[d] KU Leuven, Department of Microbiology, Immunology and Transplantation, Rega Institute for Medical Research, Molecular Genetics and Therapeutics in Virology and Oncology Research Group, Herestraat 49, postbus 1043, 3000 Leuven, Belgium
* tamara.rinkovec@irb.hr

Receptor-interacting protein kinase 2 (RIPK2) is a key mediator of innate immune signaling and an attractive therapeutic target for inflammatory disorders. A recently developed series of benzoxazole-derived acrylonitriles (Figure 1) has demonstrated potent RIPK2 inhibitory activity, with several hydroxy-substituted derivatives exhibiting low nanomolar potency. To elucidate the structural basis of their activity and guide further optimization, we applied an integrated computational approach combining molecular docking, all-atom molecular dynamics (MD) simulations, and MM-GBSA binding free-energy calculations. Docking identified binding poses within the RIPK2 ATP-binding site, which were further evaluated by MD simulations to characterize complex stability and protein-ligand interactions (Figure 2). The results support a type I inhibition mechanism, with the most active derivatives adopting stable binding modes driven by key interactions within the ATP-binding pocket. In particular, the phenolic hydroxyl group was found to enhance binding through hydrogen bonding with Thr95, while bromine substitution on the benzoxazole core contributed to complex stabilization through halogen-mediated interactions with Tyr97 and reduced ligand flexibility. Comparison of active and less active analogues revealed how structural modifications influence ligand orientation, interaction patterns, and calculated binding free energies, providing a molecular explanation for the observed structure-activity relationships. Building on these findings, we are applying the same computational strategy to newly designed derivatives to identify modifications that improve RIPK2 binding. The most promising candidates will be synthesized and experimentally evaluated, establishing an iterative computational-experimental framework for the development of improved RIPK2 inhibitors.

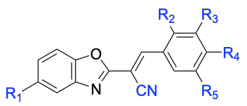


Figure 1. General chemical structure of studied ligands.

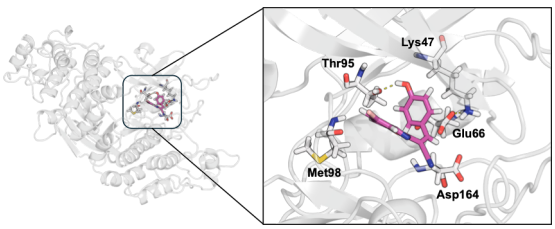


Figure 2. Representative structure of type I inhibitor within the ATP-binding site of RIPK2 as obtained from MD simulations.

CHARACTERIZATION OF "PLAVAC MALI" AND "GRAŠEVINA" WINE VARIETIES BY ICP-MS

Kora Sertić,[a] Ivan Nemet,[a] Nikolina Ilić,[a] Ana-Marija Jagatić Korenika[b]

[a] University of Zagreb, Faculty of Science, Department of Chemistry, Horvatovac 102a, HR-10000 Zagreb, Croatia, [b] University of Zagreb, Faculty of Agriculture, Department of Viticulture and Enology, Svetošimunska cesta 25, HR-10000 Zagreb, Croatia
* kora.sertic@student.pmf.hr

As the chemical composition of a wine serves as a unique geographic fingerprint, the authenticity and geographical traceability of wine are crucial for maintaining its market value.[1,2] This research focuses on the two most significant grape varieties in the Republic of Croatia: “Graševina”, cultivated in Slavonia and the Croatian Danube region and “Plavac mali”, cultivated in central and southern Dalmatia. Given their market dominance, these varieties are essential for establishing a robust database. ICP-MS is a highly sensitive analytical technique that enables accurate multi-element trace analysis. Resulting datasets combined with Deep Reinforcement Learning (DRL) analysis, are used to support further development of powerful tools that allow characterization based on grape variety and geographical origin.[3]

In our study, inductively coupled plasma mass spectrometry (ICP-MS) was used to analyze “Graševina” and “Plavac mali” wine samples. ICP-MS was applied to determine the elemental composition of the wines. The elemental composition was used as a chemical fingerprint for the characterization of the analyzed samples. The results showed that the concentrations of all analyzed elements were within the permitted limits. No potentially toxic elements exceeded the maximum allowed concentrations. The obtained results confirmed that the analyzed wines complied with food safety requirements regarding elemental content. Differences in the elemental profiles were observed between the samples. These elemental profiles enabled the classification of the “Graševina” and “Plavac mali” wines. It was demonstrated that ICP-MS is a suitable method for the elemental characterization of wines. Furthermore, the results highlighted the importance of statistical analysis for the successful classification and differentiation of wine samples based on their elemental composition.

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PREPARATION OF ADAMANTYL NORBORNADIENES FOR ENERGY STORAGE APPLICATIONS

Margareta Sohora, Marina Šekutor

Department of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia
* Margareta.Sohora@irb.hr

In the modern age the quest for renewable energy and efficient energy storage is one of the top challenges. One possible solution is to design molecular solar thermal (MOST) energy storage systems which can trap and release the stored energy on demand. These molecular photo-switches change their structure upon irradiation, resulting in high energy bonds and/or molecular strain, while energy release is usually triggered by heat or by light of differing wavelength.[1-2]

We therefore designed a series of derivatives with a norbornadiene subunit as a harvesting part of the molecule, and with diamondoids (adamantane or diamantane) as an anchor which will keep the molecule on the carrier surface through London dispersion interactions. Namely, diamondoids are excellent scaffolds in nanomaterial design due to their rigidness and good dispersion energy donor properties.[3-6] On the other hand, attractiveness of norbornadiene photoisomerization lies in the fact that a large amount of energy can be chemically stored in strained small rings that form through a photo-induced [2+2] cycloaddition. Since this isomerization reaction is reversible, either by thermal of catalytic means, it is a suitable candidate for repeating reaction cycles and continuous conversion of sunlight to heat.[1-2] Herein we report a synthesis of novel adamantyl norbornadienes that we plan to test as potential on-surface self-assembled MOST systems.

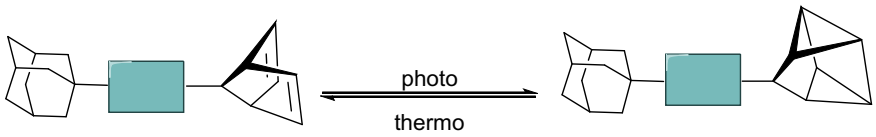


Figure 1. Adamantyl norbornadienes as candidates for MOST system.

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MODEL-GUIDED ASSESSMENT OF DASATINIB RELEASE FROM Zr-BASED METAL–ORGANIC FRAMEWORKS: IMPLICATIONS FOR CARDIAC SAFETY

Katarina Sokač Pogrmilović,[a] Przemysław J. Jodłowski,[b] Witold Piskorz,[c] Krunoslav Žižek[a]

[a] Department of Mechanical and Thermal Process Engineering, University of Zagreb Faculty of Chemical Engineering and Technology, Trg Marka Marulića 19, Zagreb, Croatia, [b] Department of Organic Chemistry and Technology, Faculty of Chemical Engineering and Technology, Cracow University of Technology, Warszawska 24, Cracow, Poland, [c] Department of Inorganic Chemistry, Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, Cracow, Poland
* ksokac@fkit.unizg.hr

A series of zirconium-based metal–organic frameworks (MOFs), including UiO-66, differently functionalized UiO-66 derivatives, UiO-67, MOF-808, and NU-1000, was investigated as a platform for controlled dasatinib (DAS) delivery. The materials were evaluated in terms of pore architecture, surface functionality, drug-loading capacity, and release behavior. Pronounced differences across the series demonstrated that framework structure and pore accessibility strongly affected DAS encapsulation and release. Among the investigated systems, NU-1000 and UiO-67 exhibited the most favorable controlled-release profiles and were therefore selected for biological evaluation. Studies in H9c2 cardiomyoblasts and *Danio rerio* embryos demonstrated markedly reduced cardiotoxicity of the DAS-loaded MOFs compared with free DAS, including preservation of heart rate and the absence of developmental abnormalities despite exposure to substantially higher formulation concentrations.[1] Following the identification of the most promising carriers, their release profiles were analyzed using empirical and semi-empirical mathematical models. The modeling revealed distinct release patterns for NU-1000 and UiO-67, consistent with differences in pore architecture, drug loading, and accessibility of the encapsulated drug. Computational modeling was additionally employed to investigate DAS localization and drug–framework interactions within the selected MOFs, providing molecular-level support for the experimentally observed differences in release behavior. Overall, the findings demonstrate that the structural characteristics of Zr-based MOFs govern DAS loading and release and are associated with differences in biological response. Mathematical and computational modeling provided complementary insight into the performance of the selected carriers, supporting Zr-based MOFs as promising platforms for controlled DAS delivery with improved cardiac safety.

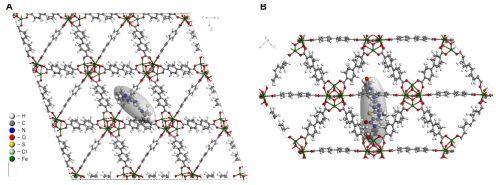


Figure 1. DAS@UiO-67: (A) general view and (B) detailed view.

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NOVEL CATIONIC IMIDAZOLE-BASED AMPHIPHILES: SYNTHESIS AND POTENTIAL ANTIMICROBIAL ACTIVITY

Terezija Som,[a] Hanna Zhukouskaya,[b,c] Martin Hrubý,[c] Jiří Pánek,[c] Domagoj Drenjančević,[d,e] Nikola Sakač,[f] Marija Karaševac Sakač,[f] Marija Jozanović[a]

[a] Department of Chemistry, Josip Juraj Strossmayer University of Osijek, Cara Hadrijana 8, HR-31000 Osijek, Croatia, [b] Institute of Macromolecular Chemistry, Czech Academy of Sciences, Heyrovského náměstí 2, 162 00 Prague 6, Czech Republic, [c] Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University, Hlavova 8, Prague, 128 43, Czech Republic, [d] Clinic for Infectious Diseases, University Hospital Centre Osijek, 31000 Osijek, Croatia, [e] Department of Medical Microbiology and Infectology, Faculty of Medicine Osijek, Josip Juraj Strossmayer University of Osijek, 31000 Osijek, Croatia, [f] Faculty of Geotechnical Engineering, University of Zagreb, Hallerova aleja 7, 42000 Varaždin, Croatia
* terezijasom2003@gmail.com

In this research, novel cationic imidazole-based amphiphiles with potential antimicrobial properties were synthesized. The synthesized compounds belong to quaternary ammonium salts, which have found many useful applications across different fields. For example, they can be used as lubricants, additives in shampoos, detergents, fabric softeners, etc. Some of them come in the form of ionic liquids and are used as green solvents in synthesis and different extraction procedures, as well as catalysts in synthesis. Since a lot of quaternary ammonium salts possess amphiphilic properties, they can interact with the cell membrane of different microorganisms, disrupt its structure, and cause cell death. The properties and uses of quaternary ammonium salts depend on their structure, which is easy to change. The reactions in this work were conducted without the use of a solvent. The synthetic approach where no solvent is used is called the ‘’neat synthesis’’ and it is in agreement with the principles of green chemistry. Antibacterial and antifungal properties of the synthesized compounds were determined.[1–4] Depending on the bacterial and fungal strain, compounds with C12–C18 alkyl chains exhibited the highest antimicrobial activity. The obtained products were characterized using nuclear magnetic resonance (NMR) spectroscopy, infrared (IR) spectroscopy, and mass spectrometry (MS). Changing the structure of quaternary ammonium salts impacts their physical and chemical properties. The results demonstrate that neat synthesis is an effective approach for preparing amphiphilic cationic compounds active against Gram-positive bacteria, Gram-negative bacteria, and fungi, highlighting their potential as disinfectants for surfaces, skin, and equipment.

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EVALUATION AND OPTIMIZATION OF RESPONSE CHARACTERISTICS POTENTIOMETRIC SENSORS FOR ANALYSIS SURFACE ACTIVE SUBSTANCES

Ana Stanisavljev, Marija Stanković

City Institute for Public Health, Bulevar Despota Stefana 54a, Belgrade, Serbia
* ana.stanisavljev@zdravlje.org.rs

The wide use of surfactants demands the development of modern methodologies for their accurate determination.[1] The mostly used technique in ionic surfactant analysis is the two-phase titration method [2] with a mixed indicator, which suffers from many drawbacks.[3]

Potentiometry with ion-selective electrodes (ISE) used as sensors is a simple, fast and inexpensive method for determining surfactants and avoids most of the limitations of classical titrimetric methods.[4-10]

In these investigations, theoretical models for potentiometric titration curves of some ionic (cationic, anionic) surfactants are proposed and their estimations of response parameters for a few surfactant sensors are reported. The generated potentiometric experimental data were then incorporated into calculations using mass and charge balance equations.[11] The models were optimized using Solver (Microsoft Excel).

Potentiometric titration data were used to estimate and optimize sensor response parameters and analyte properties (sensor slope, constant potential term, solubility product constant, and analyte concentration). The two commercial sensors and one self-made sensor of the own construction were used for all the measurements. The analytically usable titration curves are obtained with all three sensors, but the highest potential change in the equivalence point was obtained using DMI-TPB sensor, which only exhibited Nernstian behaviour of the sensors investigated.

Solver (Excel) was used to find the values for those variables that minimize the sum of the squares of the differences between the theoretical and experimental curves. The initial parameter settings were defined, and no constraints were applied on the variables.

The theoretical models fit satisfactorily to the experimental values obtained using DMI-TPB and CS-1 sensor, whereas CS-2 sensor revealed slightly higher deviations.

The proposed methodology gives the insight in the sensor condition and its acceptability for analytical application.

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EFFECTS OF POLYETHYLENE GLYCOL CROWDING ON AMINO ACID AND γD-CRYSTALLIN ASSOCIATION IN AQUEOUS SOLUTIONS

Zala Štefanič,* Barbara Hribar-Lee

Faculty of Chemistry and Chemical Technology, University of Ljubljana, Ljubljana, Slovenia
* zala.stefanic@fkkt.uni-lj.si

The conformational stability of proteins, and therefore their functionality, is strongly influenced by the surrounding environment. Cells are crowded molecular environments in which the space available to biomolecules is reduced, altering their local interactions.[1] To explore protein properties that are challenging to investigate directly, amino acids are often utilised as model systems. Potentials of mean force (PMFs) can be used to describe molecular association along a reaction coordinate. Determining a suitable reaction coordinate is challenging for proteins because their interactions depend on separation and orientation. PMFs have been applied to characterise amino acid side-chain interactions in water,[2] while atomistic approaches have been developed to quantify protein–protein interactions and model the phase behaviour of γ-crystallins.[3,4] In this work, we use an orientation-resolved PMF approach to study the association of amino acids and γD-crystallin in aqueous and crowded solutions.

All-atom molecular dynamics simulations were performed for arginine, aspartate, glutamate, glycine, lysine, serine, tryptophan, and γD-crystallin in aqueous solutions and in the presence of polyethylene glycol (PEG) at a volume fraction of 0.3. These amino acids were selected to compare the effects of different side-chain properties on association. Pair configurations were described by the distance between molecular reference points and three Euler angles. From these distributions, orientation-resolved and radial PMFs were calculated. The systems with and without PEG were compared by examining the positions and depths of the main PMF minima. For γD-crystallin, the radius of gyration and protein–protein separation distributions were also analysed.

Analysis of the complete amino acid series showed that PEG affected each solute differently. Although the presence of PEG produced only minor changes in the position of the short-range PMF minimum, it affected the strength of attraction and the orientational distributions of close-contact configurations. Association was stronger for most of the studied amino acids, weaker for arginine, and showed mixed behaviour for glycine and lysine. For γD-crystallin, visual analysis suggested tighter packing and more clustered configurations in the presence of the crowder; however, the mean radius of gyration remained practically unchanged. Overall, the results provide a systematic molecular-level description of how a polymeric crowded environment reshapes biomolecular association.

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PREPARATION OF MANNOSE-TRIAZOLE PRECURSOR FOR THE SYNTHESIS OF NOVEL DESMURAMYL PEPTIDE ADJUVANTS

Luka Sumić,[a]* Vesna Petrović Peroković,[a] Željka Car,[a] Rosana Ribić[b]

[a] Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, 10000 Zagreb, Croatia, [b] University North, University Center Varaždin, Jurja Križanića 31b, 42000 Varaždin, Croatia

* lsumic@student.chem.pmf.hr

The triazole structural motif is one of the most important heterocyclic fragments in medicinal chemistry due to its chemical stability, favorable electronic properties, and ability to form specific interactions with biological targets. It is incorporated into numerous biologically active molecules and drugs with antifungal, antibacterial, antiviral, anti-inflammatory, antitumor and other biological activities.[1] Lipophilic mannosylated derivatives of desmuramyl peptide (L-Ala-D-*iso*Gln, DMP) and their adjuvant activity are the subject of our long-term research. The mannose subunit is attached to the amino group of L-Ala, while lipophilic subunits, such as adamantyl, cholesteryl or alkyl chains, are introduced to the α- or γ-position of *iso*Gln.[2] In the structure of mannosylated DMP derivatives, the triazole subunit can be introduced in several places (Figure 1). Our previous research has shown that mannosylated DMPs with triazole part introduced between lipophilic subunits and a-position of *iso*Gln have good *in vivo* adjuvant activity in mouse model.[2] Herein, the focus is on the introduction of a triazole motif between mannose part and DMP. For this purpose, a new mannose-triazole precursor was prepared whose terminal carboxyl group will be used to bind to the amino group of alanine of various DMP derivatives.

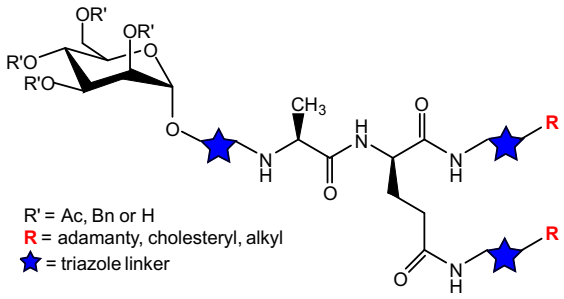


Figure 1. General structure of mannosylated DMP derivatives with indicated positions for the introduction of the triazole motif.

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

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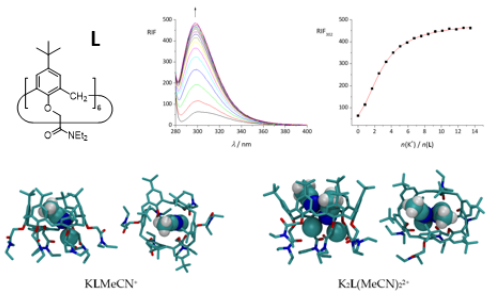
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INTRINSIC FLUORESCENCE OF A CALIX[6]ARENE DERIVATIVE: INSIGHTS INTO METAL CATION COMPLEXATION

Franka Sunjka,[a] Luka Klemen,[a] Andrea Usenik,[a] Karla Kukina Gradečak,[a] Katarina Leko,[a] Mateja Belovari,[b] Nikola Cindro,[a] Gordan Horvat,[a] Ivo Piantanida,[b] Vladislav Tomišić[a]

[a] Department of Chemistry, University of Zagreb Faculty of Science, Horvatovac 102a, HR-10000, Zagreb, Croatia, [b] Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička cesta 54, HR-10000, Zagreb, Croatia
* fsunjka.chem@pmf.hr, lklemen.chem@pmf.hr

The intrinsic fluorescence of the tertiary-amide calix[6]arene derivative **L** and its complexes with group I and group II metal cations was investigated using steady-state and time-resolved fluorescence spectroscopy. As previously shown for the calix[4]arene analogue,[1] despite the absence of an appended fluorophore, **L** exhibits intrinsic fluorescence that is significantly affected by cation complexation. The stability constants of the 1:1 and 2:1 (cation:ligand) complexes were determined by spectrofluorimetric titrations and compared with those obtained using absorption spectrophotometry and microcalorimetry, showing very good agreement. The stoichiometries and structures of the complexes were further studied by means of ^{1}H NMR spectroscopy and mass spectrometry, whereas molecular dynamics simulations provided additional insight into the cation-binding processes and the structures of the complex species. The observed changes in emission upon cation binding demonstrate that the intrinsic fluorescence of a calix[6]arene derivative can be effectively used to monitor and quantitatively characterize complexation processes in the micromolar concentration range. The findings emphasise the advantages of fluorimetry owing to its higher sensitivity and lower required receptor concentration compared to other commonly used methods. Therefore, the presented results highlight the potential of using intrinsic calix[6]arene fluorescence as a powerful approach for the sensitive detection and differentiation of alkali and alkaline earth metal cations in solution.



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VALIDATION OF A NUMERICAL INNER FILTER EFFECT CORRECTION METHOD FOR QUANTITATIVE FLUORESCENCE SPECTROSCOPY

Davor Šakić, Tin Weitner, Tino Šeba, Domagoj Kifer

Faculty of Pharmacy and Biochemistry University of Zagreb, Ante Kovačića 1, 10000 Zagreb, Croatia

* davor.sakic@pharma.unizg.hr

The inner filter effect (IFE) is a major source of systematic error in fluorescence spectroscopy, causing signal attenuation and loss of linearity in absorbing samples.[1,2] Although numerous correction approaches have been proposed, including empirical absorbance-based methods, their performance depends strongly on sample composition and measurement geometry, highlighting the need for rigorous experimental validation. Building on a previously reported variable-focus approach for IFE correction,[3] we evaluated an automated spectral correction workflow (SpecIFE) using a structured laboratory validation protocol. Validation was performed using fluorescein as a reference fluorophore and red wine as a complex analytical matrix. Fluorescence measurements were acquired at multiple optical configurations in microplates and verified on independent spectrofluorimeters. Correction performance was assessed by restoration of the linear relationship between fluorescence intensity and analyte concentration and compared with uncorrected data and the classical Lakowicz correction.For fluorescein, SpecIFE consistently produced the highest linearity, reaching a median coefficient of determination of R^2 = 0.998 under the optimal measurement configuration, compared with 0.35 – 0.66 for uncorrected data, while the classical Lakowicz correction showed little or no improvement. In the red wine matrix, where optical interference was substantially greater, SpecIFE again outperformed the empirical correction and achieved a median R^2 of 0.969 under the optimal configuration, although performance remained dependent on measurement geometry. These results demonstrate that successful IFE correction depends on both the correction algorithm and experimental design, particularly the measurement geometry. The proposed validation strategy combines controlled reference systems, complex real-world matrices and independent instrumental platforms to provide a robust framework for evaluating IFE correction methods. Beyond the present algorithm, this approach offers a practical methodology for validating quantitative fluorescence measurements in optically challenging samples.

ACKNOWLEDGEMENTS This work was supported by the Proof of Concept (PoC III) Programme grant NPOO.C3.2.R3-I1.06.0259, co-financed by the European Union through the European Regional Development Fund (ERDF) and the Ministry of Science, Education and Youth of the Republic of Croatia. The views and opinions expressed are those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them.

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ORTHOGONAL VALIDATION OF PROTEIN–LIGAND INTERACTIONS: INTEGRATED BIOPHYSICAL CHARACTERIZATION OF THE G-ACTIN–LATRUNCULIN A INTERACTION

Tino Šeba,[a] Mario Gabričević,[a] Robert Kerep,[b] Zvonimir Mlinarić,[a] Tin Weitner[a]

[a] Faculty of Pharmacy and Biochemistry University of Zagreb, Ante Kovačića 1, 10000 Zagreb, Croatia,

[b] Faculty of Science University of Zagreb, Horvatovac 102A, 10000 Zagreb, Croatia

* tino.seba@pharma.unizg.hr

Reliable determination of protein–ligand affinity remains a significant analytical challenge because different biophysical techniques probe distinct physicochemical aspects of the same interaction and are therefore subject to different experimental limitations. The G-actin–Latrunculin A complex represents an excellent reference system for method validation, as its 1:1 binding stoichiometry and submicromolar affinity (K_D ≈ 0.2 – 0.4 μM) have been established by complementary biochemical and structural studies.[1]

An orthogonal analytical workflow combining isothermal titration calorimetry (ITC), bio-layer interferometry (BLI), microscale thermophoresis (MST), nano differential scanning fluorimetry (nanoDSF) and pyrene-actin polymerization assays was applied to assess the consistency and limitations of contemporary protein–ligand binding measurements. These methods independently probe binding thermodynamics, surface interactions, thermophoretic behaviour, thermal stabilization and functional activity.

ITC provided the primary affinity determination (K_D = 0.22 ± 0.08 μM), in excellent agreement with the literature benchmark. Functional inhibition measured by the pyrene assay (EC_{50} = 0.610 ± 0.046 μM) independently supported the calorimetric results. Additionally, nanoDSF detected ligand-induced stabilization of G-actin (ΔT_m ≈ 4.3 °C), confirming complex formation. BLI revealed concentration-dependent binding with an apparent affinity of approximately 1 μM, but also measurable nonspecific background that limited quantitative interpretation. In contrast, MST failed to produce a reliable binding isotherm despite acceptable signal quality, illustrating that the absence of a measurable response in a single assay should not be interpreted as the absence of binding.

The study demonstrates that robust protein–ligand characterization requires convergence of orthogonal analytical methods rather than reliance on a single technique. Combining complementary biophysical assays enables discrimination between true molecular recognition and method-dependent artefacts, providing a transferable framework for affinity validation and quality assessment of biomolecular interactions.

ACKNOWLEDGEMENTS This work was financially supported by Selvita Ltd., Zagreb, Croatia.

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ON-SURFACE SELF-ASSEMBLY OF DIAMONDOID ESTERS

Marina Šekutor,[a] Nataša Burić,[a] Cosme González Ayani,[b] Tomislav Vuletić,[b] Margareta Sohora,[a] Zoran Štefanić,[c] Ida Delač[b]

[a] Department of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia, [b] Centre for Advanced Laser Techniques, Institute of Physics, Bijenička cesta 46, 10000 Zagreb, Croatia, [c] Department of Physical Chemistry, Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia
* msekutor@irb.hr

Spontaneous self-assembly of non-aromatic organics on carrier surfaces is still an underexplored area of nanomaterial design. For that purpose we have been exploring the on-surface deposits of diamondoids,[1] rigid saturated cage scaffolds, and we have found that such compounds are capable of forming highly ordered supramolecular systems on various substrates.[2–5]

Here we present a systematic characterization of diamondoid ester (Figure 1) self-assemblies on a highly oriented pyrolytic graphite (HOPG) that was achieved through a combination of experimental and computational tools.[6] AFM imaging afforded discernment of mosaic-like fused on-surface islands built up from molecular chain structures. Computational examination of the systems revealed the most stable molecular on-surface orientations, in which the ester carbonyls preferentially pointed towards the surface while retaining the highest possible system symmetry. An excellent data match between experimental and theoretical approaches was observed and we identified London dispersion interactions as a driving force for the observed molecular chain formation, that later led to more complex on-surface domains of noticeable structural periodicity. Our findings demonstrate the applicability of a bottom-up strategy for designing ordered non-aromatic supramolecular architectures on carrier surfaces.

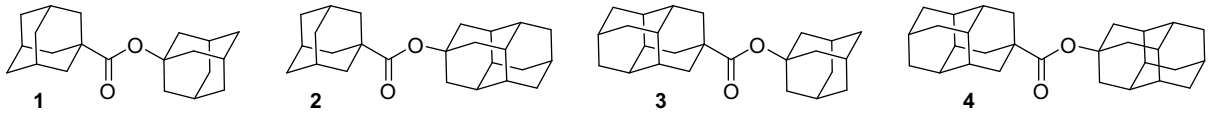


Figure 1. Structures of studied diamondoid esters.

ACKNOWLEDGEMENTS This work was supported by the Croatian Science Foundation under the project numbers HRZZ-UIP-2017-05-9653 and HRZZ-UIP-2020-02-8891.

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CHIRAL MESOGENIC DIMERS: FROM MOLECULAR DESIGN TO SELF-ASSEMBLY

Aleksandra Šimanović, Andreja Lesac
Department of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička cesta 54, Zagreb, Croatia
* asimanov@irb.hr

Liquid crystals are soft materials that combine the molecular order of crystalline solids with the fluidity of liquids, making them attractive for applications ranging from display technologies to advanced photonic devices. Their self-organization is highly sensitive to molecular structure and chirality, giving rise to a variety of mesophases with unique structural and optical properties. Among them, mesogenic dimers represent an important class of liquid crystalline materials owing to their conformational flexibility and rich mesomorphic behaviour.

In this work, a homologous series of chiral non-symmetric mesogenic dimers containing a cyanobiphenyl mesogenic unit and an (*S*)-3-aryl-3-hydroxypropanoate moiety as the source of chirality was synthesized. The effects of terminal alkyl chain length and enantiomeric excess on mesomorphic behaviour were investigated to establish structure–property relationships in these systems. Furthermore, the ability of the synthesized dimers to transfer chirality to structurally different achiral liquid crystal hosts was explored to gain insight into the mechanisms governing supramolecular organization.

The obtained results reveal that subtle variations in molecular structure and composition strongly influence the self-assembly and mesomorphic behaviour of these materials. The presentation will highlight unusual chiral phenomena, including the formation of Blue Phase III and temperature-induced helix inversion, and discuss their significance for understanding chirality transfer and self-assembly in liquid crystalline systems.

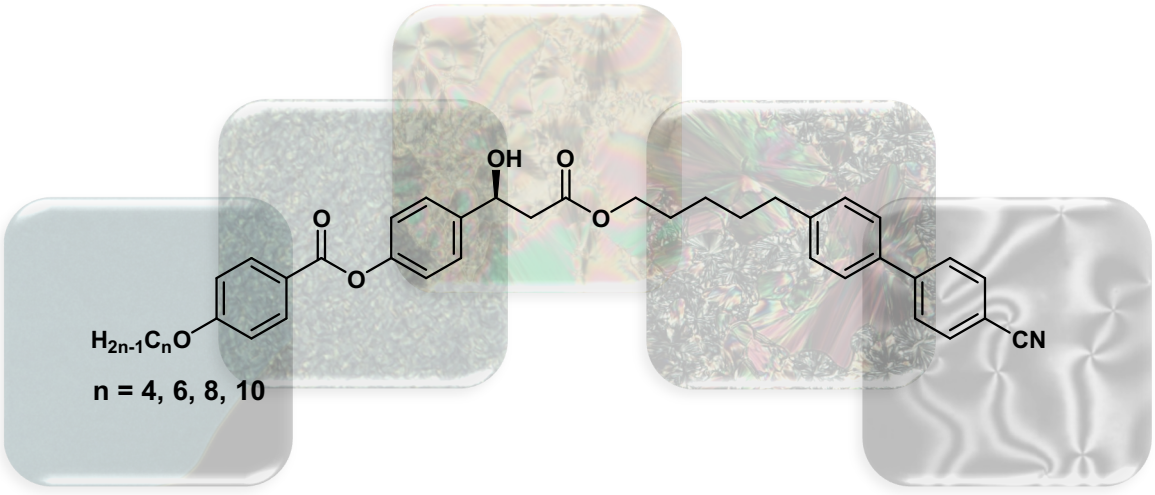


Figure 1. Molecular structure and the rich mesomorphic behaviour of the synthesized dimers.

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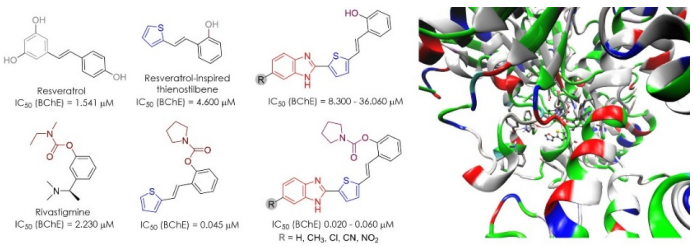
SYNTHESIS, COMPUTATIONAL STUDY, AND BIOLOGICAL ASSESSMENT OF NOVEL BENZIMIDAZOLE AND OXAZOLE DERIVATIVES OF PHENOLS AND CARBAMATES INCORPORATING DIARYLETHENE MOTIF

Irena Škorić,[a] Milena Mlakić,[a] Ilijana Odak,[b] Stanislava Talić,[b] Danijela Barić[c]

[a] Department of Organic chemistry, University of Zagreb Faculty of Chemical Engineering and Technology, Trg Marka Marulića 19, HR-10 000 Zagreb, Croatia, [b] Department of Chemistry, Faculty of Science and Education, University of Mostar, Matice Hrvatske bb, 88 000 Mostar, Bosnia and Herzegovina, [c] Group for Computational Life Sciences, Division of Physical Chemistry, Ruđer Bošković Institute, Bijenička cesta 54, HR-10 000 Zagreb, Croatia

* iskoric@fkit.unizg.hr

This study reports the design, synthesis, and biological evaluation of novel resveratrol-inspired thieno-benzimidazole and thieno-oxazole derivatives as potential therapeutics for Alzheimer's disease (AD). The research is grounded in the cholinergic hypothesis, which links cognitive decline to reduced acetylcholine levels due to enzymatic degradation by acetylcholinesterase (AChE) and butyrylcholinesterase (BChE).[1-3] Given the increasing relevance of BChE in later disease stages, the focus was placed on developing selective BChE inhibitors. A series of phenols and carbamates incorporating diarylethene motif was synthesized using multi-step organic reactions, including Wittig reactions, Vilsmeier formylation, and cyclization strategies. Structural confirmation was achieved through NMR and mass spectrometry. The studied compounds exhibit photochemical instability due to efficient trans–cis isomerization and subsequent secondary processes under UV irradiation, necessitating strict light protection during handling, storage, and application. Biological evaluation revealed that all compounds selectively inhibited BChE, with no significant AChE inhibition observed. Among them, carbamate derivatives exhibited much higher inhibition potency over hydroxy analogues, but all of them outperforming the reference drugs galantamine or rivastigmine. In addition to enzyme inhibition, antioxidant activity was assessed using the DPPH and CUPRAC assays. Some of the phenols exhibited very strong radical-scavenging activity, comparable to that of Trolox. Molecular docking and dynamics simulations provided insight into binding interactions, highlighting key π–π stacking and hydrogen bonding within the BChE active site. Overall, the study identifies promising multifunctional candidates combining selective BChE inhibition, antioxidant properties, and favorable safety profiles, supporting their potential as lead compounds for AD therapy.



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COMPUTATIONAL ANALYSIS OF POLYCYCLIC GUANIDINE DERIVATIVES

Petar Štrbac, Ian Horvat, Zoran Glasovac, Davor Margetić

Laboratory for physical-organic chemistry, Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička cesta 54

* pstrbac@irb.hr

Polycyclic guanidine derivatives constitute an important class of nitrogen-containing heterocycles with significant synthetic and potential biological relevance.[1,2] In this study, density functional theory (DFT) calculations were employed to investigate the structural and spectroscopic properties of a series of polycyclic guanidine adducts. The Diels-Alder cycloaddition reactions leading to the formation of the polycyclic guanidine adducts[3] were investigated computationally by locating transition states and calculating activation free energies and reaction energies. Conformational analysis was performed to identify the most stable molecular geometries at the selected stationary points along the reaction path.

These calculations provide insight into the energetics of the cyclization process and the factors governing the formation and stability of the resulting polycyclic systems. The optimized structures of polycyclic guanidines (Fig. 1) were subsequently used to calculate electronic absorption (UV–Vis) spectra using the PBE0 functional, allowing the relationship between molecular structure and spectroscopic properties to be established.

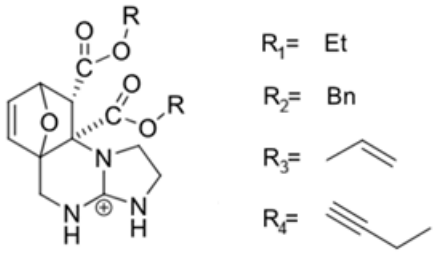


Figure 1. Structure of the polycyclic guanidines investigated in this work.

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DEFECT-DRIVEN SOLAR CO_2 CONVERSION IN CERIA-BASED HIGH-ENTROPY OXIDES

Dalibor Tatar,[a] Jakov Babić,[a] Stjepan Šarić,[a] Petra Šušak,[a] Jelena Kojčinović,[a] Anamarija Stanković,[a] Ronen Gottesman,[b] Doron Azulay,[c] Oded Millo,[d] Igor Djerdj[a]

[a] Department of Chemistry, University J. J. Strossmayer Osijek, Cara Hadrijana 8/A, 31000 Osijek, Croatia, [b] Institute of Chemistry, The Hebrew University of Jerusalem, Edmond J. Safra Campus, Givat Ram, 9190401 Jerusalem, Israel, [c] Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, Edmond J. Safra Campus, Givat Ram, 9190401 Jerusalem, Israel, [d] Department of Physics, Azrieli College of Engineering Jerusalem, POB 3566, 9103501 Jerusalem, Israel

* dtatar@kemija.unios.hr

Solar-driven conversion of CO_2 into useful chemicals has emerged as an attractive approach for reducing greenhouse gas emissions while simultaneously producing sustainable fuels. In this study, ceria-based high-entropy oxides (HEOs) containing Ce, Zr, La, Pr, and selected rare-earth elements (Y, Nd, or Sm) were synthesized and evaluated as visible-light photocatalysts for CO_2 conversion.[1] Structural characterization confirmed the formation of single-phase fluorite-type materials with a highly disordered lattice and abundant oxygen-deficient sites. Detailed spectroscopic analyses showed that the coexistence of Ce^{3+}/Ce^{4+} and Pr^{3+}/Pr^{4+} redox couples promote the formation of oxygen vacancies, improve charge separation, and enhance visible-light absorption. The presence of these defect sites had a major role in activating CO_2 molecules and suppressing electron-hole recombination during the photocatalytic process. Among the investigated materials, $Ce_{0.2}Zr_{0.2}La_{0.2}Pr_{0.2}Sm_{0.2}O_{2-\delta}$ (CZLPS) exhibited the best photocatalytic performance, achieving a CO_2 conversion of 20.3% under visible-light irradiation, significantly higher than pure CeO_2. The reaction mainly produced CO, accompanied by smaller amounts of CH_4 and CH_3OH. Density functional theory calculations revealed that Zr sites provide the most favorable adsorption and activation centers for CO_2 reduction, while oxygen vacancies facilitate electron transfer and stabilize reaction intermediates. The improved catalytic activity was therefore attributed to the combined effects of configurational entropy, lattice defects, and multivalent rare-earth cations.

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METALLOSUPRAMOLECULAR ISOMERISM AND POLYMORPHISM IN NICOTINOYLHYDRAZONATO VANADIUM COMPLEXES

Edi Topić, Josipa Sarjanović, Dino Kuzman, Andrea Cocut, Tomica Hrenar, Jana Pisk, Višnja Vrdoljak

University of Zagreb Faculty of Science, Department of Chemistry, Horvatovac 102A, 10000 Zagreb, Croatia
*edi.topic@chem.pmf.unizg.hr

Coordination-driven self-assembly of vanadium(V) with *o*-vanillin nicotinoylhydrazone (H_2VanNH) was investigated to establish how auxiliary alkoxides and crystallization conditions control nuclearity and solid state form. Reactions in C_1-C_5 alcohols afforded tetranuclear metallacycles $[VO(VanNH)(OR)]_4$ and one-dimensional polymers $[VO(VanNH)(OR)]_n$. Single-crystal X-ray diffraction identified supramolecular isomers and polymorphs that fall into three types according to pyridyl orientation: alternating *syn*/*anti* (I), all-*anti* (II), and all-*syn* (III). Two *n*-pentoxide tetramer polymorphs show a rare reversible temperature-dependent transformation.

Density-functional calculations showed that alternating *syn*/*anti* chains are thermodynamically preferred across the alkoxide series because of more exothermic binding enthalpies. All-*anti* chains gain relative stability with longer alkoxides, while cyclic tetramers receive modest stabilization, demonstrating how electronic, steric, and crystal-packing effects direct assembly.

Catalytic oxidation of 4-chloro- and 4-nitrobenzyl alcohols with aqueous *t*-butyl hydroperoxide exposed a nuclearity-dependent activity-selectivity tradeoff. Polymeric propoxide and butoxide systems gave the highest conversions (up to 79% and 87% after 120 min for the chloro and nitro substrates, respectively) but progressively lost aldehyde selectivity. Tetranuclear propoxide complex reached 88% conversion and the highest initial TOF for 4-nitrobenzyl alcohol, whereas *n*-pentoxide tetramer gave 35% conversion with >91% selectivity. Alkoxide chain length and steric bulk therefore provide practical handles for tuning vanadium oxidation catalysts.[1]

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BIO-BASED COATINGS FOR FLAME RETARDANCY AND UV PROTECTION OF COTTON AND NYCO FABRICS

Karlo Vojtkuf,[a] Helena Biljanić,[a] Jelena Kosanović,[a] Lea Botteri,[b] Marijan Marciuš,[a] Katarina Marušić,[a] Nives Matijaković Mlinarić[a]

[a]Division of Materials Chemistry, Ruđer Bošković Institute, Bijenička cesta 54, Zagreb, Croatia,
[b]Department of Textile Chemistry and Ecology, University of Zagreb, Faculty of Textile Technology, Prilaz baruna Filipovića 28a, Zagreb, Croatia
* kavojtkuf@irb.hr

Protective textiles must combine fire safety with additional functions such as UV protection, while retaining the comfort and mechanical performance of the underlying fabric. Cotton and nylon/cotton (NyCo) blends are attractive for these applications but are inherently flammable. In NyCo, combustion may be further promoted by the scaffolding effect, in which molten nylon is retained by the cotton-derived char.[1] Surface coatings provide an effective approach to localising protective components at the fibre interface, where ignition and flame propagation occur, while preserving the bulk properties of the textile.[2] Phytic acid (PA) and tannic acid (TA) provide complementary bio-based functionalities: phosphorus-rich PA promotes acid-catalysed dehydration and char formation, whereas polyphenolic TA acts as a carbon source and UV-absorbing agent and can participate in coordination with metal ions.[3] In this study, cotton and NyCo fabrics were functionalised with a PA/TA coating coordinated with Zn^{2+} and Y^{3+} ions.

The surface morphology and elemental composition of the treated fabrics were characterised by scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM-EDS). Flame-retardant performance was evaluated using limiting oxygen index (LOI) measurements and horizontal and vertical flame tests, while UV-protective performance was assessed by determining the ultraviolet protection factor (UPF) and UVA and UVB transmittance.

The treatment increased the LOI from 17.4 to 28.6% for cotton and from 17.8 to 26.8% for NyCo. SEM-EDS showed surface deposits on both substrates and the spatial distribution of Zn and Y atoms across the treated fibres. The UPF increased from 1.32 to 17.83 for cotton and from 11.78 to 23.25 for NyCo, accompanied by pronounced reductions in UVA and UVB transmittance. These findings demonstrate that the developed PA/TA-Zn/Y coating strategy provides an effective multifunctional surface treatment for cotton and NyCo fabrics, combining improved flame-retardant behaviour with enhanced UV protection.

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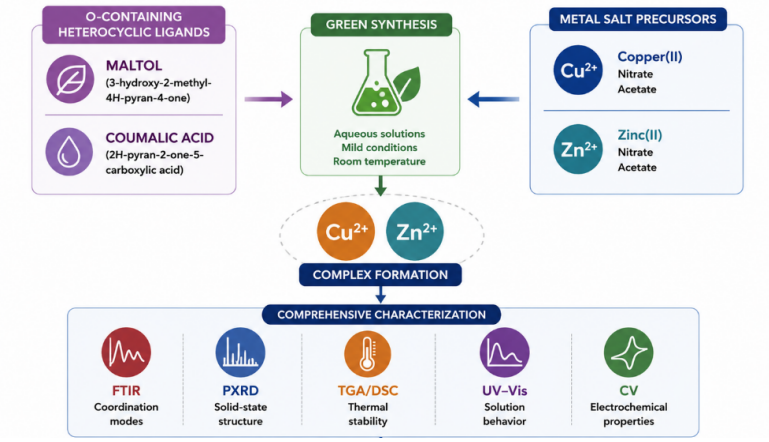
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COORDINATION BEHAVIOR OF TRANSITION METAL IONS WITH *O*-CONTAINING HETEROCYCLIC LIGANDS

Gala Bereš,* Tea Kozić, Anamarija Stanković, Tomislav Balić, Nikolina Filipović,*

Department of Chemistry, University of Osijek, Ulica cara Hadrijana 8/A, 31 000, Osijek
* nfilipovic@kemija.unios.hr

Oxygen-containing heterocyclic compounds are versatile ligands capable of coordinating metal ions through hydroxyl, carbonyl, and carboxylate donor groups. Their structural diversity and ability to form stable coordination compounds make them attractive systems for studying metal–ligand interactions and structure–property relationships.[1] In this work, the coordination behavior of two *O*-containing heterocyclic ligands, maltol (3-hydroxy-2-methyl-4*H*-pyran-4-one) and coumalic acid (2*H*-pyran-2-one-5-carboxylic acid), toward transition metal ions was investigated. Copper(II) and zinc(II) complexes were synthesized from nitrate and acetate precursors under mild aqueous conditions. The resulting products were characterized using Fourier transform infrared spectroscopy (FT-IR), powder X-ray diffraction (PXRD), thermogravimetric and differential scanning calorimetry (TGA/DSC), and UV–Vis spectroscopy. These techniques provided insight into coordination modes, structural organization, thermal stability, and solution behavior of the synthesized compounds. The obtained results confirmed successful complex formation in all investigated systems. For Cu(II)–maltol complexes, coordination occurs through hydroxyl and carbonyl groups, leading to the formation of stable *O*,*O*-chelate structures. In Zn(II)–coumalate complexes, coordination primarily involves the deprotonated carboxylate group, with possible participation of the lactone carbonyl oxygen. Spectroscopic and thermal analyses indicate the formation of structurally well-defined coordination compounds with characteristic physicochemical properties. The study demonstrates the versatility of *O*-containing heterocyclic ligands in stabilizing transition metal ions through different coordination modes. Furthermore, the results highlight the influence of ligand functionality on coordination behavior and structural organization, providing additional insight into the chemistry of oxygen-donor ligands and their coordination compounds.



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A RADIATION BASED APPROACH TO DEVELOPING FUNCTIONAL COATINGS FOR MILITARY TEXTILES

Helena Biljanić, Karlo Vojtkuf, Jelena Kosanović, Katarina Marušić, Nives Matijaković Mlinarić

Division of Materials Chemistry, Ruđer Bošković Institute, Bijenička cesta 54, Zagreb, Croatia
* hbachroj@irb.hr

Ionizing gamma irradiation is a well-established technique for textile activation, generating free radicals both within the fiber bulk and its surface. These radicals break existing chemical bonds and introduce reactive functional groups, which serve as anchor points for the covalent attachment of various compounds to the fiber surface without resorting to aggressive chemical treatments. The procedure takes place at room temperature and avoids the use of toxic reagents, positioning it as an energy-efficient and ecologically favorable route to textile functionalization. In recent years, naturally derived polyphenolic acids have gained considerable interest as functional agents for textile finishing. Phytic acid, a non-toxic and readily biodegradable compound, displays notable flame-retardant capacity attributed to its elevated phosphorus content and its role in promoting char development. Tannic acid, on the other hand, functions as an efficient UV-absorbing agent and demonstrates antimicrobial activity, thereby improving both the protective and hygienic qualities of treated fabrics. Coupling gamma irradiation with polyphenolic acids offers a pathway toward multifunctional textiles that combine enhanced durability, improved safety profiles, and greater sustainability, meeting the demanding requirements of military use.

This study introduces a novel strategy for functionalizing a range of textile substrates (cotton, nylon, polyester, and nylon-cotton blend) through gamma irradiation, assisted by tannic acid complexed with iron ions and phytic acid. Irradiation was performed across a range of doses and conditions. Functionalization was achieved through a one-pot synthesis as well as a layer-by-layer deposition approach. Color properties were assessed via colorimetric analysis and visual inspection of coloration intensity. Surface wettability was characterized by water contact angle measurements, and elemental distribution and coating uniformity were verified through energy-dispersive X-ray spectroscopy. The findings reveal that both irradiation dose and treatment conditions exert a significant influence on coating adhesion to the textile surface. The radiation-assisted procedure produced a homogeneous elemental distribution across the fabric surfaces and induced measurable changes in surface properties.

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FATTY ACID NANOCOATINGS: A RADIATION-CROSSLINKING APPROACH TO IMPLANT SURFACE ENGINEERING

Helena Biljanić,[a]* James Mcfarlane Hoad,[b] Atiđa Selmani,[b] Eva Roblegg,[b] Katarina Marušić[a]

[a] Division of Materials Chemistry, Ruđer Bošković Institute, Bijenička cesta 54, Zagreb, Croatia, [b] Institute of Pharmaceutical Sciences, University of Graz, Universitatplatz 1, Graz, Austria

* hbachroj@irb.hr

Biomedical stainless steel is a widely used material for orthopedic and vascular implants, valued for its mechanical strength and established biocompatibility. However, its susceptibility to corrosion in physiological environments remains a challenge for long-term implant reliability. Therefore, surface functionalization with durable, biocompatible coatings is required to improve corrosion resistance without altering bulk properties. Fatty acids can form self-assembled monolayers (SAMs) on metal surfaces, providing a hydrophobic barrier that results in only limited improvement in corrosion resistance. High-energy ionizing radiation can induce intermolecular crosslinking within these monolayers, transforming SAMs into more robust polymer nanocoatings (PNCs) via radical polymerization.

This study investigates fatty-acid SAMs and radiation-crosslinked PNCs as a surface-functionalization strategy to enhance the corrosion resistance of SS316L stainless steel. SAMs were prepared from various fatty acids on SS316L surfaces and subsequently irradiated to convert them into crosslinked PNCs. Their electrochemical performance was evaluated using electrochemical impedance spectroscopy and potentiodynamic polarization with Tafel extrapolation. Biocompatibility was evaluated via direct contact assays using the human endothelial cell line Ea.hy926, in accordance with ISO 10993-5 standard.

The results demonstrate that radiation-crosslinked fatty acid-based PNCs provide significant enhancement in corrosion resistance compared to untreated surfaces while maintaining excellent cytocompatibility. This approach presents a versatile and environmentally friendly route for engineering durable, biocompatible surface modifications for the next generation of biomedical implants.

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CD26 DEFICIENCY DIFFERENTIALLY MODULATES PYY AND SUBSTANCE P SIGNALING IN EXPERIMENTAL COLITIS

Sunčica Buljević,[a] Iva Vukelić,[a] Sara Borovac,[b] Gabriela Petrić,[b] Lea Lukšić,[a] Dijana Detel[a]

[a] Department of Medical Chemistry, Biochemistry and Clinical Chemistry, Faculty of Medicine, University of Rijeka, Rijeka, Croatia, [b] Faculty of Medicine, University of Rijeka, Rijeka, Croatia
* suncica.buljevic@uniri.hr

CD26 (dipeptidyl peptidase 4; DPP4) is a multifunctional serine protease that regulates the biological activity of numerous peptide substrates through N-terminal cleavage.[1] Among its physiologically relevant targets are the neuropeptides peptide YY (PYY) and substance P (SP), whose receptor interactions and downstream signaling are altered following DPP4-mediated processing.[2] However, the contribution of CD26 to neuropeptide-dependent signaling in inflammatory conditions remains incompletely understood.

The present study investigated the impact of CD26 deficiency on the PYY–Y1R/Y2R–EGFR–ERK and SP–NK-1R–TGF-β/SMAD signaling pathways in a TNBS-induced murine model of Crohn's-like colitis. Male C57BL/6 and $CD26^{-/-}$ mice received intrarectal TNBS and were sacrificed during the acute (day 2) and resolution (day 7) phases. Gene expression, protein abundance, and peptide concentrations were assessed using quantitative PCR, Western blotting, immunohistochemistry, ELISA, and enzymatic activity assays.

CD26 deficiency resulted in preferential engagement of Y1R over Y2R signaling, accompanied by sustained ERK activation and enhanced EGFR expression independent of PKCα. In parallel, CD26-deficient animals exhibited increased NK-1R protein expression, elevated TGF-β receptor 2 abundance, and enhanced SMAD2/3 phosphorylation despite increased SMAD7 expression. Furthermore, DPP4 activity was markedly reduced during colitis without corresponding changes in DPP4 transcription, indicating predominantly post-transcriptional regulation.

Our findings demonstrate that CD26-dependent proteolytic processing critically influences neuropeptide receptor selection and downstream signaling. The results provide novel insights into the role of DPP4 as a regulator of peptide-mediated communication and highlight neuropeptide–receptor interactions as important modulators of intracellular signaling networks.

Keywords: CD26/DPP4, peptide YY, substance P, neuropeptides, receptor signaling, EGFR

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SYNTHESIS OF CATIONIC AB_3 *MESO*-(4-(*N*,*N*-DIETHYLAMINO)PHENYL)PORPHYRINS AS PHOTOSENSITIZERS FOR PHOTODYNAMIC THERAPY

Melisa Ciglarić, Martina Mušković Lukić, Nela Malatesti*
Faculty of Biotechnology and Drug Development, University of Rijeka, Rijeka, Radmile Matejčić 2, Croatia
* melisa.ciglaric@biotech.uniri.hr, martina.muskovic@biotech.uniri.hr, nela.malatesti@biotech.uniri.hr

Photodynamic therapy (PDT) is a minimally invasive therapeutic approach that combines a photosensitizer, light of an appropriate wavelength, and molecular oxygen to generate reactive oxygen species, primarily singlet oxygen, which induce localized oxidative damage and selective cell death. Porphyrins are among the most studied photosensitizers due to their strong visible absorption, high singlet oxygen generation efficiency, and tuneable structure. The development of novel porphyrin derivatives with optimized amphiphilic properties remains important for improving cellular uptake and photodynamic efficiency.[1]

Previous research has shown that increasing porphyrin lipophilicity through long alkyl chains significantly influences cellular uptake and photodynamic activity. In our earlier work, *N*-methylated tricationic pyridinium porphyrins bearing C14 and C18 alkyl chains exhibited distinct biological activities against melanoma cell lines, with the C14 derivative showing pronounced tumor selectivity and the C18 analogue the highest overall cytotoxicity.[2] Building on these findings, the present study explores amphiphilic porphyrins in which pyridyl substituents are replaced with *N*,*N*-diethylaniline moieties while retaining C14 and C18 alkyl chains, to assess the effect of peripheral substituents on physicochemical and photophysical properties.

In this work, our aim was to synthesize AB_3 porphyrins bearing three *N*,*N*-diethylaniline and one 4-acetamidophenyl substituent *via* the Adler–Longo condensation. Hydrolysis of the acetamido group afforded the corresponding amino derivative, which was subsequently functionalized by nucleophilic acyl substitution using tetradecanoyl chloride ($C_{13}H_{27}COCl$) and octadecanoyl chloride ($C_{17}H_{35}COCl$) to introduce C14 and C18 alkyl chains, respectively. Finally, *N*-methylation with methyl iodide yielded the corresponding quaternized amphiphilic porphyrin derivatives.

The structures of all newly synthesized compounds were confirmed by ^{1}H NMR, ^{13}C NMR, and high-resolution mass spectrometry (HRMS). Their photophysical properties were investigated by UV–Vis absorption and fluorescence spectroscopy to evaluate the effect of structural modifications and alkyl chain length on their absorption and emission characteristics. The results provide insight into the relationship between molecular structure and photophysical behavior, supporting the rational design of porphyrin-based photosensitizers. Preliminary in vitro MTT assay results on melanoma and non-tumor cell lines will also be presented to provide an initial assessment of biological activity.

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THE IMPACT OF TOURISM SEASONALITY ON THE DESIGN AND OPERATIONAL MANAGEMENT OF A BIOREACTOR SYSTEM FOR BIOWASTE TREATMENT: A CASE STUDY OF ISTRIA COUNTY

Tomislav Domanovac,[a] Dajana Kučić Grgić,[b] Monika Šabić Runjavec,[b] Marija Vuković Domanovac[b]

[a] IPZ Uniprojekt TERRA, Voćarska cesta 68, HR-10000 Zagreb, [b] University of Zagreb Faculty of Chemical Engineering and Technology, Trg Marka Marulića 19, HR-10000 Zagreb
* tomislav@ipz-uniprojekt.hr

Biowaste accounts for a significant share of total biodegradable waste in the Republic of Croatia. In regions with developed tourism, such as Istria County, which records over 26 million overnight stays per year, waste treatment systems must be designed to withstand extreme seasonal fluctuations. The aim of this work is to analyse the dynamics of biowaste generation and define optimal operating parameters for the bioreactor to achieve process stability.[1]

The analysis uses data from 2019, assuming that about 55% of total kitchen biowaste generated by households is collected for processing. An estimated annual volume of 9,519 tonnes, including food and green waste, was processed at a fixed density of 0.609 t/m^3.[2] A bioreactor system (7.0 × 3.5 × 3.5 m) was designed with the key criterion that the filling time of an individual unit should be between 1 and 2 days.[3]

The research identified pronounced seasonality, with volumes ranging from 547 t/month in January to 947 t/month in July. To cover the peak summer load, a capacity of 19 bioreactors is required which, with a filling height of 2.50 m, ensures a filling time of 1.4 days per unit. Off-season operating options were analysed, including running all 19 bioreactors at a lower filling height and intensive use of 14 bioreactors while maintaining the standard filling height.

The strategy of intensive use of 14 bioreactors in the off-season (with a filling time of 1.3 days) proved more effective for maintaining stable biological processes. The remaining five bioreactors are recommended as operational reserve or for regular system maintenance. This management model enables high flexibility and efficiency of the system despite variations in incoming waste volumes.

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FOOD INDUSTRY BY-PRODUCT ASH AS A GREEN CATALYST IN THE SYNTHESIS OF ACETYLSALICYLIC ACID

Dajana Gašo-Sokač, Valentina Bušić, Dora Zobundžija, Anamarija Bilavčić

Josip Juraj Strossmayer University of Osijek, Faculty of Food Technology Osijek, Franje Kuhača 18, Osijek, Croatia
* dajana.gaso@ptfos.hr

Green chemistry aims to develop more sustainable and environmentally friendly chemical processes by reducing waste, minimising the use of toxic substances, and lowering the consumption of hazardous reagents, with particular emphasis on identifying alternative catalysts and raw materials derived from renewable sources. In organic synthesis, catalysts that are toxic, flammable, or corrosive are often used. Numerous studies show that by-products from the food industry can serve as a sustainable alternative to such catalysts. This study investigates the use of ash from a by-product of oil production technology as a substitute for phosphoric acid in esterification reactions. Ash samples obtained from residues of cold-pressed oil production were tested and compared using the following raw materials: camelina seed (*Camelina sativa*), apricot kernel (*Prunus armeniaca*), and coconut (*Cocos nucifera*). It is hypothesised that the metals present in the ash act as Lewis acids, thereby enabling catalysis of the reaction. Acetylsalicylic acid was synthesised from salicylic acid and acetic anhydride with the addition of 20 mg of the catalyst at a reaction temperature of 80–100 °C, yielding products in the range of 30–59%. The results confirm that ash catalyses the esterification reaction, offering a low-cost, bio-based alternative to conventional mineral acid catalysts. Overall, these findings highlight the potential of oil-industry ash as a sustainable catalytic material, supporting the valorisation of food-industry waste in line with the principles of green chemistry.

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CONTROLLING PRODUCT DISTRIBUTION IN ADLER-LONGO CONDENSATION VIA UPLC-GUIDED OPTIMIZATION

Dora Grgurić,[a,b,*] Martina Mušković Lukić,[b] Nela Malatesti[b]

[a] Research and Development, Pliva Croatia, Prilaz Baruna Filipovića 25, Zagreb, Croatia, [b] Faculty of Biotechnology and Drug Development, University of Rijeka, Radmile Matejčić 2, Rijeka, Croatia
* dora.grguric@pliva.com

Photodynamic therapy (PDT) is an emerging anticancer treatment that relies on three individually non-toxic components: a photosensitizer (PS), light irradiation, and oxygen.[1] Among PSs, porphyrins represent the largest class investigated in preclinical and clinical studies, including several compounds approved for PDT.[2] The Adler–Longo condensation is a widely used method for porphyrin synthesis; however, the resulting complex reaction mixtures often complicate product isolation and lead to low yields. Differentially functionalized porphyrins are commonly prepared using two different aldehydes, but these reactions can generate up to six porphyrin products. In this study, an ultra-performance liquid chromatography (UPLC) method was developed to monitor and optimize reaction conditions for the synthesis of new *cis*- and *trans*-A_2B_2 pyridylporphyrins (Figure 1.).

The UPLC method employed a multi-step gradient of 0.1% formic acid and acetonitrile on an Acquity UPLC HSS T3 column (1.8 µm, 2.1 × 100 mm), with UV detection at 420 nm. The developed method enabled the separation of all six porphyrins formed during the Adler–Longo condensation and was subsequently applied to reaction optimization studies. The optimized analytical approach allowed rapid evaluation of reaction parameters and identification of conditions that increased the relative abundance (Area %) of the desired *cis*- and *trans*-A_2B_2 pyridylporphyrins in the reaction mixture. The developed UPLC method therefore represents a valuable tool for monitoring porphyrin synthesis and facilitating reaction optimization.

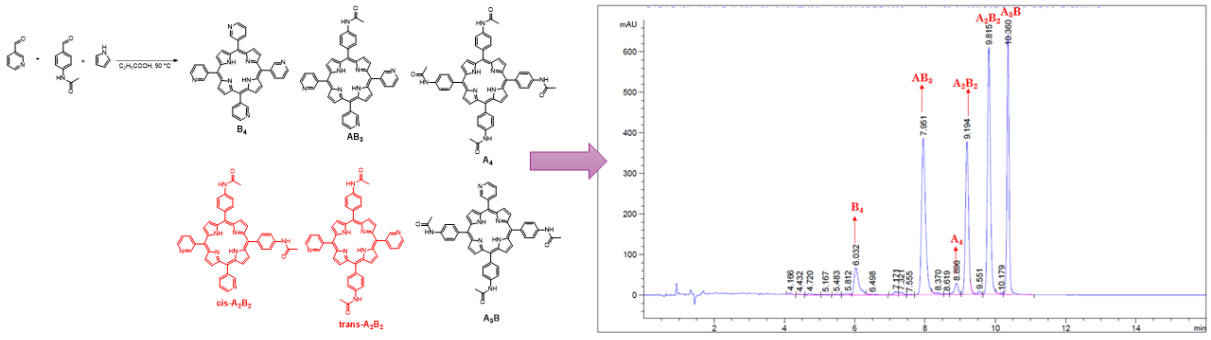


Figure 1. Experimental workflow for UPLC-guided optimization of the Adler–Longo condensation. Synthesis of *cis*- and *trans*-A_2B_2 pyridylporphyrins (left). Representative chromatogram showing separation of porphyrin products (right).

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PHYTOCHEMICAL CHARACTERIZATION AND BIOACTIVE POTENTIAL OF DEEP EUTECTIC SOLVENT EXTRACTS FROM CHAMOMILE WASTE

Martina Jakovljević Kovač,[a] Mario Komar,[a] Maja Karnaš Babić,[b] Ema Pavičić,[a] Mia Gotal,[a] Maja Molnar,[a] Stela Jokić,[a] Jelena Vladić[c]

[a] Josip Juraj Strossmayer University of Osijek, Faculty of Food Technology Osijek, Franje Kuhača 18, 31000 Osijek, Croatia, [b] Josip Juraj Strossmayer University of Osijek, Faculty of Agrobiotechnical Sciences, Vladimira Preloga 1, 31000 Osijek, Croatia, [c] NOVA University Lisbon, NOVA School of Science and Technology, Department of Chemistry, Campus de Caparica, 2829-516 Caparica, Portugal

* mjakovljevic@ptfos.hr

Chamomile herbal dust, a by-product of chamomile processing, represents a valuable source of bioactive compounds that can be recovered using sustainable extraction approaches.[1] This study evaluated the suitability of five deep eutectic solvents (DESs) for the extraction of bioactive compounds from chamomile herbal dust using either ultrasound-assisted extraction with an ultrasonic probe or conventional extraction by magnetic stirring at 40 and 60 °C. The extracts were characterized by determining apigenin content using HPLC, total phenolic content (TPC) by the Folin–Ciocalteu method, total flavonoid content (TFC) using the $AlCl_3$ assay, and antiradical activity using DPPH and ABTS assays.

The extraction efficiency depended on both the DES composition and the extraction technique. Overall, ultrasound-assisted extraction provided the highest recovery of bioactive compounds and antioxidant activity, while extraction at 60 °C generally outperformed extraction at 40 °C when magnetic stirring was applied. The highest apigenin content (3.25 ± 0.15 mg g^{-1} plant material) was achieved using the malic acid:betaine:water (1:2:3) in combination with ultrasound-assisted extraction. In contrast, the lactic acid:proline (2:1) yielded the highest total phenolic and total flavonoid contents, as well as the strongest DPPH and ABTS radical scavenging activities when ultrasound-assisted extraction was employed. Correlation analysis revealed a strong positive relationship between apigenin and ABTS values (r = 0.91), as well as between apigenin and total flavonoid content (r = 0.85), suggesting that flavonoids, including apigenin, substantially contribute to the antioxidant potential of the extracts.

These findings demonstrate that the extraction performance of DESs is highly dependent on both solvent composition and extraction technique. The possibility of tailoring DES composition according to the target compounds highlights their considerable potential as sustainable and versatile extraction media for the valorization of chamomile processing by-products.

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MECHANOCHEMICAL ANION EXCHANGE FOR TAILORING IMIDAZOLIUM-BASED CATIONIC AMPHIPHILES

Aleksandar Čeke Trišler,[a] Nikolina Filipović,[a] Hanna Zhukouskaya,[b,c] Martin Hrubý,[b] Jiří Pánek,[b] Nikola Sakač,[d] Dean Marković,[e] Brunislav Matasović,[a] Marija Jozanović[a]*

[a] Department of Chemistry, Josip Juraj Strossmayer University of Osijek, Cara Hadrijana 8, 31000 Osijek, Croatia, [b] Institute of Macromolecular Chemistry, Czech Academy of Sciences, Heyrovského náměstí 2, 162 00 Prague 6, Czech Republic, [c] Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University, Hlavova 8, 128 43 Prague, Czech Republic, [d] Faculty of Geotechnical Engineering, University of Zagreb, Hallerova 7, 42000 Varaždin, Croatia, [e] Department of Biotechnology, University of Rijeka, Radmile Matejčić 2, 51000 Rijeka, Croatia

* mjozanovic@kemija.unios.hr

Cationic amphiphiles based on quaternary ammonium compounds (QACs) represent a versatile class of compounds whose physicochemical properties can be tailored through modification of both cationic and anionic components.[1] Their combination of a permanently charged group and hydrophobic moieties makes them attractive for applications requiring surface activity and potential biological activity.

In this study, imidazolium-based QACs were first synthesized by conventional quaternization of imidazole derivatives with appropriate alkyl halides. The obtained salts were subsequently subjected to anion exchange with sodium tetraphenylborate using a mechanochemical approach. The anion-exchange reactions were performed in a planetary ball mill under solvent-free conditions, providing a more sustainable alternative to conventional solution-based metathesis. Mechanochemical approaches have been successfully applied to ion-exchange reactions, demonstrating their potential for solvent-free modification of ionic systems.[2]

The synthesized compounds were characterized by nuclear magnetic resonance (NMR) and infrared (IR) spectroscopy, mass spectrometry (MS), and X-ray diffraction (XRD). The analytical data confirmed the formation of the targeted compounds and structural changes associated with quaternization and subsequent anion exchange. Modification of the counterion provides an additional strategy for tuning the ionic, structural, and amphiphilic properties of imidazolium-based QACs.

The results demonstrate that combining conventional quaternization with mechanochemical anion exchange represents an efficient approach for the synthesis and structural modification of cationic amphiphiles. Their tunable properties make these compounds promising candidates for further investigation as surface-active materials and in electrochemical, catalytic, and antimicrobial applications.

ACKNOWLEDGEMENTS This work was supported by the Ministry of Education, Youth and Sports of the Czech Republic, under the project 'Polymer 2D-orthogonal sensors with highly chemoselective responses to micropollutants' (grant INTER-COST-LUC25 No. LUC25093, PolyChemSens.

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TRIPHENYLPHOSPHINES AND PYRIDINES AS LEAVING GROUPS IN SOLVOLYTIC REACTION

Sandra Jurić

University of Zagreb, Faculty of Pharmacy and Biochemistry, Zagreb, Croatia
* sandra.juric@pharma.unizg.hr

The leaving group abilities (nucleofugalities) of triphenylphosphine (Ph_3P) have been derived from the S_N1 solvolysis rate constants of the corresponding ferrocenyl-X-phenylmethyltriphenylphosphonium salts by applying the *Linear Free Energy Relationship* (*LFER*) equation: log *k* (25 ºC) = s_f (E_f + N_f)[1,2] and compared with leaving group abilities of pyridines.[3–5] In this work a series of ferrocenylphenylmethyltriphenylphosphonium salts, which were prepared from corresponding ferrocenylphenylmethanol were subjected to solvolysis in variety of hydroxylic solvents and aqueous mixture. The solvolysis rates were measured titrimetrically at 25°C. The rate constants of some triphenylphosphonium salts were measured for at least three different lower temperatures and extrapolated to 25°C by using the Eyring plot. The logarithms of the first-order rate constants in the given solvents were plotted against E_f for the corresponding ferrocenylphenymethyl cations and nucleofugality parameters (N_f and s_f) for triphenylphosphine in variety of hydroxylic solvents and aqueous mixture were derived. According to *LFER* equation N_f is the negative intercept on the abscissa, whereas s_f is the slope of the log *k* versus E_f plot. E_f is the electrofugality parameter of the corresponding ferrocenylphenylmethyl cations determined earlier.[6] All plots of log *k* against E_f for ferrocenylphenylmethyltriphenylphosphonium ions resulted in linear correlations with correlation coefficients R > 0.998. The reasonably good log *k* versus E_f correlation makes it possible to relate the leaving group ability of triphenylphosphines to leaving group ability of other neutral leaving groups (pyridines). Knowing that the difference in N_f of one unit corresponds approximately to a reactivity difference in an order of magnitude, triphenylphosphine are less reactive leaving group than 4-methoxypyridine for about an order of magnitude of one, less reactive than pyridine by about an order of magnitude of three, and less reactive than 4-chloropyridine for about an order of magnitude of five. The N_f values for 4-methoxypyridine and tris(4-chlorophenyl)phosphine are the same in 80% aqueous acetonitrile while N_f value for 4-methoxypyridine is slightly higher than N_f value for tris(4-chlorophenyl)phosphine in 80% aqueous acetone. Tris(4-methoxyphenyl)phosphine is less reactive than 4-methoxypyridine for about an order of magnitude of two. Therefore, pyridine is a better leaving group than triphenylphosphine which is strong bulky nucleophile which forms highly basic conjugate base. According to N_f values of triphenylphosphine obtained in this work, now it is easy to predict that any substrate with a nucleofuge structure equivalent to triphenylphosphine is stable at ambient temperature to be handled safely in given solvent mixtures, regardless of the electrofuge moiety. For example, 4-methoxybenzhydryltriphenylphosphonium salt which is the combination of moderate electrofuge (E_f = -2.09) and a very weak nucleofuge is stable compound, whose half-live of reaction in various solvent is about 1 year, while the half-live of reaction of 4-methoxybenzhydrylpyridinium salt which is the combination of moderate electrofuge and moderate nucleofuge is about 40 hours.

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

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ENANTIOSELECTIVE OXIDATION AND CHIRAL CHROMATOGRAPHIC PROFILING OF SULFOXIDES FOR CHIRAL BIOANALYSIS

Rusudan Kakava, Mariam Sikharulidze, Khatia Chagalidze, Gabriel Sarishvili, Bezhan Chankvetadze

Institute of Physical and Analytical Chemistry, School of Exact and Natural Sciences, Ivane Javakhishvili Tbilisi State University, Tbilisi, Georgia
rusudan.kakava@tsu.ge

Chiral sulfoxides are valuable motifs in organic synthesis, medicinal chemistry, and pharmaceutical research. The present study addresses a central methodological challenge in biochirality research: how to control, monitor, and analytically resolve stereochemical outcomes in small chiral molecules. A series of aryl sulfides bearing electron-donating and electron-withdrawing substituents at different aromatic positions was subjected to enantioselective oxidation in order to evaluate the influence of substrate electronics and substitution pattern on reactivity and stereochemical induction.[1]
Preliminary experiments indicate that suppression of non-selective background oxidation and optimization of the Ti:DET ratio are important for maintaining enantiomeric enrichment. Use of opposite diethyl tartrate enantiomers, *R*,*R*-DET and *S*,*S*-DET, in separate catalyst-complex formation experiments led to a reversal of enantioselectivity, with the opposite sulfoxide enantiomer becoming predominant in each case. The products are profiled by chiral HPLC on polysaccharide-based chiral stationary phases to determine enantiomeric excess and evaluate structure-selector relationships. Presented as an ongoing methodological project rather than a fully completed study, this work invites discussion on improving catalyst assembly, asymmetric oxidation conditions, and chromatographic strategies for reliable profiling of small chiral molecules relevant to biochirality research.

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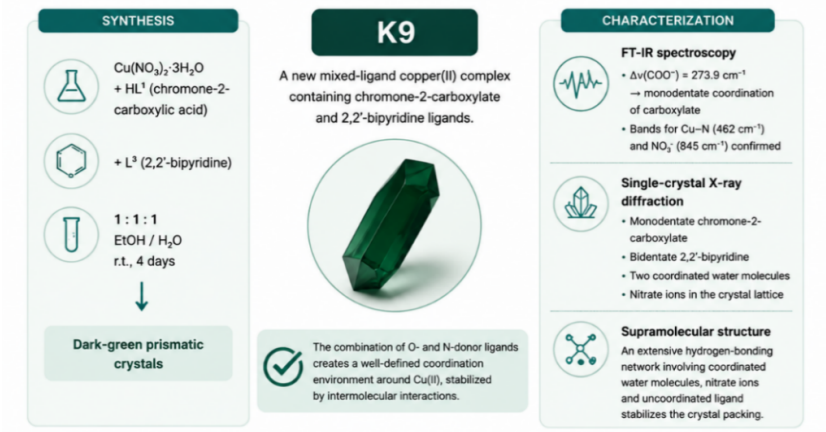
SYNTHESIS AND CRYSTAL STRUCTURE OF A TERNARY COPPER(II) COMPLEX CONTAINING CHROMONE-2-CARBOXYLATE AND 2,2'-BIPYRIDINE

Tea Kozić,* Gala Bereš, Anamarija Stanković, Tomislav Balić, Nikolina Filipović,*

Department of Chemistry, University of Osijek, Ulica cara Hadrijana 8/A, 31 000, Osijek

* tkozic@kemija.unios.hr

Ternary copper(II) complexes containing O- and N-donor ligands attract considerable attention due to their structural diversity and potential applications in coordination, catalytic, and medicinal chemistry. In particular, chromone-derived ligands are of interest due to their versatile coordination modes and ability to participate in supramolecular interactions. In this work, a novel ternary copper(II) complex, K9, containing chromone-2-carboxylate (HL1) and 2,2'-bipyridine (L3) ligands, was synthesized from copper(II) nitrate trihydrate and the corresponding ligands in a 1:1:1 molar ratio. Dark-green prismatic crystals suitable for single-crystal X-ray diffraction were obtained after four days. FT-IR spectroscopy confirmed coordination of the chromone-2-carboxylate ligand through its carboxylate group. The difference between the asymmetric and symmetric stretching vibrations of the carboxylate group ($\Delta\nu$ = 273.9 cm^{-1}) indicated ligand deprotonation and monodentate coordination to the Cu(II) center. The absorption band at 462 cm^{-1} was assigned to the Cu–N stretching vibration, while the band at 845 cm^{-1} confirmed the presence of nitrate ions. Single-crystal X-ray diffraction revealed that the Cu(II) ion is coordinated by one monodentately bound chromone-2-carboxylate ligand and one bidentate 2,2'-bipyridine ligand through both nitrogen donor atoms. The coordination sphere is completed by two water molecules. In addition, an uncoordinated chromone-2-carboxylic acid molecule is present in the crystal lattice and connected to the coordinated ligand through hydrogen-bonding. Nitrate ions are also incorporated into the crystal structure, contributing to the stabilization of the supramolecular assembly. These results demonstrate that the combination of chromone-2-carboxylate and 2,2'-bipyridine ligands enables the formation of a structurally well-defined ternary copper(II) complex stabilized by coordination and hydrogen-bonding interactions.



Scheme 1. Graphical representation of the synthesis and characterization of K9.

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MAGNETIC CMC-BASED HYDROGELS: RADIOLYTIC SYNTHESIS VIA ONE- AND TWO-STEP APPROACHES

Ivana Landripet,[a] Ivan Marić,[a] Nataša Šijaković Vujičić,[b] Tanja Jurkin[a]

[a] Radiation Chemistry and Dosimetry Laboratory, Division of Materials Chemistry, Ruđer Bošković Institute, Bijenička cesta 54, Zagreb, Croatia, [b] Laboratory for Rheology and Material Synthesis, Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička cesta 54, Zagreb, Croatia
* ilandrip@irb.hr

Biocompatible magnetic nanocomposites based on a naturally derived polymer, carboxymethyl cellulose (CMC), were synthesized using ^{60}Co γ-irradiation at the Ruđer Bošković Institute. γ-irradiation offers the advantage of inducing both the reduction of metal cations and polymer chain crosslinking, depending on the synthesis parameters, without the need for any external reducing or crosslinking agents.

Our research systematically explores the critical conditions, including pH and the concentrations of the Fe^{3+} precursor, polymer, and scavenger, that direct the system toward forming either stable ferrofluids or crosslinked hydrogels.

Building on the previous synthesis of poly(ethylene oxide) (PEO)/magnetite nanocomposite hydrogels using a one-step γ-irradiation technique[1], this work establishes conditions to suppress radiation-induced polysaccharide degradation. In the one-step approach, high CMC concentrations yielded orange, non-magnetic gels due to incomplete Fe^{3+} reduction and rapid oxidation upon air exposure. However, lower concentrations successfully produced stable ferrofluids.

In a two-step approach, these ferrofluids served as ideal precursors for radiation-induced crosslinking, yielding dark, homogeneous magnetic hydrogels with uniform nanoparticle distribution. Pure CMC hydrogel behaves as a rigid but brittle elastic network, whereas in magnetic CMC hydrogels incorporation of the magnetite nanoparticles increases deformability dramatically together with higher yield stress, indicating the formation of a softer yet viscoelastic network capable of sustaining large deformation before yielding. The synthesized materials display outstanding thixotropic properties and rapid self-healing behavior.

This dual strategy allows precise tuning from flowable ferrofluids to magnetic hydrogels, opening new possibilities for targeted drug delivery, magnetic hyperthermia, and tissue engineering.

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DEVELOPMENT OF A BREATHING SIMULATION SYSTEM IN A LUNG-ON-A-CHIP PLATFORM

Tea Leskovar,[a] Anđela Marković,[a] Dora Malešević,[a] Iris Frlan,[a] Donna Danijela Dragun,[a] Iva Rezić Meštrović,[b] Ernest Meštrović[a]

[a] University of Zagreb, Faculty of Chemical Engineering and Technology, Trg Marka Marulića 19, 10000 Zagreb, Croatia, [b] University of Zagreb, Faculty of Textile Technology, Prilaz brauna Filipovića 28, 10000 Zagreb, Croatia

* tleskovar@fkit.hr

Modern drug discovery is facing an urgent need for more reliable testing models, driven by the ethical constraints, prohibitive costs, and poor translational success of traditional animal studies.[1] When it comes to evaluating respiratory therapies, traditional 2D culture systems cannot adequately reproduce the dynamic conditions of the human lung, particularly during inhalation, where airflow patterns, particle size, and mechanical stretching of the tissue critically influence drug absorption. In a living lung, these microenvironmental factors dictate exactly how an inhaled formulation behaves, making static culture dishes obsolete for predictive testing. Organ-on-a-chip technologies represent a major leap forward, acting as advanced biomimetic platforms that enable precise control over the microenvironment and faithful reproduction of these key physiological functions.[2] In this study, a compact lung-on-a-chip system was developed with an integrated breathing simulation module specifically designed for testing inhalation drug formulations under realistic conditions. The basal membrane separating the epithelial and endothelial compartments was fabricated from an electrospun polycaprolactone membrane, while the connective tissue layer was simulated using a hydrogel coating.[3] A key innovation of the developed system is the seamless integration of controlled airflow and cyclic membrane stretching with a dedicated aerosol-delivery module. Furthermore, real-time tracking of the platform's microenvironment is achieved via an integrated potentiometric sensor that monitors system functionality by measuring the potential difference between a polyaniline-coated graphite working electrode and an Ag/AgCl reference electrode, mapping local pH variations directly. This combination allows us to replicate true respiratory mechanics and assess drug deposition, absorption, and overall barrier performance in an environment that closely mirrors the human alveolus. Ultimately, this platform provides a reliable, human-relevant tool for early-stage formulation optimization, offering a promising avenue to reduce animal use in preclinical respiratory research.

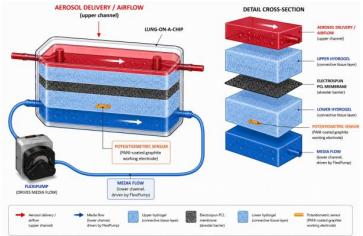


Figure 1. Schematic illustration of the microfluidic chip setup. (OpenAI, ChatGPT with image generation).

ACKNOWLEDGEMENTS: This work was funded by the Croatian Science Foundation under the project IP-2024-05-4339 entitled "The 'Coffee Ring' Effect in a Lab on a Chip Environment for the Development of Novel Drug Formulations" (project leader: Prof. Ernest Meštrović), as well as by the University of Zagreb through the institutional research project "Advanced Technologies for the Fabrication of (Bio)chemical Sensors and Lab on a Chip Devices" (112103).

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UV ABSORPTION PROPERTIES OF THE π-CONJUGATED SYSTEM OF DIBENZALACETONE

Gordana Majstorović, Sandro Vuk

Prirodoslovna škola Vladimira Preloga, Ulica grada Vukovara 269, Zagreb
* majstorovicg@gmail.com

Ultraviolet (UV) radiation absorption in organic molecules is governed by their electronic structure, with increased conjugation causing a bathochromic shift of the absorption maximum toward longer wavelengths. Owing to its extended conjugated π-system, dibenzalacetone (DBA) represents a suitable model compound for investigating optical properties and evaluating its potential application as an organic UV filter. The aim of this study was to investigate the optical properties of synthesized DBA using UV–Vis spectrophotometry, compare its absorption maximum with those of the starting reactants, and assess its photostability upon exposure to UV radiation.

DBA was synthesized via the Claisen–Schmidt condensation of benzaldehyde and acetone. The purity of the synthesized product was confirmed by melting point determination, followed by spectroscopic characterization. UV–Vis spectrophotometry was used to measure the absorbance of five different DBA concentrations, as well as the absorbance of benzaldehyde and acetone. In addition, the absorbance of DBA was recorded before and after UV irradiation to evaluate possible changes in the absorption maximum and the photostability of the compound. The sun protection factor (SPF) was subsequently calculated from the obtained absorbance values.

The results demonstrated a linear relationship between absorbance and concentration, consistent with the Beer–Lambert law. The absorption maximum of DBA was observed at 330 nm, whereas the absorption maxima of acetone and benzaldehyde were recorded at 272 nm and 279 nm, respectively. The observed bathochromic shift confirms the influence of the extended conjugated π-system on the optical properties of DBA. No significant change in the position of the absorption maximum was detected following UV irradiation, indicating the relative photostability of the synthesized compound. These findings demonstrate that dibenzalacetone exhibits favorable optical properties and good stability under UV exposure, highlighting its potential as a model compound for the development of organic UV filters.

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TAILORING HIGH MOLECULAR DIVERSITY THROUGH CARBENE CHEMISTRY AND REACTIVITY SUPPRESSION

Josip Mikulić,[a] Marko Purić,[b] Nikola Topolovčan[b]

[a] Department of Chemistry, Faculty of Science, Horvatovac 102a, 10 000 Zagreb, Croatia, [b] Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička cesta 54, 10 000 Zagreb, Croatia

* jmikulic.chem@pmf.hr

Utilization of carbenes as highly reactive intermediates proves to be a valuable method for rapid construction of a diverse carbon scaffold. Thus, a number of innovative methodologies regarding their *in-situ* generation were consequently developed. Such a method is the visible-light-induced generation of carbenes from diazoesters – a high-yielding transformation under mild conditions.[1] This methodology was readily applied in generating substituted norcaradienes which can further undergo oxidation and ultimately provide synthetically valuable, highly functionalized compounds (Figure 1a).[2]

Though mentioned carbenes are nowadays easy to generate, directing their reactivity remains a challenge. In this work, we explore means of directing their selectivity in a diversely functionalized system (Figure 1b). With carbazole as a model substrate, a series of organic bases and inorganic salts were utilized to investigate hydrogen bonding as a method of transient non-covalent protection. Furthermore, carbazole's reactivity relative to previously investigated carbene-trapping agents was explored to screen functionalities whose reactivity can further be selectively directed upon.

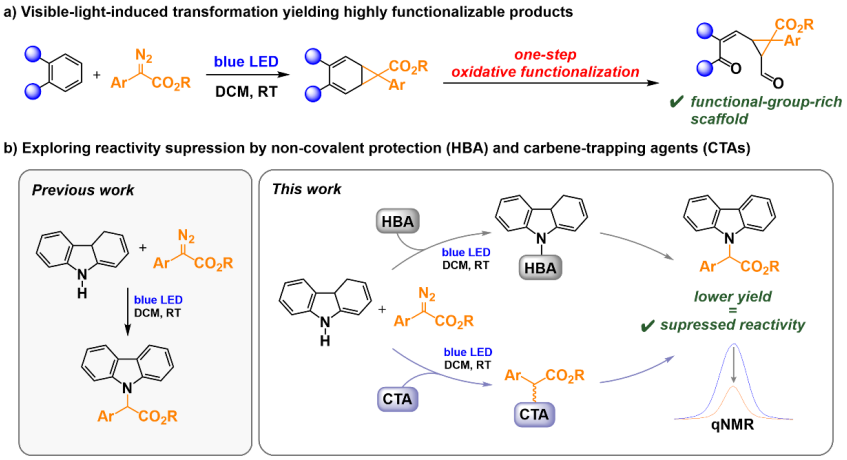


Figure 1. a) Implementing photochemically generated carbenes in constructing highly functionalized synthetic precursors; **b)** investigating possibilities for carbazole reactivity suppression by applying transient non-covalent protection and carbene-trapping agents.

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SYNTHESIS AND INVESTIGATION OF THE ELECTROCHEMICAL PROPERTIES OF TWO QUINAZOLINONE SCHIFF BASES

Maja Molnar,[a] Ivana Tomac,[a] Mario Komar,[a] Leonarda Marković,[a] Martina Jakovljević Kovač,[a] Dajana Gašo-Sokač,[a] Mirna Habuda-Stanić,[a] Damir Magdić,[a] Lahorka Budić,[a] Valentina Bušić,[a] Dragica Suknović[b]

[a] Josip Juraj Strossmayer University of Osijek, Faculty of Food Technology Osijek, F. Kuhača 18, 31000 Osijek, [b] University Hospital Centre Osijek, Clinical Institute of Nuclear Medicine and Radiation Protection, Josipa Huttlera 4 Osijek, Croatia
* mmolnar@ptfos.hr

Two selected quinazolinone derivatives, (*E*)-3-((2-hydroxybenzylidene)amino)-2-methylquinazolin-4(3*H*)-one and (*E*)-6,8-dichloro-3-((2-hydroxybenzylidene)amino)-2-methylquinazolin-4(3*H*)-one, were synthesized using green chemistry methods. A synthesis was performed from substituted 3-amino-2-methylquinazolin-4(3*H*)-ones in reaction with corresponding aldehydes, using deep eutectic solvents both as solvents and catalysts.[1] Electrochemical properties of synthesized compounds were investigated. They were characterized electrochemically in a non-aqueous medium by cyclic voltammetry. The effects of scan rate, chemical structure, and concentration on the electrochemical response were evaluated, together with their influence on the performance of an electrochemical DNA biosensor. The electrochemical studies revealed that a scan rate of 50 mV s^{-1} provided the optimal analytical response. Both quinazolinone derivatives exhibited a linear relationship between peak current and concentration within the range of 2.5×10^{-5} to 2.35×10^{-4} mol L^{-1}. Analysis of the voltammetric behavior indicated the presence of two oxidation peaks. The peak observed at approximately 0.30 V was attributed to the oxidation of the quinazolinone aromatic system, while the peak at approximately 0.75 V was associated with the oxidation of the carbonyl group within the quinazolinone ring. Evaluation of the interaction between the synthesized compounds and the electrochemical DNA biosensor demonstrated a relative proportion of DNA of approximately 87% for both derivatives, indicating a reduced degree of DNA damage. Overall, the synthesized quinazolinones exhibited favorable electrochemical characteristics, good concentration-dependent linearity, and a protective effect toward DNA under the investigated experimental conditions.

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SYNTHESIS AND PHOTOPHYSICAL CHARACTERIZATION OF QUINAZOLINE-BASED ESIPT CHROMOPHORES

Marko Pećina,[a] Đani Škalamera,[a] Iva Džeba[b]

[a] Department of Chemistry, University of Zagreb Faculty of Science, Horvatovac 102a, 10000 Zagreb, [b] Division of Materials Chemistry, Ruđer Bošković Institute, Bijenička 54, 10000 Zagreb
* mpecina.chem@pmf.hr

Compounds containing a quinazoline backbone have been extensively studied due to their broad utility in biological systems and importance as pharmacological agents.[1]
In recent years there has been a growing interest in the photophysical properties of these, and similar, compounds as excited state intramolecular proton transfer (ESIPT)-based emitters due to their broad scope of applications in sensing, imaging and lighting materials research.[2] Predicting the emissive properties of such a compound proves daunting without computational support as ESIPT depends on numerous factors some of which are hydrogen-bond strength, conformational changes, solvent effects and aggregation.[3], [4] We present our approach to designing potential quinazoline-based ESIPT emitters.

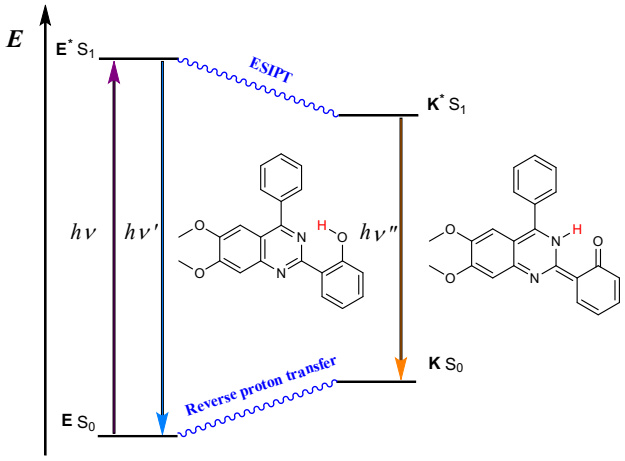


Figure 1. Schematic representation of quinazoline-based ESIPT emission.

A synthetic pathway to these derivatives was developed, [5] providing the desired products in good yields. Furthermore, the photophysical characterization of the derivatives, including steady-state and time-resolved absorption and emission spectroscopy in both solution and the solid state, will be presented.

ACKNOWLEDGEMENTS: This research was supported by the European Union – NextGenerationEU through the National Recovery and Resilience Plan 2021-2026 Institutional grant of Ruđer Bošković Institute KP1-2026 01-1112/1-2026 (I. Dž.), and European Union – NextGenerationEU through the National Recovery and Resilience Plan 2021-2026 Institutional grants of University of Zagreb Faculty of Science (ProPubFO, PMF-CROFUND, GOUT PMF).

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DECODING PHARMACEUTICAL FORMULATIONS THROUGH COFFEE-RING MORPHOLOGY

Nika Šajković,[a] Bruno Mikan,[b] Donna Danijela Dragun,[a] Zlatko Smole,[c] Domagoj Begušić,[c] Damir Pintar,[c] Ernest Meštrović[a]

[a] Faculty of Chemical Engineering and Technology, University of Zagreb, Marulićev trg 19, 10000 Zagreb, Croatia, [b] Faculty of Electrical Engineering and Computing, University of Zagreb, Unska 3, 10000 Zagreb, Croatia, [c] Modalis d.o.o., Vinogradska cesta 103A, 10000 Zagreb, Croatia
* nsajkovic@fkit.hr

The coffee-ring effect is an evaporation-driven self-assembly phenomenon in which the final morphology of a dried droplet emerges from the interplay between capillary flow, evaporation dynamics, crystallization, particle redistribution, and physicochemical interactions within the solution. Rather than being a simple drying artifact, the resulting deposition pattern represents a complex fingerprint reflecting formulation composition. In this study, the coffee-ring effect was investigated as a non-destructive platform for characterizing pharmaceutical formulations containing pantoprazole formulated with different excipients. Since excipients influence intermolecular interactions, crystallization behavior, and particle transport during evaporation, their effect on deposition morphology was systematically evaluated. Microdroplets of each formulation were deposited onto glass substrates and dried under controlled environmental conditions to ensure reproducible evaporation. The resulting deposits were digitized using automated optical microscopy and subjected to computational image analysis. Image preprocessing and extraction of morphometric descriptors enabled quantitative characterization of the resulting drying patterns. Computational analysis was used to identify formulation-dependent morphological signatures and objectively compare the formulations. Distinct differences between formulations were observed, demonstrating that relatively small variations in formulation composition significantly influence evaporation-induced self-assembly. These findings emphasize that coffee-ring formation is controlled by a combination of fluid dynamics and formulation-specific physicochemical properties rather than evaporation alone, making it a promising tool for investigating formulation behavior and development.

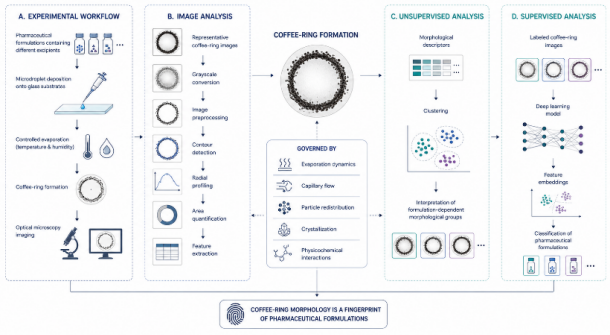


Figure 1. Experimental and analytical workflow for coffee-ring characterization of pharmaceutical formulations.

ACKNOWLEDGEMENTS This work was funded by the Croatian Science Foundation under the project IP-2024-05-4339 entitled "The 'Coffee Ring' Effect in a Lab on a Chip Environment for the Development of Novel Drug Formulations" (project leader: Prof. Ernest Meštrović), as well as by the University of Zagreb through the institutional research project "Advanced Technologies for the Fabrication of (Bio)chemical Sensors and Lab on a Chip Devices" (112103).

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COORDINATION CHEMISTRY OF COPPER(II) COMPLEXES WITH O-CONTAINING LIGANDS: STRUCTURAL AND PHYSICOCHEMICAL INSIGHTS

Stjepan Šarić,* Iva Jozinović, Tomislav Balić, Martina Šrajer Gajdošik, Nikolina Filipović,* Elvira Kovač-Andrić

Department of Chemistry, University of Osijek, cara Hadrijana 8/A, 31 000, Osijek
* nfilipovic@kemija.unios.hr

Chromone derivatives represent an important class of oxygen-containing heterocyclic compounds with a strong ability to coordinate transition metal ions through carboxylate and carbonyl functional groups.[1] In this work, a series of copper(II) complexes containing chromone-2-carboxylate ligands were synthesized following environmentally friendly synthetic procedures (Figure 1). The obtained compounds were investigated in order to establish the influence of ligand environment on the structural and physicochemical properties of the resulting coordination compounds. Three copper(II) complexes with chromone-2-carboxylate ligands were synthesized and characterized using Fourier-transform infrared spectroscopy (FT-IR), nuclear magnetic resonance spectroscopy, cyclic voltammetry, and thermal analysis (TGA/DSC). The results indicated the formation of both mononuclear and hydroxo-bridged dinuclear copper(II) species. Electrochemical studies confirmed the presence of copper in the +2-oxidation state in all investigated compounds. In addition, a new copper(II) complex containing chromone-2-carboxylate and coordinated pyridine molecules was successfully crystallized and structurally characterized by single-crystal X-ray diffraction analysis. The crystal structure revealed a mononuclear complex with a distorted square-pyramidal geometry around the central Cu(II) ion. The coordination environment consists of oxygen donor atoms from the chromone-2-carboxylate ligand and nitrogen donor atoms from pyridine molecules, resulting in a five-coordinate metal center. Structural findings were further supported by FT-IR, UV–Vis spectroscopy, elemental analysis, cyclic voltammetry, and thermal analysis. The combined results demonstrate the versatility of chromone-2-carboxylate as a ligand capable of stabilizing different copper(II) coordination motifs, ranging from mononuclear to dinuclear architectures. Furthermore, the study highlights the relationship between coordination environment, crystal structure, thermal stability, and electrochemical behavior of copper(II) chromone derivatives, contributing to a better understanding of structure–property relationships in chromone-based coordination compounds.

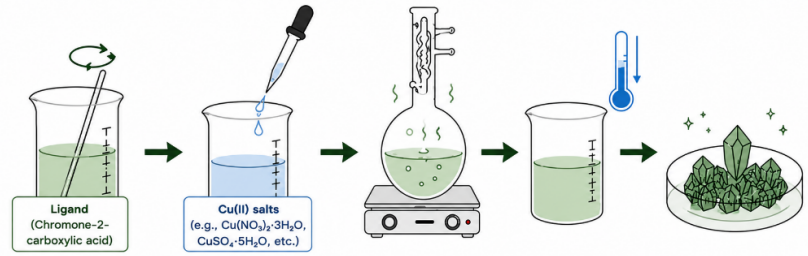


Figure 1. Green synthetic route to the copper(II) complexes.

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THE EFFECT OF ZINC(II) AND COPPER(II) IONS INSERTION INTO TETRAKIS(*N*-METHYLPYRIDINIUM-3-YL)PORPHYRIN ON PHOTODYNAMIC INACTIVATION

Nika Škokić,[a] Lucia Bajakić,[a] Martina Mušković Lukić,[a] Gabrijela Begić,[b] Nela Malatesti[a,*]

[a] Faculty of Biotechnology and Drug Development, University of Rijeka, Rijeka, Radmile Matejčić 2, Croatia, [b] Faculty of Medicine, University of Rijeka, Braće Branchetta 20/1, Croatia
*e-mail: nela.malatesti@biotech.uniri.hr

Porphyrins are well-established class of photosensitizers with strong potential in photodynamic inactivation (PDI). Previous work from our group demonstrated the efficacy of amphiphilic long-chain porphyrins against opportunistic waterborne pathogens.[1] However, the multistep synthesis, low yields, and high costs of those derivates prompted a shift towards symmetric cationic porphyrins and their metal analogues, as more accessible alternatives.[2] Metal chelation influences the key photophysical properties of porphyrins - intersystem crossing efficiency, triplet state lifetime and singlet oxygen quantum yield - and therefore their photodynamic efficacy.[3]

In this study, the free-base, 5,10,15,20-tetrakis(*N*-methylpyridinium-3-yl) porphyrin tetrachloride (TMPyP3) was synthesised by *N*-methylation of TPyP3 precursor. Zn(II) and Cu(II) derivatives were obtained by metalation with $ZnCl_2$ and $CuCl_2$ salts, under alkaline aqueous conditions with mild heating. All compounds were confirmed by ^{1}H NMR spectroscopy and HRMS. Their spectroscopic properties were analyzed by UV-Vis and fluorescence spectroscopy. As the Type II mechanism is the dominant ROS production pathway for porphyrin-based photosensitizers, singlet oxygen production was evaluated by measuring the photodegradation of ABMDMA in PBS (λ = 426 nm). Due to the limited aqueous solubility of the Cu(II) complex, complementary measurements were performed using DPBF in methanol (λ = 592 nm).

PDI activity was assessed against two opportunistic waterborne pathogens – *Pseudomonas aeruginosa PAO1* as Gram-negative and *Enterococcus faecalis ATCC 29212* as Gram-positive bacteria. All assays were conducted in PBS and tap water, under violet-light irradiation (λ = 394 nm, 20 mW/cm^2). Both strains are known for their capacity of forming biofilms, which represents an additional challenge in water disinfection, due to the increased resistance of biofilm-associated bacteria to conventional antimicrobial treatments.[4] PDI assays showed that TMPyP3 exhibited the lowest MEC values against both bacterial strains, followed by Zn(II)-TMPyP3, while Cu(II)-TMPyP3 showed negligible photodynamic activity. This trend is consistent with singlet oxygen/ROS production measurements, where free-base showed the highest generation, followed by Zn(II) and Cu(II) complex.[5]

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ZETA POTENTIAL OF URINARY EXTRACELLULAR VESICLES DIFFERENTIATES DIABETES FROM DIABETIC KIDNEY DISEASE

Melanie Tepuš Petršorić,[a,b] Maria Pia Savoca,[a] Elisabetta Verderio Edwards[a,c]

[a] Centre for Systems Health and integrated Metabolic Research (SHiMR), School of Science and Technology, Nottingham Trent University, Clifton Ln, Clifton, Nottingham NG11 8NS, Nottingham, United Kingdom, [b] Department of Medical Chemistry, Biochemistry, and Clinical Chemistry, Faculty of Medicine, University of Rijeka, Braće Branchetta 20, 51000 Rijeka. Croatia, [c] Department of Biological, Geological, and Environmental Sciences, Alma Mater Studiorum, University of Bologna, Via Zamboni, 33 - 40126 Bologna, Italy

* melanietp@uniri.hr

Diabetic kidney disease (DKD) is the most common type of chronic kidney disease (CKD), often leading to kidney failure. Clinical manifestations typically appear only after substantial renal damage has occurred, so early diagnosis is essential to enable timely intervention and improve outcomes. Urinary extracellular vesicles (uEVs) are membrane-enclosed carriers of biomolecules with a key role in intercellular communication. As their molecular cargo reflects the pathophysiology of their cells of origin, uEVs represent an attractive source of biomarkers for kidney diseases. Unlike their molecular cargo, the surface charge of uEVs remains underexplored. Zeta potential, or surface charge, may mirror the characteristics of their cells of origin and serve as an indicator of pathological alterations. In diabetes and DKD, post-translational modifications including glycosylation and phosphorylation can further modulate cellular surface charge. We hypothesized that uEVs zeta potential discriminates between DKD, diabetes without CKD, and healthy controls, with potential utility for stratifying DKD. Cell-free urine samples were obtained from the Sheffield Kidney Institute (UK) and Patras University Hospital (Greece) with informed consent, comprising DKD (n = 36), diabetes without CKD (n = 16), and healthy control (n = 18) cohorts. The DKD group was further stratified according to the rate of eGFR decline into stable (<2 mL/min/year) and progressive (>5 mL/min/year) subgroups. Differences in zeta potential, size distribution, and concentration of small and large uEVs were assessed using nanoparticle tracking analysis. The uEVs were further characterized by immunoblotting, transmission electron microscopy, and single-particle interferometric reflectance imaging sensing (SP-IRIS/ExoView) using heparan sulphate-binding capture. Significant differences in zeta potential were observed in large uEVs fraction, but not in small uEVs fraction. Large uEVs from individuals with diabetes exhibited a less negative zeta potential than those from healthy controls and patients with progressive DKD. This reduction in negative surface charge may reflect the loss of the negatively charged glycocalyx, a well-established feature of diabetes. As DKD progresses, glycocalyx depletion may be accompanied by increased HS deposition associated with renal fibrosis, potentially leading to restoration of the negative surface charge and a more negative zeta potential compared with diabetes without CKD. Consistent with this, uEVs from patients with DKD exhibited higher HS levels than those from individuals with diabetes without CKD, as determined by SP-IRIS/ExoView.

Our findings identify the zeta potential of large uEVs as a novel physicochemical parameter capable of differentiating diabetes from DKD. Although it did not significantly discriminate between stable and progressive DKD, an observable trend suggests potential utility that warrants further investigation.

OPTIMIZATION OF ACTIVATED SLUDGE CONCENTRATION FOR THE BIOREMEDIATION OF MODEL BIOWASTE LEACHATE

Mirela Volf, Ana Coban, Marta Jerneić, Monika Šabić Runjavec, Marija Vuković Domanovac

University of Zagreb Faculty of Chemical Engineering and Technology, Trg Marka Marulića 19, HR-10000 Zagreb, Croatia

* volf.mirela@gmail.com

Leachate derived from model biowaste is characterized by a high organic load and requires efficient treatment due to its elevated concentration of organic contaminants.[1] Bioremediation using activated sludge is a sustainable and environmentally friendly biological treatment in which the metabolic activity of microorganisms facilitates the degradation of organic contaminants into less harmful compounds.[2]

The aim of this study was to investigate the effect of the initial activated sludge concentration on the efficiency of aerobic leachate biodegradation in a batch reactor over a 7-day treatment period. Changes in chemical oxygen demand (COD), as an indicator of organic load, and mixed liquor suspended solids (MLSS), as an indicator of biomass growth, were monitored throughout the experiment. Regardless of the initial activated sludge concentration, COD decreased from an initial value of 17,212 mg O_2/L to approximately 2,790 mg O_2/L, corresponding to an average organic load removal efficiency of about 84 %. A higher initial activated sludge concentration resulted in faster initial degradation of organic pollutants and enhanced biomass growth. Although no significant differences in the final COD removal efficiency were observed among the investigated conditions, the results indicate that increasing the initial activated sludge concentration improves the kinetics of aerobic biodegradation and contributes to greater process stability.

These findings provide a valuable basis for optimizing the biological treatment of leachate and determining the optimal biomass concentration for the bioaugmentation process.

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FUNGAL BIOSYNTHESIS OF SILVER NANOPARTICLES: THE ROLE OF MEDIUM COMPOSITION AND PHENOL OXIDASE INDUCTION

Mislav Vorkapić,[a] Gabriela Galić,[b] Goran Palijan,[b] Nikolina Filipović,[a] Anamarija Stanković[a]

[a] Department of Chemistry, University of Osijek, Ulica cara Hadrijana 8/a, 31000 Osijek, Croatia,

[b] Department of Biology, University of Osijek, Ulica cara Hadrijana 8/a, 31000 Osijek, Croatia

* mvorkapic@kemija.unios.hr

Green synthesis has emerged as a promising environmentally friendly alternative to conventional chemical methods for nanoparticle production.[1] Among biological approaches, fungal-mediated synthesis of silver nanoparticles (AgNPs) has gained considerable attention because fungi efficiently reduce metal ions and secrete biomolecules that facilitate nanoparticle stabilization.[2] In this study, the effect of enhanced phenol oxidase activity on the biosynthesis of AgNPs by the filamentous fungus *Aspergillus niger* was investigated. Six modified Czapek–Dox media were prepared using sucrose, starch, or glucose as carbon sources. To stimulate phenol oxidase production, media variants 2, 4, and 6 were supplemented with copper(II) sulfate, oak sawdust, and hydrogen peroxide. After 72 hours of cultivation, fungal biomass was harvested and transferred to ultrapure water to induce the release of extracellular metabolites. Following a further 72-hour incubation, the biomass was removed and 1 mM silver nitrate was added to the resulting cell-free filtrates. AgNP synthesis was monitored for 120 hours by UV–Vis spectroscopy. Functional groups involved in nanoparticle formation were analyzed using FTIR spectroscopy, while X-ray diffraction (XRD) was employed to verify crystallinity. All samples exhibited a characteristic AgNP surface plasmon resonance peak near 420 nm. Filtrates obtained from media containing phenol oxidase inducers showed increased absorbance and accelerated nanoparticle formation compared with the corresponding controls. FTIR analysis revealed the presence of protein-, enzyme-, and carbohydrate-associated functional groups contributing to nanoparticle capping and stabilization, whereas XRD confirmed the crystalline structure of AgNPs in all variants. The results demonstrate that phenol oxidase induction enhances the kinetics of AgNP biosynthesis without affecting nanoparticle crystallinity, highlighting the importance of culture-condition optimization for large-scale production and industrial implementation.

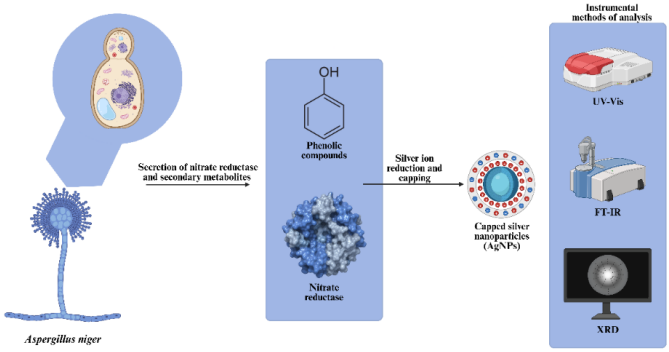


Figure 1. Schematic representation of AgNP biosynthesis and instrumental analytical methods.

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ANTIMICROBIAL ACTIVITY OF INDOLE SCHIFF BASES

Dragana Vuk,[a] Vilma Lovrinčević,[a] Marija Vuković Domanovac,[b] and Ines Despotović[c]

[a] Department of Organic Chemistry, University of Zagreb Faculty of Chemical Engineering and Technology, Trg Marka Marulića 19, 10000 Zagreb, Croatia, [b] Department of Industrial Ecology, University of Zagreb Faculty of Chemical Engineering and Technology, Trg Marka Marulića 19, 10000 Zagreb, Croatia, [c] Division of Physical Chemistry, Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia
* dvuk@fkit.unizg.hr

The antimicrobial activity[1] of natural and synthetic substances is considered as one of the fundamental area of research in modern medicine. The discovery and application of antimicrobial drugs2 have brought enormous progress in the treatment of infectious diseases, leading to a reduction in mortality and an extension of human lifespan. However, the emergence of antimicrobial resistance[2] has compromised the effectiveness of these therapies and re-established the threat posed by microorganisms.
Therefore, continued research into the mechanisms of action, spectrum of activity and clinical application of novel antimicrobial agents is continuously needed. In this work, as part of the continuation of the study and expansion of the library of new antimicrobial agents, extended conjugation indole Shiff bases were designed as new antimicrobial precursors. Antibacterial activity was tested against *Bacillus subtilis*[3] 3020, while antifungal activity was tested against *Candida lipolytica* 59 and *Aspergillus niger* 405. Molecular docking simulations were conducted to characterize the binding of the synthesized molecules to the target enzyme. The analysis provided valuable information regarding their binding potential and identified specific interactions within the enzyme active site that are likely to influence complex stability and support the antimicrobial efficacy of these compounds.

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IL-29 AND AIM IN OBESITY: ASSOCIATIONS WITH METABOLIC DYSFUNCTION AND THEIR POTENTIAL AS BIOMARKERS

Iva Vukelić,[a] Mattea Simonelli,[b] Lea Lukšić,[a] Sunčica Buljević,[a] Sanja Klobučar,[c,d] Dijana Detel[a]

[a] Department of Medical Chemistry, Biochemistry and Clinical Chemistry, Faculty of Medicine, University of Rijeka, Rijeka, Croatia, [b] Faculty of Medicine, University of Rijeka, Rijeka, Croatia, [c] Department of Endocrinology, Diabetes and Metabolic Diseases, Clinical Hospital Centre Rijeka, Rijeka, Croatia, [d] Department of Internal Medicine, Faculty of Medicine, University of Rijeka, Rijeka, Croatia

* iva.vukelic@uniri.hr

Obesity is a multifactorial chronic disease and a major global health challenge, associated with an increased risk of obesity-related metabolic complications, including type 2 diabetes (T2D).[1] Adipose tissue expansion promotes chronic low-grade inflammation characterized by increased production of pro-inflammatory mediators that contribute to insulin resistance, dyslipidemia, endothelial dysfunction, and impaired metabolic homeostasis, highlighting their central role in the pathogenesis of obesity and related complications.[1] Among these, interleukin-29 (IL-29) and apoptosis inhibitor of macrophage (AIM/CD5L) have attracted particular attention due to their potential roles in inflammatory signaling, adipose tissue dysfunction, and obesity-related metabolic abnormalities. IL-29 has emerged as a cytokine potentially involved in obesity-associated inflammation[2] and immune regulation,[3] while AIM, a macrophage-derived circulating protein, has been implicated in adipose tissue remodeling, lipid metabolism, and inflammatory pathways,[4] making both promising candidate biomarkers and potential therapeutic targets in obesity-related metabolic disorders. This study aimed to investigate the potential of serum IL-29 and AIM as biomarkers of obesity, to examine their association with anthropometric and metabolic parameters, and to evaluate alterations in key metabolic indicators among individuals diagnosed with overweight and obesity. Results demonstrated a positive correlation of BMI and body fat, blood pressure, inflammatory status, and metabolic disturbances. Individuals with obesity exhibited increased levels of C-reactive protein, triglycerides, insulin, HOMA-IR, IL-29 (r_s = 0.264, p = 0.131), and AIM (r_s = 0.331, p = 0.033), alongside reduced HDL cholesterol and insulin sensitivity. Increasing BMI was accompanied by unfavorable alterations in lipid metabolism, hyperinsulinemia, and evidence of chronic low-grade inflammation, indicating elevated cardiometabolic risk and impaired glucose homeostasis in overweight and obese participants. The observed associations between obesity, metabolic dysregulation, and increased circulating levels of IL-29 and AIM support their potential as novel biomarkers of obesity-related inflammation and metabolic impairment. Their assessment may improve early identification of individuals at increased cardiometabolic risk and monitoring of disease progression or response to weight-loss interventions. Furthermore, IL-29 and AIM may provide insights into the inflammatory mechanisms underlying obesity and represent potential therapeutic targets for reducing metabolic and cardiovascular complications. Larger longitudinal studies are warranted to validate their clinical utility and establish their role in precision medicine approaches for obesity management.

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FERROCYANIDE-BASED COMPLEXES OF *N*-SUBSTITUTED PYRIDINIUM OXIMES AND RELATED NON-OXIME ANALOGUES

Igor Picek, Danijela Musija, Vladimir Damjanović, Blaženka Foretić

Department of Chemistry and Biochemistry, School of Medicine, University of Zagreb, Šalata 3, Croatia

* ipicek@mef.hr

Supramolecular ferrocyanide-based charge-transfer complexes (CTCs) with pyridinium oximes have emerged as promising stimuli-responsive metallo-organic materials owing to their tunable optical and redox properties.[1–3] The ferrocyanide anion, with its rigid octahedral geometry, strong electron-donating character, and multiple hydrogen-bonding sites capable of forming bifurcated interactions, provides an effective platform for the construction of multidimensional supramolecular architectures. In these assemblies, pyridinium oximes function as electron acceptors and hydrogen-bond donors, giving rise to extended networks stabilized by hydrogen bonding and π–π interactions. The interplay between crystal packing, noncovalent interactions, and redox activity governs the optical properties of these materials.[1–4]

Herein, we present a comparative spectroscopic investigation of ferrocyanide-based assemblies incorporating N-benzoylethyl and N-phenacyl substituents on pyridinium and pyridinium oxime cationic systems. By comparing oxime- and non-oxime analogues, we aim to elucidate how the presence or absence of oxime functionality influences the nature of donor–acceptor interactions, directing the formation of conventional ionic salts and/or charge-transfer assemblies, and governs their resulting electronic and optical properties.

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CHEMICAL PROFILING AND BIOLOGICAL EVALUATION OF ORGANIC EXTRACTS FROM ADRIATIC *CYSTOSEIRA BARBATA*

Iris Car Kubaska[a*], Hrvoje Zadravec[a], Nikolina Vidović[a], Valerije Vrček[b], Maria Kolympadi Markovic[c], Dean Marković[a]

[a] Faculty of Biotechnology and Drug Development, University of Rijeka, Rijeka, Croatia,

[b] Faculty of Pharmacy and Biochemistry, University of Zagreb, Zagreb, Croatia

[c] Faculty of Physics, University of Rijeka, Rijeka, Croatia.

* iris.car.kubaska@uniri.hr

Marine invertebrates and algae are rich sources of bioactive secondary metabolites. Brown algae of the genus *Cystoseira* have recently gained attention for pharmaceutical exploitation[1,2], but studies on the biological activities of Adriatic Sea *Cystoseira barbata* extracts remain scarce, with most research focusing on its ecology[3] and distribution[4].

We performed bioactivity-guided fractionation of dichloromethane (DCM) and methanolic (MeOH) organic extracts of *C. barbata*. The *in vitro* antiproliferative and cytotoxic effects were evaluated in several human cancer cell lines (A375 melanoma, A549 lung carcinoma, SW620 colon carcinoma) and one normal human cell line (HEK293 embryonic kidney). The DCM extract showed stronger cytotoxic effects than the MeOH extract across all cell lines. Notably, the DCM extract exhibited a lower IC_{50} value in SW620 cancer cells compared to HEK293 normal cells, indicating selective activity against colon carcinoma. In contrast, for A375 and A549 cells, the IC_{50} values of both extracts were higher than in HEK293 cells, showing no selectivity for these cancer types. Beyond cytotoxicity, antioxidant capacity was assessed via DPPH and ABTS assays. The DCM extract demonstrated markedly stronger ABTS radical scavenging activity than the MeOH extract, while both extracts showed only weak DPPH scavenging, revealing a clear selectivity for ABTS over DPPH radicals. Qualitative phytochemical screening identified major compound classes, and subsequent purification by column and preparative thin-layer chromatography yielded a major compound from the DCM extract, identified as fucosterol by ^{1}H and ^{13}C NMR spectroscopy. The DCM extract of *C. barbata* demonstrates selective cytotoxicity against SW620 colon cancer cells relative to normal HEK293 cells, with fucosterol identified as a major constituent. Further investigations will focus on confirming fucosterol's contribution to this selective effect, and testing the extracts and purified compound against a broader panel of cancer cell lines.

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