THE **CROATIAN CHEMICAL SOCIETY**
PROUDLY PRESENTS

THE COMPILATION OF THIS YEAR'S NEW

SOLUTIONS IN CHEMISTRY

11–15 November 2024 · Sveti Martin na Muri, Croatia

BOOK OF ABSTRACTS

SOLUTIONS IN CHEMISTRY

SOLUTIONS IN CHEMISTRY 2024

11–15 November 2024

Hotel Terme Sveti Martin☆☆☆☆

Sveti Martin na Muri, Croatia

BOOK OF ABSTRACTS

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Welcome from the Chairmen of the Organising Committee

On behalf of the Organising Committee, it is our great pleasure to welcome you to the Solutions in Chemistry 2024 conference taking place in Sveti Martin na Muri from 11 to 15 November 2024. The focus of the Conference organized by the Croatian Chemical Society can be deduced from the two meanings of the word "Solutions" in its title. The first one refers to the solution as a phase and comprises the experimental and computational studies of the processes occurring in liquid media. The second one is concerned with general solutions to chemical problems which are met in academia and various branches of industry. Thus, the Conference aims to gather the scientists dealing with different fields of chemistry and to deepen and strengthen the collaboration of the experts from universities, research institutes, schools, and chemistry-related companies.

This biennial conference will be held this year for the second time. The first launch in 2022 was a resounding success with more than 200 participants from 14 countries, and we strongly believe that the second edition will be even more fruitful. A number of plenary, invited, and section lectures will be delivered by top-tier scientists, and various sponsor presentations will be held as well. These will provide a new insight into the current problems in chemical science and industry, and an opportunity to learn and obtain new skills from prominent chemists and entrepreneurs. In addition, the Conference participants will have a chance to find out more about the newest instruments and consumables available from our numerous sponsors to whom we are grateful for their support. The poster session will give everyone the opportunity to present their work: from undergraduate students to experienced scientists in diverse fields of chemistry and chemical engineering. The education section will be held as well, focusing on finding new solutions in teaching new generations of chemists. This year's news is student-oriented day focused on the future career paths of students and young scientists in chemistry. For that purpose, the Conference will comprise an event entitled Career Accelerator.

A significant emphasis will also be put on an irreplaceable part of every great conference: social activities. Thus, we plan to organize various social events and encourage the participants to interact in a non-formal manner as well as to take the opportunity to discover the beauty of the picturesque Međimurje County and taste the local delicacies.

LET'S FIND THE NEW SOLUTIONS IN CHEMISTRY!

Ernest Meštrović & Vladislav Tomišić

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PLENARY LECTURES

PL1

NEW DEVELOPMENTS IN SYNTHETIC ANION TRANSPORTER SYSTEMS

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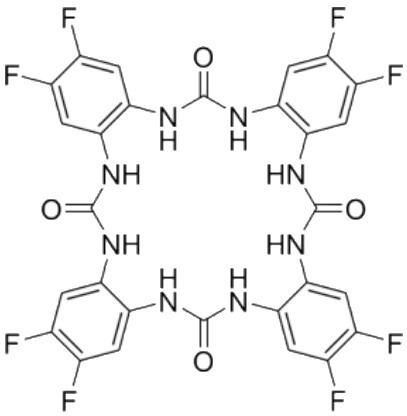
The development of synthetic anion transporters is the focus of several groups worldwide due to the potential application of these compounds in the treatment of diseases caused by faulty anion transport (e.g., cystic fibrosis)[1] and in disrupting anion concentration gradients and pH gradients leading to apoptosis and disruption of autophagy.[2]



This presentation will give an overview of work in the Gale group over the last few years and in particular focus on the development of new assays to measure membrane transport, the development of selective transporters[3,4] such as the tetraurea macrocycle shown[5] and the development of switchable[6] transporters and targeted transporters.[7]

ACKNOWLEDGEMENTS：This work was supported by the Australian Research Council (DP180100612, DP200100453, DP210100039) and the University of Sydney.

REFERENCES

1. P.A. Gale, J.T. Davis, R. Quesada, *Chem. Soc. Rev.,* **2017**, *46*, 2497-2519; H. Li, H. Valkenier, A.G. Thorne, C.M. Dias, J.A. Cooper, M. Kieffer, N. Busschaert, P.A. Gale, D.N. Sheppard, A.P. Davis, *Chem. Sci.,* **2019**, *42*, 9663-9672.
2. N. Busschaert, S.-H. Park, K.-H. Baek, Y.P. Choi, J. Park, E.N.W. Howe, J.R. Hiscock, L.E. Karagiannidis, I. Marques, V. Félix, W. Namkung, J.L. Sessler, P.A. Gale, I. Shin, *Nature Chem.*, **2017**, *9*, 667-675; S. Cheung, D. Wu, H.C. Daly, N. Busschaert, M. Morgunova, J.C. Simpson, D. Scholz, P.A. Gale, D.F. O'Shea, *Chem*, **2018**, *4,* 879-895; S.-H. Park, S.-H. Park, E.N.W. Howe, J.Y. Hyun, L.-J. Chen, I. Huang, G. Vargas-Zuñiga, N. Busschaert, P.A. Gale, J.L. Sessler, I. Shin, *Chem,* **2019**, *5*, 2079-2098.
3. X. Wu, L.W. Judd, E.N.W. Howe, A.M. Withecombe, V. Soto-Cerrato, H. Li, N. Busschaert, H. Valkenier, R. Perez-Tomas, D.N. Sheppard, Y.-B. Jiang, A.P. Davis, P.A. Gale, *Chem*, **2016**, *1*, 127-146.
4. X. Wu, P. Wang, W. Lewis Y.-B. Jiang, P.A Gale, *Nature Commun.* **2022**, *13*, 4623.
5. X. Wu, J.R. Small, A. Cataldo, A.M. Withecombe, P. Turner, P.A. Gale, *Angew. Chem. Int. Ed.,* **2019**, *58*, 15142-15147.
6. S.J. Wezenberg, L.-J. Chen, J.E. Bos, B.L. Feringa, E.N.W. Howe, X. Wu, M.A. Siegler, P.A. Gale, *J. Am. Chem. Soc*. **2022**, *144*, 331-338.
7. W. G. Ryder, M.E. Graziotto, A. Levina, B.A. Hawkins, D.E. Hibbs, E.J. New, P.A. Gale, *Chem*, **2025**, *in press*.

PL2

DNA TANDEM REPEATS: NMR STRUCTURAL STUDIES

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Quadruplex DNA, such as G-quadruplexes (G4), i-motifs and AGCGA-quadruplexes, are non-canonical DNA structures formed by tandem repeat sequences. Quadruplexes can form at various locations in the genome, including telomeres, promoter regions of oncogenes and other regulatory regions. Their structural details are influenced by factors such as the presence of monovalent cations (*e.g.,* K^+ or Na^+), the length of the G-rich sequence and the loop sequences connecting the G-quartets, as well as molecular crowding. Due to their unique structural properties and biological functions, quadruplex DNA structures have become attractive targets for therapeutic intervention, especially in cancer.

NMR studies are essential for elucidating the interactions between quadruplex DNA and ligands, offering detailed structural and dynamic insights at the atomic level. The bis-quinolinium ligand 360A, which has a high affinity for G4 structures, binds strongly to VK2, d[G_3(AGCGAG_3)$_3$AGCG]-3', a member of the AGCGA-quadruplex family. Notably, binding of 360A does not induce a conformational change from the anticipated G4 structure. Instead, NMR structural analysis revealed the first high-resolution structure of a G4 ligand intercalating into a G-rich tetrahelical fold (pdb 6SX3). The ligand Phen-DC_3, on the other hand, induces a structural transition in d[TAGGG(TTAGGG)$_3$] in a KCl solution from a hybrid-1 to an antiparallel chair structure, intercalating between two G-quartets (pdb 7Z9L). This high-resolution NMR structure provides unprecedented evidence of true ligand intercalation within an intramolecular G4.

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REFERENCES

1. J. Plavec, in *Handbook of Chemical Biology of Nucleic Acids* (Ed.: N. Sugimoto), Springer Nature Singapore, Singapore, **2023**, pp. 169-212.

2. M. Trajkovski, A. Pastore, J. Plavec, *Nucleic Acids Res.* **2024**, *52*, 1591.

3. B. R. Sahoo, V. Kocman, N. Clark, N. Myers, X. Deng, Ee L. Wong, H. J. Yang, A. Kotar, B. B. Guzman, D. Dominguez, J. Plavec, J. C. A. Bardwell, *Nucleic Acids Res.* **2024**, *52*, 4702.

4. M. Orehova, J. Plavec, V. Kocman, *ACS Omega* **2024**, *9*, 7215.

5. M. Juribašić Kulcsár, V. Gabelica, J. Plavec, *Chem. Eur. J.* **2024**, *30*, e202401190.

6. S. Hadži, Z. Živič, M. Kovačič, U. Zavrtanik, S. Haeserts, D. Charlier, J. Plavec, A. N. Volkov, J. Lah, R. Loris, *Nat. Commun.* **2024**, *15*, 3105.

7. T. Endoh, S. Satpathi, Y. Chen, S. Matsumoto, T. Ohyama, P. Podbevšek, J. Plavec, K. Onizuka, F. Nagatsugi, N. Sugimoto, *New J. Chem.* **2024**, *48*, 8529.

8. E. Chen, M. Trajkovski, H. K. Lee, S. Nyovanie, K. N. Martin, W. L. Dean, M. Tahiliani, J. Plavec, Liliya A. Yatsunyk, *Nucleic Acids Res.* **2024**, *52*, 3390.

PL3

ONE MOLECULE TO BIND THEM ALL: ORGANIC DYES SIMULTANEOUSLY TARGETING DNA, RNA OR PROTEINS, FOR EACH TARGET GIVING A SELECTIVE RESPONSE

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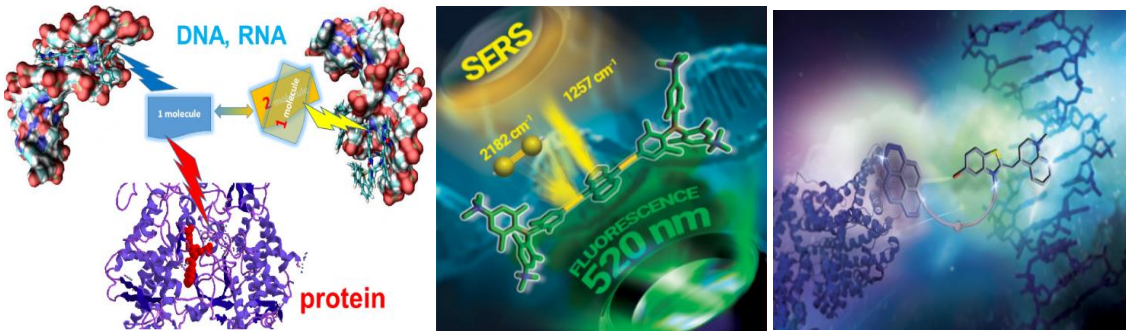
Bioimaging methods are essential for the advancement of life sciences; therefore, novel imaging techniques and tools are continuously studied, bringing novel modalities for the characterization of molecular mechanisms and biophysical properties[1]. The fluorescence-based techniques are by far the most used (<70%) due to the very high sensitivity combined with easy and safe application. However, fluorescent dyes or emissive biomacromolecules (proteins and others) also have many drawbacks[1,2], which could be solved by single probe that non-selectively binds to all systems and produces distinct spectroscopic signals for each (Scheme 1a).



a) b) c)

Scheme 1 a) dye simultaneously targeting various DNA, RNA or proteins, each with a selective response, *b) Fluorimetric and Raman sensing of various DNAs and RNAs[4], c) schematic presentation of chromophore preferences to protein or DNA, respectively.[5]*

Three strategies for achieving this goal will be discussed: i) Designing a single chromophore with the appropriate hydrophobicity and binding properties for interaction with DNA, RNA, and proteins (Scheme 1b)[4]; including application of one of the emerging bioimaging techniques based on Raman spectroscopy, which made significant progress in live-cell and tissue imaging, approaching the sensitivity and resolution of confocal fluorescence microscopy;[3] ii) Connecting two chromophores, each selective for different biomacromolecule, with an inert or active linker (Scheme 1c)[5] iii) Utilizing chromophores that can aggregate, where the monomer and aggregate forms show different preferences for biotargets and produce distinct spectrometric responses (Scheme 1a).

REFERENCES

[1] A. Walter, J. Mannheim, C. J Caruana, Imaging Modalities for Biological and Preclinical Research: A Compendium, 2021, IOP Publishing.
[2] T. Niehorster *et al*., *Nat Methods 13*, (2016) 257-262.
[3] F. Hu, L. Shi and W. Min, *Nat Methods 16*, (2019) 830-842.
[4] M. Ferger, *et al*., *Chem. Eur. J.* 27, (2021) 5142-5159.
[5] T. Smidlehner, M. Badovinac, I. Piantanida, *New J Chem*. 42, (2018) 6655-6663.

PL4

SOLUTIONS FOR CAREER DEVELOPMENT AND MENTORSHIP IN THE PHARMACEUTICAL INDUSTRY FOR CHEMISTS

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The pharmaceutical industry offers chemists an array of career paths, each with unique challenges and growth opportunities, particularly in the high-stakes field of drug discovery. This lecture delves into effective strategies for career development and mentorship that empower chemists to excel in this dynamic area. We will explore the competencies essential for success in drug discovery, including interdisciplinary collaboration, innovation-driven thinking, and the agility to navigate technological advancements like AI and automation.

Emphasizing mentorship, we will discuss how seasoned professionals can guide emerging chemists in cultivating specialized skills and fostering an entrepreneurial mindset critical to scientific and commercial achievements. Additionally, we will highlight structured mentorship models and career development frameworks that leading organizations employ to prepare the next generation of chemists for the evolving drug discovery landscape. This session aims to equip participants with actionable insights and best practices to forge meaningful career trajectories within the pharmaceutical sector and contribute to advancing therapeutic solutions.

PL5

PUSHING THE LIMITS OF CHEMICAL SENSING WITH SYNTHETIC LIGANDS AND NANOSTRUCTURES

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This talk intends to present a snapshot of our results in enabling novel chemical sensing concepts and highly improved sensing performances by rationally designed nanostructures and synthetic ligands. In terms of nanostructures, we will focus on solid-state nanopores, which offer a highly sensitive label-free transduction mechanism for the detection of single species. One of the most promising practical applications of single nanopore sensors is the counting and sizing nanoparticles and viruses. For this purpose, we introduced cost-effective quartz nanopores and calibration-free resistive pulse sensing methodologies.[1] Despite the wealth of information (e.g., size, charge, shape) and excellent size resolution that nanopore sensing can provide on single species, complex samples generally require the use of selective ligands. Therefore, the talk will address the chemical modification of gold nanopores[2] and their application for quantitative analysis. Most importantly, it will introduce potentiometric transduction with chemically modified permselective nanopore arrays and single nanopores that enable the selective measurement of ions[3,4] and polyions (e.g. microRNAs)[5]. In this respect we will report on the smallest sensing surface potentiometric ion-selective nanoelectrodes ever fabricated. However, nanopores can be used not only for transduction, but also as nanoreactors that led us to the synthesis of surface imprinted polymers for selective protein recognition.[6] Surface imprinting is a major enabling technology for the preparation of molecularly imprinted polymers (MIPs) for macromolecules. We then further developed the concept of surface imprinting to ultimately enable the high-throughput synthesis of protein chips based on MIPs. This has been realized through gradually refining the synthetic approaches, that includes nanosphere lithography,[7] microelectrospotting,[8] as well as a combination of microcontact printing, peptide epitope imprinting and polymer electrosynthesis[9].

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REFERENCES

1. Terejánszky, P.; Makra, I.; Fürjes, P.; Gyurcsányi, R. E. *Anal Chem* **2014**, *86*, 4688.
2. Jagerszki, G.; Gyurcsányi, R. E.; Höfler, L.; Pretsch, E. *Nano Lett* **2007**, *7*, 1609.
3. Papp, S.; Jágerszki, G.; Gyurcsányi, R. E. *Angew Chem Int Ed.* **2018**, *57*, 4752.
4. Jagerszki, G.; Takács, A.; Bitter, I.; Gyurcsányi, R. E. *Angew Chem Int Ed Engl* **2011**, *50*, 1656.
5. Makra, I.; Brajnovits, A.; Jágerszki, G.; Fürjes, P. t.; Gyurcsányi, R. E. *Nanoscale* **2017**, *9*, 739..
6. Menaker, A.; Syritski, V.; Reut, J.; Oepik, A.; Horvath, V.; Gyurcsányi, R. E. *Adv Mater* **2009**, *21*, 2271.
7. Bognár, J.; Szűcs, J.; Dorkó, Z.; Horváth, V.; Gyurcsányi, R. E. *Adv Funct Mater* **2013**, *23*, 4641.
8. Bosserdt, M.; Erdőssy, J.; Lautner, G.; Witt, J.; Kohler, K.; Gajovic-Eichelmann, N.; Yarman, A.; Wittstock, G.; Scheller, F. W.; Gyurcsányi, R. E. *Biosens Bioelectron* **2015**, *73*, 123.
9. Bognár, Z.; Supala, E.; Yarman, A.; Zhang, X.; Bier, F. F.; Scheller, F. W.; Gyurcsányi, E. R. *Chem Sci* **2022**, *13*, 1263.

PL6

MANIPULATION OF IMMUNE CELLS FOR IMMUNOTHERAPY

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Cellular immunotherapy with human immune cells has shown promise in the treatment of a number of aggressive disorders, particularly cancers, owing to the ability of immune cells to eliminate pathogens. Among immune effectors formulated as cell-therapeutics are natural killer (NK) cells, attractive in large party owing to their safety and potential for allogeneic use. Severe immunosuppression in the microenvironment of solid tumors causes dysfunction, metabolic reprogramming and exhaustion of immune effectors. To improve NK cell persistence and responses, we have employed chemical, pharmacological and biological tools to reprogram immune behavior. We have engineered multi-specific, gate-based constructs which enable NK cells to multi-specifically target and respond to mechanisms of immune evasion, and achieve homing via improved chemokine production. We have demonstrated that the use of chemical compounds with pharmacological activity, such as inhibitors of autophagy and cancer metabolism, can reprogram the microenvironment in favor of immune activation.[1,2] In addition, the us NK cells necessitates the cryopreservation of cell therapy products. A challenge with cryopreservation is the loss of potency of the cells post-thaw, as cells lose viability due to water-induced effects, including dehydration and intracellular ice crystal formation. Additionally, freezing and thawing rates affect cryopreservation. DMSO, the most commonly used cryoprotectant (CPA), has been effective in protecting immune cells during freezing and thawing, as it acts to intracellularly limit freezing and ice crystal formation. However, its ability to induce molecular and genetic changes to immune cells, as well as its toxicity, has stimulated interest in alternative CPAs. Replacing DMSO's ability to act intracellularly has been difficult. In order to develop formulation of cryoprotectants which can effectively cryopreserve human cells, we have investigated the potential of using non-cell-penetrating and cell-penetrating CPAs to recover NK cells post-thaw without DMSO. We have found that cryoprotection using CPA compounds with cell-penetrating ability can retain the viability and cytotoxicity of human peripheral blood-derived NK cells to a comparable degree to DMSO, owing to their intracellular freezing mechanisms being controlled. This talk discusses the potential of chemical and biochemical manipulations of immune cells for immunotherapies of complex diseases.

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REFERENCES

1. Lupo KB, Yao X, Borde S, Wang J, Torregrosa-Allen S, Elzey BD, Utturkar S, Attalah Lanman N, McIntosh M, Matosevic S. synNotch-programmed iPSC-derived NK cells usurp TIGIT and CD73 activities for glioblastoma therapy. 2024, *Nature Communications*, 15, 1909.

2. Wang J, Torregrosa-Allen S, Elzey BD, Utturkar S, Atallah Lanman N, Bernal-Crespo V, Behymer MM, Knipp GS, Yun Y, Veronesi MC, Sinn AL, Pollok KE, Brutkiewicz R, Nevel KS, Matosevic S. Multispecific targeting of glioblastoma with tumor microenvironment-responsive multifunctional engineered NK cells. 2021, *Proceedings of the National Academy of Sciences USA*, 118 (45):e2107507118.

PL7

G-QUADRUPLEX-FORMING APTAMERS

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Many known aptamers are based on guanine-rich oligonucleotides,[1-3] which share a distinctive ability to fold into stable but also extremely different G-quadruplex (G4) structures. Thus, even very similar DNA sequences can exhibit an extraordinarily wide structural variability and provide precious scaffolds to evolve effective aptamers with different biological effects.

In this frame, we recently investigated several G4-forming aptamers specifically targeting cancer-related[4-10] proteins. Our recent results concerning cancer protein-targeting aptamers will be here presented. Special focus will be devoted to G4-forming aptamers selectively recognizing: i) $VEGF_{165}$, a widely studied biomarker protein of different cancer forms,[9] and ii) HMGB1, a cromatin-associated, non-histonic protein released under inflammatory conditions in the extracellular environment, where it acts as a cytokine contributing to the pathogenesis of cancer.[10] Both the anti-VEGF V7t1[4,11,12] and the newly discovered anti-HMGB1 L12[7,8] are highly polymorphic aptamers and their conformational behaviour indeed dramatically depends on the sample manipulation and the chosen buffer. In physiological buffers mimicking the extracellular media and without annealing, both aptamers, though having different sequence and bioactivities, exhibit a similar overall conformational behaviour, folding into very stable dimeric parallel G-quadruplex structures, which recognize their respective target with much higher affinity than their monomeric counterpart. These dimeric aptamers can be efficient therapeutic tools, also inspiring the design of more effective modified analogues for *in vivo* studies.

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REFERENCES

1. J. Zhou, J. Rossi, *Nat. Rev. Drug. Discov.* **2017**, *16*, 181.
2. C. Platella, C. Riccardi, D. Montesarchio, *et al.*, *Biochim. Biophys. Acta - Gen. Subj.* **2017**, *1861*, 1429.
3. D. Musumeci, D. Montesarchio, *Handbook of Chemical Biology of Nucleic Acids* **2023**, 2421.
4. F. Moccia, C. Riccardi, D. Musumeci, L. Petraccone, D. Montesarchio, *Nucleic Acids Res.* **2019**, *47*, 8318.
5. C. Riccardi, D. Musumeci, C. Platella, A. Arciello, D. Montesarchio, *Int. J. Mol. Sci.* **2020**, *21*, 1963.
6. E. Napolitano, *et al.*, *Int. J. Biol. Macromol.* **2023**, *224*, 344.
7. E. Napolitano, *et al.*, *Angew. Chem. Int. Ed.* **2024**, *63*, e202319828.
8. E. Napolitano, *et al.*, *Int. J. Biol. Macromol., under review*.
9. C. Riccardi, E. Napolitano, C. Platella, D. Musumeci, M.A.B. Melone, D. Montesarchio, *Med. Res. Rev.* **2021**, *41*, 464.
10. D. Musumeci, G.N. Roviello, D. Montesarchio, *Pharmacol. Ther.* **2014**, *141*, 347.
11. S.L. Edwards, *et al.*, *Chem. Commun*. **2015**, *55*, 9499.
12. M. Marušič, R.N. Veedu, J. Wengel, J. Plavec, *Nucleic Acids Res.* **2013**, *41*, 9524.

PL8

ENZYMATIC SYNTHESIS AND STRUCTURAL MODELLING OF BIO-BASED OLIGOESTERS AS AN APPROACH FOR THE ECODESIGN OF NEW SUSTAINABLE POLYMERS

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The interest in polymers derived from renewable sources has amplified as demonstrated by the large number of recent patents and publications. The material and polymer sectors are facing the challenge of integrating the sustainability of both processes and products, including their management after disposal. To minimize the effects of their dispersal in open environments due to specific applications (cosmetics and fishing nets, food packaging) stringent eco-design criteria focused on biodegradability and ecotoxicity are required. Our approach integrates experimental and computational methods, analyzing short oligomers to rapidly screen for sustainable alternatives, particularly bio-based ones. Enzymatic polycondensation was used for the preparation of an array of polyesters with controlled structures. These biocatalyzed processes allowed to obtain also functionalized polymers by working at mild temperatures (50-70°C) and under solvent-less conditions. This integrated study sheds light on the relationship between chemical structure and properties, including biodegradability in marine environments and eco-toxicity.

ACKNOWLEDGEMENTS This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 101029444 (RenEcoPol), from ICSC – Centro Nazionale di Ricerca in High Performance Computing, Big Data and Quantum Computing, funded by European Union – NextGenerationEU - PNRR, Missione 4 Componente 2 Investimento 1.4 Grant number CN00000013 and Bruschi R . is grateful to CAFC S.p.A and to NextGenerationEU PNRR (Missione 4, Componente 1, Investimento 3.4 and 4.1).

PL9

INNOVATIVE INTERDISCIPLINARY SCIENCE AND ENGINEERING PROGRAMMES TO EDUCATE THE FUTURE GENERATION CHANGEMAKERS

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Maastricht University (UM) is known for its innovative educational model, international character and transdisciplinary approach to research and education. Within Maastricht University, the faculty of Science and Engineering (FSE) is the youngest faculty established in 2018 to strengthen the STEM presence at UM and the region. At the moment, FSE houses 7 bachelor and 5 master programmes.[1] The faculty is not only located in the historical heart of Maastricht but also present at four Brightlands research and innovation campuses[2] spread over the province of Limburg. This presence aims to establish triple helix collaborations between university, industry and the public sector.

In 2026, UM will celebrate its 50th anniversary. The university started as a medical school, adopting the innovative method of problem-based learning (PBL) that was on the rise at many medical programs. UM became renowned worldwide for the way it implemented PBL as baseline educational philosophy for all educational programmes. PBL is a student-centred, small group-based form of education geared towards self-directed lifelong learning. Together with the typical international classroom at FSE, students collectively analyze and discuss problems, exchange knowledge, cultural experience and learn how to formulate solutions for relevant scientific and societal issues. PBL is an umbrella term for a number of student-centered educational methods based on the four principles known as CCCS[3] (contextual, constructive, collaborative and self-directed learning). The traditional form of PBL has an assortment of variants nowadays in the form of Research Based Learning (RBL), project based learning,… Furthermore, the development of the method continues, guaranteeing that Maastricht remains the innovative educational university it has always been.

UM is not only innovative in the teaching method used within the programmes, the programmes as well can be considered innovative. Research groups and educational programmes within the faculty are build upon societal relevant themes and not in disciplinary departments. This set-up intrinsically needs an interdisciplinary approach. Several educational programmes, for instance Circular Engineering (CE) and the Maastricht Science Programme (MSP) have an open curriculum, giving students the opportunity to fully build their own portfolio based on their interests. This plenary lecture will focus on the set-up of interdisciplinary open curricula in science and engineering, the UM teaching models and how to apply the teaching models on science and engineering courses.

REFERENCE

1. https://www.maastrichtuniversity.nl/about-um/faculties/faculty-science-and-engineering
2. www.brightlands.com
3. https://www.maastrichtuniversity.nl/education/edlab

INVITED LECTURES

IL1

"TO *B* OR NOT TO *B*" IN NUCLEIC ACIDS CHEMISTRY

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Nucleic acids (DNA and RNA) are genetic materials in living organisms and formed by a sequence of nucleobases. The stability of nucleic acids structures cannot be determined from only the sequence composition, as this property critically depends on the surrounding environment of the solution. The intracellular condition is greatly different from that of the diluted buffer typically used for standard experiments and is not constant in each local area of the cell. Thus, to make excellent nanomaterials with nucleic acids working in cells, stability predictions should reflect the situation under intracellular conditions and are required importantly. In this lecture, I will provide an overview of the basic concepts, methods, and applications of predicting the stabilities of nucleic acid structures. I explain the theory of the most successful prediction method based on a nearest-neighbor (NN) model. To improve the versality of prediction, corrections for various solution conditions considered hydration have been investigated.[1-6] I also describe advances in the prediction of non-canonical structures of G-quadruplexes and i-motifs. Finally, studies of ligands binding to canonical and non-canonical structures of nucleic acids are discussed for human health and diseases.

ACKNOWLEDGEMENTS：The author is grateful to the colleagues named in the cited papers from my laboratory, institute (FIBER), and others. This work was supported by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) and the Japan Society for the Promotion of Science (JSPS), especially for Grant-in-Aid for Scientific Research (S) (22H04975), JSPS Core-to-Core Program (JPJSCCA20220005), The Hirao Taro Foundation of Konan Gakuen for Academic Research, and The Chubei Itoh Foundation.

REFERENCES

1. H. Tateishi-Karimata, K. Kawauchi, S. Takahashi, N. Sugimoto, Development of a Pseudocellular System to Quantify Specific Interactions Determining the G-Quadruplex Function in Cells, *J. Am. Chem. Soc* **2024**, *146*, 8005–8015.

2. D. Banerjee, H. Tateishi-Karimata, M. Toplishek, T. Ohyama, S. Ghosh, S. Takahashi, M. Trajkovski, J. Plavec, N. Sugimoto, In-Cell Stability Prediction of RNA/DNA Hybrid Duplexes for Designing Oligonucleotides Aimed at Therapeutics**,** *J. Am. Chem. Soc* **2023**, *145*, 23503-23518.

3. S. Ghosh, S. Takahashi, D. Banerjee, T. Ohyama, T. Endoh, H. Tateishi-Karimata, N. Sugimoto, Nearest-neighbor parameters for the prediction of RNA duplex stability in diverse in vitro and cellular-like crowding conditions, *Nucleic Acids Res.* **2023**, *5*1, 4101-4111.

4. K. T. McQuaid, S. Takahashi, L. Baumgaertner, D. J. Cardin, N. G. Paterson, J. P. Hall, N. Sugimoto, and C. J. Cardin, Ruthenium Polypyridyl Complex Bound to a Unimolecular Chair-Form G-Quadruplex, *J. Am. Chem. Soc* **2022**, *144*, 5956-5964.

5. S. Takahashi, A. Kotar, H. Tateishi-Karimata, S. Bhowmik, Z.-F. Wang, T.-C. Chang, S, Sato, S. Takenaka, J. Plavec, N. Sugimoto, Chemical Modulation of DNA Replication along G-Quadruplex Based on Topology-Dependent Ligand Binding, *J. Am. Chem. Soc*. **2021**, *143*, 16458-16469.

6. N. Sugimoto ed., Handbook of Chemical Biology of Nucleic Acids, SPRINGER NATURE, **2023**, Vols 1- 3.

IL2

ADDING COLOUR TO ION SENSING IN SOLUTIONS

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The classical ion-selective sensors receptors composition requires presence of ionophore and ion-exchanger within plasticized polymeric matrix. Typically, none of these compounds is active in optical mode, thus typically electrochemical, potentiometric, ion-selective sensors are colorless.

Adding dyes to ion-selective membranes is attractive challenge that in principle can allow extension of application of highly selective sensors for other modes: absorption (colorimetry) or emission (fluorimetry). Even more challenging it is to achieve this using dyes that do not perturb sensing, and do not induce receptor sensitivity to pH changes. This can be accomplished using Nile blue and Nile red dyes [1]. Advantages of presence of these dyes in the ion-selective membrane include, among others, possibility of recording ratiometric signals.

REFERENCES

1. A. Konefał , P. Piątek , K. Maksymiuk, A. Michalska *Sens. Actuators: B. Chemical* **2023**, *391*, 134022.

GRAPH THEORETICAL REPRESENTATION OF CHEMICAL SYSTEMS

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Recent investigations of communications between macromolecules and corresponding molecular aggregates on the micro scale[1] afford the opportunity for the development of new approach in system studies by using simple chemical examples.

In this work such chemical communication systems are represented by using chemical graph theory,[2] the method that has already been applied in the general system studies.[3]

REFERENCES

1. J. Ventura, A. Llopie-Lorente, L. K. E. A. Abdelmohsen, J. C. M. van Hest, *Acc. Chem. Res.* **2024**, *57*, 815-830.
2. H. Vančik, *From complexity to systems*, Foundations of Chemistry, **2022**, *25*, 345-358.
3. H. Vančik, *From Complexity to Systems*, Springer Nature, Dordrecht, London, NY, **2024**.

IL4

NEW GENERATION OF QUATERNARY AMMONIUM COMPOUNDS: THE POTENT AMPHIPHILES IN COMBATING BACTERIAL RESISTANCE

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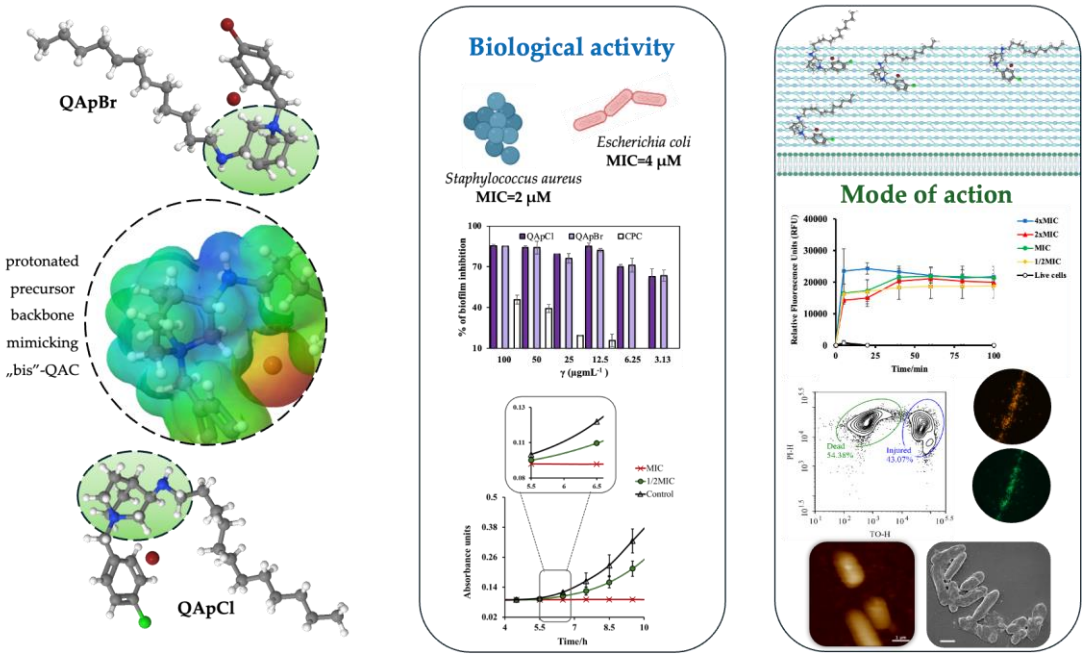
Quaternary ammonium compounds (QACs) are essential antimicrobial agents widely used for disinfection due to their ability to disrupt bacterial cell membranes. However, growing bacterial resistance and environmental persistence necessitate the development of modified "soft" QACs. Recent studies have explored structural modifications, including the introduction of hydrolyzable groups (e.g., amides and esters), to create environmentally safer QACs with reduced resistance potential. Investigations into pyridinium-4-aldoxime and 3-amidoquinuclidine derivatives have revealed critical structure-activity relationships, showing that hydrophobic-hydrophilic balance, backbone polarity, and rigidity significantly affect antimicrobial efficacy. For example, while pyridinium-4-aldoxime compounds exhibited promising antiviral properties, their antibacterial activity was limited by polar substituents, whereas 3-amidoquinuclidine compounds displayed broad antibacterial activity and lower toxicity than traditional QACs. Furthermore, comparative analyses indicate that 3-aminoquinuclidine QACs outperform other 3-substituted quinuclidine QACs in biofilm inhibition and Gram-positive bacterial activity, underscoring the importance of polarity and backbone design. These findings from recent studies offer valuable insights for designing next-generation QACs that enhance antimicrobial effectiveness while prioritizing environmental safety and minimizing resistance development.



IL5

DEVELOPMENT OF INDUSTRIAL BIOTRANSFORMATIONS BY APPLYING CHEMICAL ENGINEERING APPROACH

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Industrial biotransformations are gaining more and more attention in industry as they provide new routes to novel compounds and alternative ways to produce the existing ones.[1,2] Still, to reach the industrial scale, the timeline of research needs to be shortened, which is often a hurdle that needs to be overpassed. As the research performed today is very interdisciplinary, it is expected that the time from lab to market will become shorter, and that biocatalysis will obtain its well-deserved space in production of chemicals. From the point of chemical engineering, efforts are done to investigate these systems as well as to assess their potential viability conducting experiments at the lab scale.[3] The first line of research is the kinetics of the enzyme-catalysed reaction, which enables mathematical modelling and model-based process optimization. This implies conducting small-scale lab experiments that give an insight on important features of the system, such as inhibitions or enzyme instability making it possible to draw conclusions on the reactor setup as well as process conditions to perform the reaction. Since a great part of the work can be conducted by simulation of mathematical models, time and money can be saved. Mathematical modelling enables a thorough research of complex reaction system such as multi-enzyme cascade reactions, which is otherwise very difficult to perform.[4,5] In this talk features of the approach will be presented, and some experience from the group presented.

ACKNOWLEDGEMENTS This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101000560 (RADICALZ) and Marie Skłodowska-Curie grant agreement No 956631 (C-C Top).

REFERENCES

1. S. Wu, R. Snajdrova, J. C. Moore, K. Baldenius, U. T. Bornscheuer, *Angew. Chem. Int. Ed*. **2021**, *60*, 88.
2. E. L. Bell, W. Finnigan, S. P. France, A. P. Green, M. A. Hayes, L. J. Hepworth, S. L. Lovelock, H. Niikura, S. Osuna, E. Romero, K. S. Ryan, N. J. Turner, S. L. Flitsch, *Nat. Rev. Methods Primers*, **2021**, *1*, 46.
3. N. Milčić, M. Sudar, A.-K. Marić, K. Kos, M. Majerić Elenkov, Z. Findrik Blažević, *Ind. Eng. Chem. Res*. **2024**, *63*, 7051.
4. M. Sudar, Z. Findrik Blažević, Enzyme Cascade Kinetic Modelling, in Enzyme Cascade Design and Modelling, S. Kara, F. Rudroff (Eds.), Switzerland: Springer International Publishing, **2021**. p. 91–108.
5. M. Sudar, N. Milčić, M. Česnik Katulić, A. Szekrenyi, K. Hernandez, M. Fekete, R. Wardenga, M. Majerić Elenkov, Y. Qi, S. Charnock, Đ. Vasić-Rački, W.-D. Fessner, P. Clapes, Z. Findrik Blažević, *RSC Adv.* **2024**, *14*, 21158.

IL6

ENZYMES FOR SUSTAINABLE CHEMICAL SYNTHESIS AND BIOSENSING APPLICATIONS

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The application of enzymes in the chemical industry has been steadily increasing due to advancements in bioinformatics, metagenomics, directed evolution and rational protein engineering. These breakthroughs have had a profound impact on numerous research areas, including organic synthesis, biophotocatalysis, and bioelectrochemistry. In my group, we have primarily focused on biocatalysis for sustainable chemical synthesis, including the synthesis of (chiral) alcohols, amines, carboxylic acids, nitriles, and epoxides using oxidoreductases, transaminases, and hydrolases. For instance, we have studied the synthesis of chiral amines from ketones using ω-transaminases (ωTAs), amine dehydrogenases (AmDHs), and imine reductases (IReds).[1] In this context, we developed a new family of thermostable AmDHs, which were applied for the synthesis of API intermediates.[2] AmDHs, IReds, and ωTAs were also incorporated into biocatalytic cascades with other enzyme families for the conversion of alcohols, styrene derivatives, α-amino acids, or α,β-unsaturated ketones into chiral amines or amino alcohols containing up to two stereogenic centers.[3] Additionally, we discovered new biocatalytic reactions, including the conversion of alcohols into nitriles catalyzed by an alcohol oxidase using ammonia and air.[4] Generally, we perform all these biotransformations with isolated or immobilized enzymes in batch or flow systems, or with resting whole cells. We have also worked on developing enzyme-based bioelectrochemical systems for chemical conversions and biosensing applications. We explored the asymmetric reduction of activated alkenes using ene-reductases (EReds) in a system where the enzyme cofactor was electrochemically regenerated.[5] To meet the growing demand for affordable, robust, sensitive and selective biosensing platforms, we constructed a biosensor for detecting uric acid by immobilizing an engineered urate oxidase onto gold nanoparticles deposited on a carbon-glass electrode.[6] We also developed a strategy for creating recyclable fluorescent probes using engineered enzymes with enhanced thermo- and chemo-stability.[7] These probes maintained high diagnostic accuracy and stability, even after multiple recycling cycles and exposure to high temperature.

SELECTED REFERENCES

[1] T. Knaus, W. Böhmer, F. G. Mutti, *Green Chem.* **2017**, *19*, 453-463.
[2] V. Tseliou, T. Knaus, M. F. Masman, M. L. Corrado, F. G. Mutti, *Nat. Commun.* **2019**, *10*, 3717.
[3] a) T. Knaus, M. L. Corrado, F. G. Mutti, *ACS Catal.* **2022**, *12*, 14459-14475; b) M. L. Corrado, T. Knaus, F. G. Mutti, *Green Chem.* **2019**, *21*, 6246-6251; c) M. L. Corrado, T. Knaus, U. Schwaneberg, F. G. Mutti, *Org. Process Res. Dev.* **2022**, *26*, 2085-2095.
[4] J. Vilim, T. Knaus, F. G. Mutti, *Angew. Chem. Int. Ed.* **2018**, *57*, 14240-14244.
[5] Z. Wei, T. Knaus, M. Damian, Y. Liu, C. S. Santana, N. Yan, G. Rothenberg, F. Mutti, *ChemBioChem* **2024**, e202400458.
[6] Z. Wei, T. Knaus, Y. Liu, Z. Zhai, A. F. G. Gargano, G. Rothenberg, N. Yan, F. G. Mutti, *Chem. Commun.* **2023**, *59*, 8071-8074.
[7] Y. Liu, Z. Wei, M. Damian, X. Zhu, T. Knaus, H. Zhang, F. G. Mutti, F. F. Loeffler, *Adv. Mater.* **2023**, *35*, e2306615.

IL7

CHIRAL RESOLUTION, KINETICS AND THERMODYNAMICS IN PREFERENTIAL CRYSTALLISATION

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In preferential crystallization for chiral resolution, control over solubility in the racemic system plays a major role. In Figure 1, the process of preferential crystallization is demonstrated, for which the presence of a conglomerate (enantiomers crystallize independently in enantiopure crystals) is essential. At the starting point, the racemic mixture is in solution at saturation. Adding a crystalline seed of one of the pure enantiomers causes that enantiomer to supersaturate, which triggers its crystallization and through entrainment more crystal is recuperated than what has been added. Once a concentration imbalance among the enantiomers exists, adding more crystalline racemic mixture will trigger crystallization of the enantiomer that has subsequently become supersaturated.

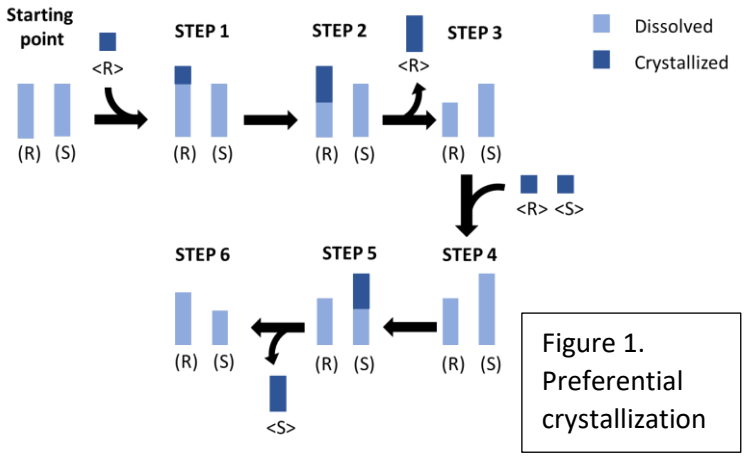
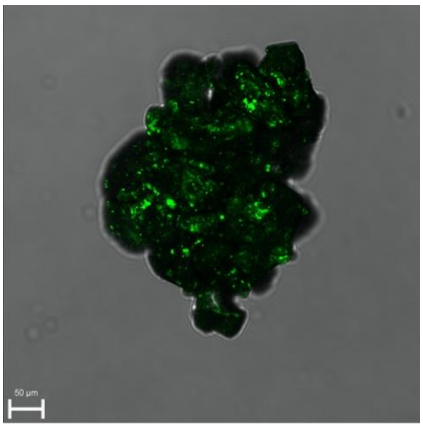


Figure 1. Preferential crystallization

This process is fully depending on thermodynamic parameters such as solubility and supersaturation. Much less is known about the crystallization kinetics of enantiomers and racemic systems. In a paper on L-histidine, pure enantiomer appears to crystallize much faster than racemic crystals. In the photograph on the right DL-histidine racemic crystals are shown after crystallization from the racemic solution. The light-green areas obtained by SHG (second harmonic generation) demonstrate the presence of enantiopure crystallites even though the racemic crystal is thermodynamically stable. Although much work remains to be done, this may open possibilities to use kinetics to steer preferential crystallization.[1] Moreover, using achiral molecules to initiate preferential crystallization will also be discussed.



ACKNOWLEDGEMENTS IBR thanks, G. Coquerel, L. Harfouche, S. Clevers, M. Hoquante, F. Painsecq, FEDER (EU) and the Normandy Region for the project NACRE and the University of Rouen for PhD grants.

REFERENCES

1. L.C. Harfouche, S. Clevers, G. Coquerel, I.B. Rietveld, *CrystEngComm* **2021,** *23*, 8379-8385.

IL8

UNVEILING NEXT-GEN CHEMISTRY EDUCATION: CURRICULUM INNOVATIONS AT INHOLLAND UNIVERSITY OF APPLIED SCIENCES

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This presentation will outline a comprehensive four-year program at the University of Applied Sciences Inholland, designed to develop students into skilled analysts and researchers. The program is structured to provide a broad foundational knowledge in the initial phase, followed by opportunities for specialization and hands-on experience in later years.[1]

The first year, known as the propaedeutic phase, focuses on the basics of laboratory research. Students follow a common curriculum with peers from Biology and Medical Laboratory Research (BML) and Biotechnology programs. This interdisciplinary approach ensures a broad perspective, essential for collaborative professional practice.

In the second year, students choose to continue with Chemistry or switch to BML or Biotechnology. Those who continue with Chemistry delve deeper into essential theories and skills required for chemical analyst. The second year culminates in a choice between two specializations: Energy and Next Generation Materials or Advanced Analytical Solutions. The former focuses on developing sustainable polymers, while the latter emphasizes precise analytical methods.

The third year combines specialization with practical experience. Students spend the first half of the third year in internships, conducting research at companies or institutes. This hands-on experience is crucial for applying theoretical knowledge in real-world settings.

The fourth year is dedicated to graduation, where students undertake an independent research project. This project can be conducted at a university, research organization, or chemical company, allowing students to integrate into professional research teams and participate in work discussions and meetings.

The program employs a variety of teaching formats, including tutorials, practica, and project groups.[2] The academic year is structured into four ten-week periods, each focused on a unique theme. Our academic program offers international students a wealth of opportunities, including a variety of courses and hands-on internship projects. Join for the presentation, where we'll dive into these possibilities.

ACKNOWLEDGEMENTS The author extends her gratitude to the Life Sciences and Chemistry team at the University of Applied Sciences Inholland for their invaluable contribution to the development of the new curriculum program.

REFERENCES

1. DAS Profile, Profile description - Domein Applied Science EN, (retrieved: 26-08-2024).
2. H.Y Samayoa-Oviedo, J. Laskin, *J. Chem. Educ.* **2022**, *12*, 4043-4050.

IL9

HARNESSING ANCESTRAL SEQUENCES TO IMPROVE THE SOLUBILITY OF PLASTIC-DEGRADING ENZYMES

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The growing concern over plastic pollution necessitates innovative biodegradation approaches,[1] particularly for biopolymers like polylactic acid (PLA).[2] In this study, we identified a novel enzyme, MGY, exhibiting PLA-degrading activity from a metagenomic database. Despite its effectiveness, the MGY enzyme suffered from low solubility and poor yield, complicating structural and functional characterization. To overcome these challenges, we utilized ancestral sequence reconstruction as a strategic design tool.[3] This approach allowed us to infer and produce ancestral enzyme variants from three distinct evolutionary nodes, all of which demonstrated significantly enhanced solubility and expression yields. Activity assays (Figure 1.) confirmed that these ancestral variants retained strong PLA-degrading activity and could be obtained in higher concentrations. This advancement facilitates downstream applications as well as detailed structural and activity studies, highlighting the potential of ancestral sequence reconstruction to enhance the use of biocatalysts for sustainable plastic degradation.

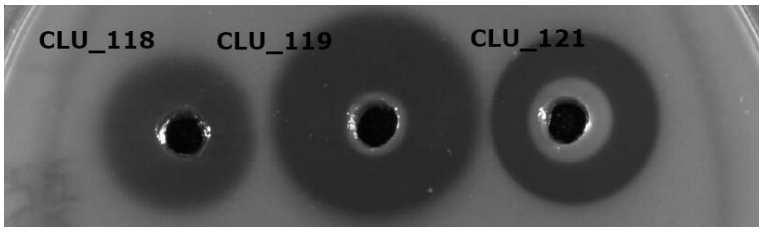

Figure 1. All three ancestral variants of MGY enzyme show robust PLA-degrading activity.

ACKNOWLEDGEMENTS

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REFERENCES

1. Rosenboom, JG., Langer, R. and Traverso, G. *Nat. Rev. Mater.* **2022**, *7*, 117.

2. Hajighasemi, M. Tchigvintsev A, Nocek B, Flick R, Popovic A, Hai T, Khusnutdinova AN, Brown G, Xu X, Cui H, Anstett J, Chernikova TN, Brüls T, Le Paslier D, Yakimov MM, Joachimiak A, Golyshina OV, Savchenko A, Golyshin PN, Edwards EA, Yakunin AF. *Environ. Sci. Technol.* **2018**, *52*, 12388.

3. Schriever K., Saenz-Mendez P., Srilakshmi Rudraraju R., Hendrikse N. M., Hudson E. P., Biundo A., Schnell R., Syrén P.-O. *J. Am. Chem. Soc.* **2021**, *143*, 3794.

IL10

ROADMAP TO ARTIFICIAL INTELLIGENCE IN CHEMISTRY: FROM BABY STEPS TO DEPLOYMENT

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This research explores the path of integrating artificial intelligence (AI) into the field of chemistry, focusing on how machine learning methods are practically applied [1]. Starting with an analysis of published studies using Scopus and VosViewer [2], it shows AI's growing impact on chemical research, highlighting early developments, major achievements, and strategies for full deployment. A case study on wine quality analysis is included, using the JASP software to demonstrate how machine learning can improve quality assessments [3]. This example illustrates how supervised learning models predict wine quality based on chemical properties, offering insights into data-driven decisions that enhance product quality, similar to Cortez et al. [4]. Finally, the roadmap for the deployment of AI in chemistry is provided clearly, proposing the step-by-step approach, ranging from vertical solutions to open-source software.

REFERENCES

1. Adams, N., Schubert, U. S. From data to knowledge: chemical data management, data mining, and modeling in polymer science. *Journal of Combinatorial Chemistry* **2004**, *6*, 12-23.

2. Van Eck, N., & Waltman, L. Software survey: VOSviewer, a computer program for bibliometric mapping. *scientometrics*, **2010**, *84*, 523-538.

3. Love, J., Selker, R., Marsman, M., Jamil, T., Dropmann, D., Verhagen, J., ... & Wagenmakers, E. J. JASP: Graphical statistical software for common statistical designs. *Journal of Statistical Software*, **2016,** *88*, 1-17.

4. Cortez, P., Teixeira, J., Cerdeira, A., Almeida, F., Matos, T., & Reis, J. Using data mining for wine quality assessment. In *Discovery Science: 12th International Conference, DS 2009, Porto, Portugal, October 3-5,* **2009** *12* (pp. 66-79), Springer Berlin Heidelberg.

IL11

SELENIUM NANOPARTICLES AS DRUG DELIVERY SYSTEM FOR LEVODOPA IN THE TREATMENT PARKINSON'S DISEASE – *IN VITRO* EVALUATION

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Parkinson's disease (PD), neurodegenerative disease that affects thinking, skilled movements, feelings, cognition and memory, is characterized by the degeneration of dopaminergic neurons which causes massive depletion of dopamine. Main therapeutic strategy for PD is to increase level of dopamine by administration of its precursor levodopa. However, levodopa treatment is responsible for different side effects in PD patients, many of them being caused by increased oxidative stress. We aimed to design safer and more efficient nanoformulation for levodopa by employing selenium nanoparticles (SeNPs) with two different stabilization agents: Tween 20 and poly(vinylpyrrolidone). Using *in vitro* 2D and 3D models of dopaminergic neurons, safety and biocompatibility of Tween-SeNP and PVP-SeNP were evaluated as nanodelivery systems of levodopa. Obtained results showed that both nanoformulations were non-toxic to dopaminergic neurons under in vitro settings. Moreover, PVP-SeNP exhibited protective action against levodopa-induced oxidative stress and cellular damages.

ACKNOWLEDGEMENTS This study was financially supported by the "Research Cooperability" Program of the Croatian Science Foundation funded by the European Union from the European Social Fund under the Operational Programme Efficient Human Resources 2014–2020 (grant HRZZ-PZS-2019-02-4323).

MECHANOCHEMISTRY: FUNDAMENTALS TO APPLICATION

IL12

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In the first part, I will talk about the role of mechanochemistry in prebiotic chemistry. For example, prebiotically plausible pathways to peptides from inactivated amino acids are unclear as most oligomerization approaches rely on thermodynamically disfavored reactions in solution. I will show how a combination of mineral surfaces and mechanochemical activation enables the oligomerization of amino acids to oligopeptides (Figure 1).[1]

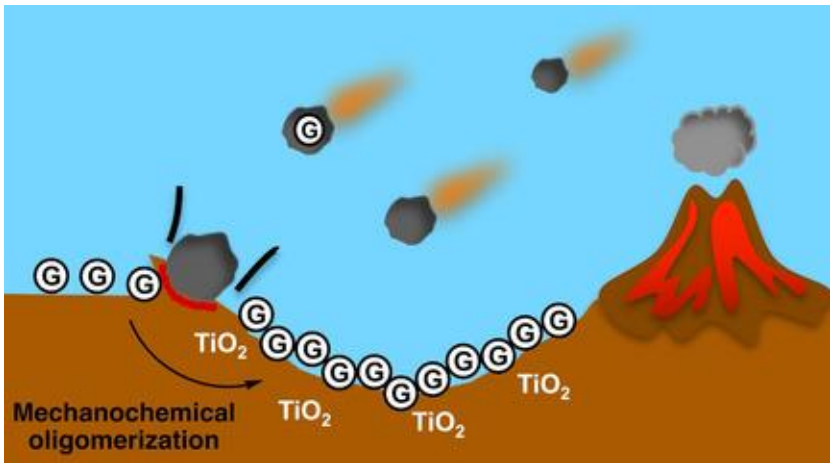

Figure 1. Mechanochemical oligomerization of amino acids on mineral surfaces.

In the second part, I will show how fundamental studies inspired to use mechanochemistry for the sustainable synthesis of commercially relevant compounds, in line with the United Nations Sustainable Development Goals.[2] We developed a solvent-free thermo-mechanochemical approach for the direct coupling of carboxylic acids and amines, which avoids activators and additives. We applied our methodology for the quantitative synthesis of the active pharmaceutical ingredient moclobemide (Figure 2).[3]

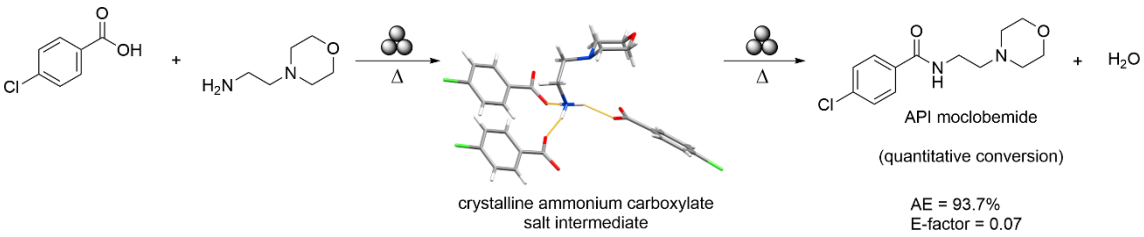

Figure 2. Thermo-mechanochemical route to moclobemide includes the formation of a supramolecular intermediate before the amide bond formation.

REFERENCES

1. T. Stolar, S. Grubešić, N. Cindro, E. Meštrović, K. Užarević, J. G. Hernández, *Angew. Chem. Int. Ed.* **2021**, *60*, 12727.

2. J. Alić, M.-C. Schlegel, F. Emmerling, T. Stolar, *Angew. Chem. Int. Ed.* **2024**, e202414745.

3. T. Stolar, J. Alić, G. Talajić, N. Cindro, M. Rubčić, K. Molčanov, K. Užarević, J. G. Hernández, *Chem. Commun*. **2023**, *59*, 13490.

SECTION LECTURES

SL1

NITROXOLINE: THE POWER OF CHELATION

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Nitroxoline (NTX, Figure 1.) is an 8-hydroxyquinoline (8-HQ) derivative, an ancient antibiotic whose use dates back to the beginning of 20th century. In the era of modern antibiotics, NTX has fallen out of use due to underestimation of its antimicrobial activities; it was kept in use only in Eastern European countries and Germany. In the last few years, with the dramatic rise of antibiotic resistance, NTX underutilisation turned out to be "advantage of backwardness", which led to a boost of research interest. Nowadays, NTX is investigated as a repurposing drug in cancer treatments, as antiviral and antifungal agent, and in combination therapies with other antibiotics.

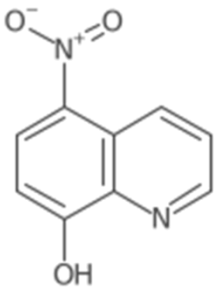

Figure 1. Nitroxoline

The 8-HQ core of NTX structure belongs to so-called "privileged structures", a concept designating molecular scaffolds with versatile binding properties, enabling a mode of action that – unlike any other class of antibiotics – rests solely on chelation[1]. It is known that NTX acts bacteriostatically by chelating divalent cations essential for bacterial growth, but this oversimplification does not suffice in explaining its pleiotropy. In our recent study[2], we investigated types of interactions between NTX and aminoglycoside antibiotic gentamicin (GEN) on 29 strains of *Enterococcus faecalis*, a bacterial species responsible for 80 – 90 % of human enterococcal infections. Besides determination of concentration combinations with synergistic/additive interactions, the results also showed antiadhesion/antibiofilm effect, disruption of cell membrane integrity and upregulation of the expression of numerous ribosomal proteins, suggesting that chelation enables not one but multiform antimicrobial activities.

ACKNOWLEDGEMENTS This research was funded by University of Rijeka grants (uniri-iskusni-prirod-23-92 and uniri-iskusni-biomed-23-110) and supported by the European Union—Next Generation EU 533-03-23-0006 (BioMolTox).

REFERENCES

1. D. Repac Antić, M. Parčina, I. Gobin, M. Petković Didović, *Antibiotics* **2022**, *11*, 1105.

2. D. Repac Antić, B. Kovač, M. Kolenc, I. Brčić Karačonji, I. Gobin, M. Petković Didović, *Antibiotics* **2024**, *13*, 829.

SL2

CHIRAL VERSUS ACHIRAL ASSEMBLIES IN MULTI-STIMULI RESPONSIVE SUPRAMOLECULAR POLYMERIZATION OF TETRA-SUBSTITUTED AZOBENZENE DYE

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The concept of self-assembly, wherein molecules organize into structured patterns driven by non-covalent interactions, has undergone thorough examination through numerous studies[1]. Manipulating the aggregation process and subsequent alterations in chirality and/or morphology can be achieved not only by adjusting supramolecular interactions but also by utilizing external stimuli, whether chemical or physical. Over recent decades, the field of supramolecular chemistry has seen an influx of systems containing photoactive components like spiropyran, diarylethene, or azobenzene, rendering materials with light-responsive properties[2]. Integrating photoswitchable components into the molecular design of supramolecular structures presents unique prospects for controlling their shape and functionality through optical stimuli. However, mastering geometric and electrical changes in response to various external stimuli at the molecular level remains a fundamental challenge. Herein, the reversible formation of the aggregates of L-tyrosine E-azobenzene-tetracarboxamide (E-ABT) is shown to be finely controlled by light, solvent, or chemical additives. The resulting assemblies vary not only in their overall shape and supramolecular interactions but also in their chirality. Depending on the applied conditions, self-assembly can produce either chiral columns or π-stacked 'achiral' oligomers. This study highlights the potential of deliberate monomer design to achieve precise control over self-assembly through chosen stimuli, thereby opening pathways for utilizing multi-responsive, sterically hindered azo-benzene aggregates in materials chemistry and nanotechnology[3].

ACKNOWLEDGEMENTS This work was financed by National Science Centre (grant SONATA BIS 2018/30/E/ST5/00032)

REFERENCES

1. J.-M. Lehn, Supramolecular Chemistry: Concepts and Perspectives, Wiley, Weinheim, Germany **1995**.
2. A. Goulet-Hanssens, F. Eisenreich, S. Hecht, Adv. Mater. **2020**, *32*, 1905966.
3. M. Conková, G .Markiewicz, Ł. Majchrzycki, A. Szmulewicz, A. R. Stefankiewicz, Small Methods, **2024**, 2301681.

SL3

BIS(TRIBENZYLAMMONIUM) FLUORIDE RECEPTOR – INTERPLAY OF STRONG AND WEAK HYDROGEN BONDS FORMING A SUPRAMOLECULAR CAPSULE

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Although molecular recognition and anion recognition had been studied since the 1960-es, the problematics of anion coordination has received greater attention only during the past several decades. This also included the design of ligands for bonding to specific anions, usually by forming a number of hydrogen bonds between the anion and the ligand. Such ion ligands or receptors may be either unique molecules with a specific hydrogen bonding donor pattern, or supramolecular complexes of several molecules. In the latter case, the desired supramolecular complex forms only in the presence of the specific anion which acts as a template.

Such a supramolecular complex acting as a fluoride receptor was detected in the crystal structure of tribenzylammonium fluoride monohydrate, where one half of fluoride ions were found to be placed within capsules composed of a pair tribenzylammonium cations hydrogen bonded to the same fluoride (d(N—H···F) = 2,467 Å). The capsule is additionally stabilized by six C—H···π contacts of 3,668 Å. When additional tribenzylammonium ions were added by co-crystallization of tribenzylammonium fluoride with other tribenzylammonium salts – thus increasing the molar ratio of tribenzylammonium cations to fluoride anions to 2:1 – all the fluoride anions were encapsulated as described above, while the various used counterions remain outside the capsule. Furthermore, the formation of such capsules was found to be specific for fluoride anion, and replacing it with other halogenides, no such capsules are formed. This can be attributed primarily to the anion radius, since the increase of central ion size makes the closing of the capsule with C—H···π contacts impossible, but also to weaker hydrogen bonding of heavier halogenides to the protonated amine in comparison to the highly basic fluoride.

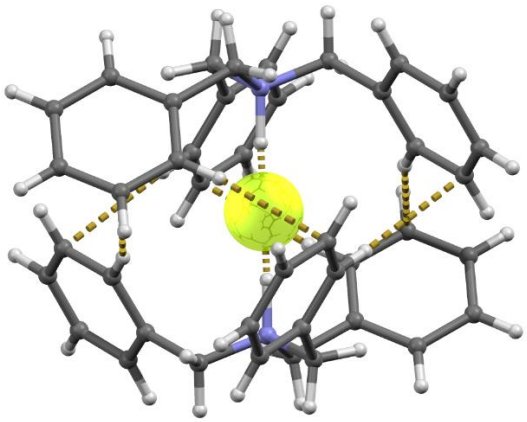

Figure 1. A fluoride anion in a bis(tribenzylammonium) capsule in the crystal structure of tribenzylammonium fluoride monohydrate.

SL4

INOVATIVE APPROACHES IN DRUG DESIGN: FROM MOLECULAR DYNAMICS TO NEURAL NETWORKS

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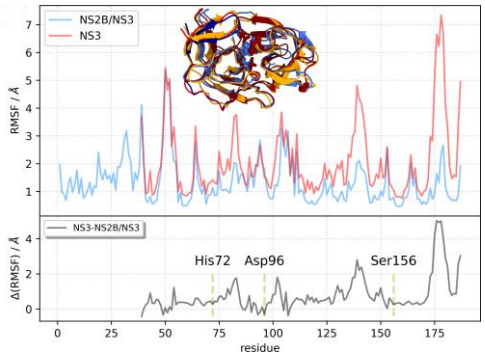
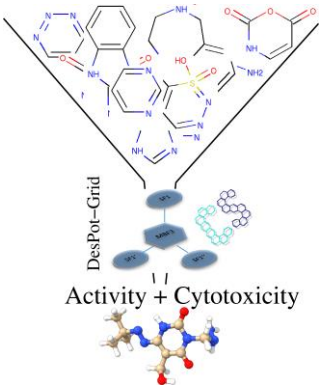
Efficiency and safety are among the most desirable characteristics of an ideal drug. The massive increase in computational power and the integration of artificial intelligence into the field of computational drug design are accelerating the processes of identification, development, and optimization of potential drugs.

We will delve into the study of the monkey fever virus (KFDV), a neglected human pathogen that causes severe hemorrhagic fever and currently lacks antiviral therapy. The focus will be on the dynamics of the NS3 viral protease and the NS2B cofactor, and the identification of potential allosteric sites in the NS2B/NS3 protease of KFDV. The applicability of these proposed allosteric binding sites will be confirmed through virtual screening and molecular dynamics simulations.[1]

Additionally, we will explore a combined approach that leverages neural networks and linear regression to build models for predicting cytotoxicity and anti-HIV activity. A genetic algorithm will be fused with the Des-Pot Grid algorithm to generate new molecules from a predefined set of molecular fragments. This innovative method will lead to the design of new molecules with high anti-HIV activity and low cytotoxicity.[2]

Join us to discover how these cutting-edge techniques are paving the way for the next generation of drug design, offering hope for new treatments and breakthroughs in combating viral diseases.





REFERENCES

1. S. Kandagalla, B. Kumbar, J. Novak, *International Journal of Molecular Sciences* ***2023***, *24*, 10907.

2. J. Novak, P. Pathak, M.A. Grishina, V.A. Potemkin, *Journal of Computational Chemistry* **2023**, *44*, 1016.

SL5

ELECTROACTIVE MOLECULARLY IMPRINTED POLYMERS IN SELECTIVE SENSING

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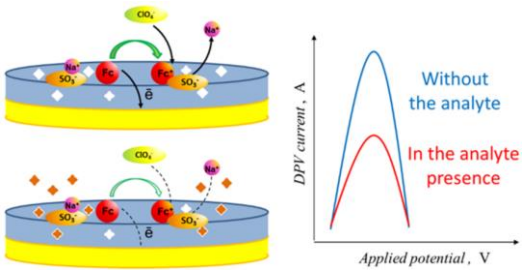
Molecularly imprinted polymers (MIPs) are bio-mimicking recognizing materials used for sensors fabrication.[1] The analytical parameters of these chemosensors, such as sensitivity, selectivity, and detectability, are almost as high as those of biosensors. Moreover, MIP-based chemosensors are superior concerning their ease of fabrication, durability, and tolerance to harsh experimental conditions, including elevated or decreased temperature, high ionic strength, extreme pH values, the presence of heavy metal ions and organic solvents in the samples. Therefore, MIP-based chemosensors found numerous applications in environmental analysis,[2] food quality control,[3] and clinical analysis.[4] For the electrochemical determination of non-electroactive analytes, some external redox probe is usually added to the test solution. It is assumed that target analyte molecules' binding into molecular cavities causes MIP film swelling or shrinking. According to the so-called "gate effect" mechanism, this polymer "breathing" causes changes in the redox probe permeability through an MIP film, thus changing faradaic current corresponding to the redox probe's oxidation in voltammetric determinations.[5] For conductive MIPs changes of the voltammetric signal originate from changes in electrochemical properties of the film.[6] We have proven that, for both conductive MIP films[7] and non-conductive MIP NPs[8] it is possible to immobilize redox probe inside of the polymer matrix by co-polymerization of monomers containing ferrocene groups. These sensors enabled label-free sensitive determination of target analytes. This may be crucial for sensors applications, especially in in-field experiments and in point-of-care devices.



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REFERENCES

1. P. S. Sharma, Z. Iskierko, A. Pietrzyk-Le, F. D'Souza, W. Kutner, *Electrochem. Commun.* **2015**, *50*, 81.
2. P. Rebelo, E. Costa-Rama, I. Seguro, J. G. Pacheco, H. P. A. Nouws, M. Cordeiro, C. Delerue-Matos, *Biosens. Bioelectron.* **2021**, *172*, 112719.
3. J. Ashley, M.-A. Shahbazi, K. Kant, V. A. Chidambara, A. Wolff, D. D. Bang, Y. Sun, *Biosens. Bioelectron.* **2017**, *91*, 606.
4. M. Feroz, P. Vadgama, *Electroanalysis* **2020**, *32*, 2361.
5. D. Korol, A. Kisiel, M. Cieplak, A. Michalska, P. S. Sharma, K. Maksymiuk, *Sens. Actuators B: Chem.* **2023**, 3821, 133476.
6. P. Lach, M. Cieplak, M. Majewska, K. R. Noworyta, P. S. Sharma, W. Kutner, *Anal. Chem.* **2019**, *91*, 7546.
7. P. Lach, M. Cieplak, K. R. Noworyta, P. Pieta, W. Lisowski, J. Kalecki, R. Chitta, F. D'Souza, W. Kutner, P. S. Sharma, *Sens. Actuators B Chem.* **2021**, *344*, 130276.
8. P. Lach, A. Garcia-Cruz, F. Canfarotta, A. Groves, J. Kalecki, D. Korol, P. Borowicz, K. Nikiforow, M. Cieplak, W. Kutner, S. A. Piletsky, P. S. Sharma, *Biosens. Bioelectron.* **2023**, *236*, 115381.

SL6

CALIX-BASED RECEPTORS: FROM FUNDAMENTAL STUDIES TO MATERIALS IN ACTION

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The field of supramolecular chemistry has been and still is the subject of extensive research mainly concerned with the synthesis, structural characterisation and host-guest complexation processes. Much less attention has been paid to detailed studies regarding thermodynamic aspects associated to these processes. Indeed, the understanding of these parameters is essential to define quantitatively the selective behaviour of a macrocyclic receptor for one species relative to another in a given medium. The Laboratory of Thermochemistry at the University of Surrey has demonstrated the importance of experimental thermodynamics in understanding the factors that contribute to complex stability in the binding process with particular emphasis on the solvation of reactants and the product in the complexation process. These fundamental studies are of paramount importance for the design of smart materials that are used for different applications. Fundamental studies on calix[4] based macrocycles namely, *meso*-octamethylcalix[4]pyrrole (CP), 21,22,23-tri(N,N-diethyl-thioacetamide)octamethyl-calix[4]pyrrole (CPII), *meso*-tetramethyl-tetrakis[(diethylthiocarbamoyl)phenoxy] calix[4]-pyrrole (CPIII) and 5,11,17,23-tetra-*tert*-butyl[25,27*bis*(diethylthiocarbamoyl)oxy]calix[4]arene (CAII) are reported along with the analytical applications.

SL7

AUTOMATED PRODUCTION OF SOLID-CONTACT ION-SELECTIVE ELECTRODES: POLYMERIC MEMBRANE DRYING ASSESMENT

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Due to minimum instrumental requirements and electrode design simplicity, open circuit potentiometry has become a promising technique in point-of-care and environmental sensing systems, as the technique includes only a working (indicator) and reference electrode. A breakthrough in solid-contact electrode (SCE) architecture led to novel production techniques that originated from the graphics industry: state-of-the-art SCEs are nowadays mass-produced by screen-printing. Well demonstrated for conductive leads deposition, screen-printing does not apply to ion-selective membrane deposition to the SCE due to the imparity of the membrane's physical characteristics to those intended for screen printing.

Herein, we demonstrate that an industrial automated dispensing machine for controllable deposition of small volumes of liquids can be used to modify screen-printed SCE with an ion-selective membrane. The proposed method is possible to significantly lower the required overall number of membrane deposition steps without altering the dry solute membrane content and improve the membrane homogeneity solely by optimizing the solvents for the ISM preparation. We observed that dry membrane uniformity strongly depends on the solvent volume ratio, i.e. tetrahydrofuran (THF) and cyclohexanone.

Colourimetric absorbance[1] measurements were used for the first time to estimate the volume of membrane deposits. With a single deposit (0.20 µL) of the potassium-selective membrane, a Nernstian response within a clinically relevant concentration range was obtained. To gather the information on time requirements for the evaporative membrane drying, we developed an experimental setup based on time-resolved impedance spectroscopy. The obtained impedance (Z) changes reflect solvent evaporation that was interpreted according to free-volume theory. With this approach, the overall production and drying of the described devices takes less than 30 minutes. The proposed membrane deposition and evaluation of the evaporative drying process should be a promising quality assessment and means of mass-production of robust potentiometric sensor arrays.

ACKNOWLEDGEMENTS This work was supported by the Croatian Science Foundation, under grants: UIP-2020-02-9139 and “Mobility Programme – outbound mobility of assistants”, the Swiss National Science Foundation (project 200021_212462).

REFERENCES

1. Y. Soda, K. J. Robinson, T. J. Cherubini, E. Bakker, *Lab on a Chip* **2020**, *20*, 1441.

DESIGN AND CHARACTERISATION OF PEROVSKITE SOLAR CELLS

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Perovskite solar technology has experienced rapid advancements, achieving an impressive energy conversion efficiency of 26.1% by 2023.[1] The distinctive characteristics of hybrid perovskite materials (Fig. 1(left)) allow for high light absorption across a broad wavelength range, as well as efficient charge transport. This leads to superior electrical performance in perovskite solar cells (PSC) (Fig. 1(right)) compared to traditional silicon-based cells.[2]

The objective of this study is to investigate how the structure and composition of perovskite materials contribute to the exceptional photovoltaic properties of perovskite solar cells. Key methods used for thin layer deposition in this research will be outlined, and the significant impact of layer morphology on both the efficiency and operational longevity of the resulting solar cells will be explored.

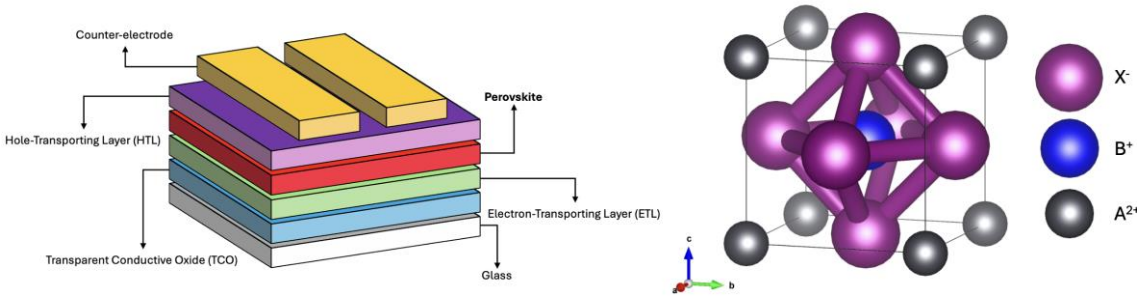

Figure 1. (left) thin layers in perovskite solar cell, (right) hybrid perovskite crystal structure.

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

REFERENCES

1. https://www.nrel.gov/pv/cell-efficiency.html (accessed 7th July 2024)
2. M. T. Bhatt, J. S. Lee, *New. J. Chem.* **41** (2017) 10508–10527.

SL9

HARNESSING THE POWER OF PEP-DEPENDENT LYASES: KINETIC CHARACTERIZATION AND MODEL-BASED OPTIMIZATION FOR *N*-ACETYLNEURAMINIC ACID SYNTHESIS

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Sialic acids (SAs), a diverse group of α-keto acids, play pivotal roles in biological processes such as development, cell signaling, immune response, and pathogen-host interactions. Among the various types of SAs, *N*-acetylneuraminic acid (Neu5Ac) stands out as the most studied due to its significance in neural development, cancer metastasis, and bacterial immune evasion.[1] Neu5Ac is synthesized through the aldol-like condensation of phosphoenolpyruvate (PEP) and *N*-acetylmannosamine (ManNAc), catalyzed by Neu5Ac synthase (NeuS)[2].

This work integrates the kinetic characterization and model-based optimization of Neu5Ac synthesis. NeuS from *Neisseria meningitidis* and a promising homolog from a metagenomic library were evaluated as biocatalysts, with comprehensive kinetic studies identifying key parameters in the biocatalytic process. Beyond Neu5Ac, we investigated the broader synthetic applicability of PEP-dependent lyases in catalyzing stereoselective aldol addition reactions with various aliphatic and aromatic aldehydes.

By leveraging these enzymes, we aim to unlock new pathways for C–C bond formation in synthetic organic chemistry. Finally, model-based optimization approaches were employed to enhance Neu5Ac biosynthesis, addressing bottlenecks in enzymatic reactions and optimizing conditions for scalable production. This integrative approach paves the way for novel biocatalytic applications, expanding the synthetic utility of PEP-dependent lyases and Neu5Ac production for biomedical and industrial uses.

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REFERENCES

1. A. Varki, *Glycobiology* **1993**, *3*, 97.
2. R. Schauer, *Carbohydr. Chem. Biol.* **2008,** *3-4*, 227.

SL10

CARBON DIOXIDE IN THE SYNTHESIS OF ORGANIC CARBONATES

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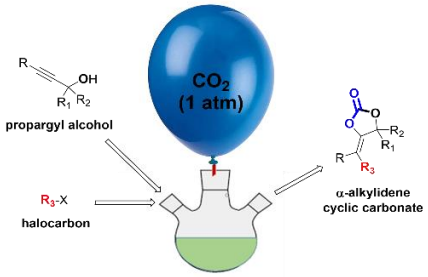
Carbon dioxide (CO_2) is an atmospheric gas (in molar ratios 420 ppm) that is responsible for the greenhouse effect. Its constantly increasing quantities released into the atmosphere through the burning of fossil fuels are considered to be the main cause of global warming and climate change. Capturing CO_2 and converting it into high-value organic compounds is particularly challenging due to its increased kinetic and thermodynamic inertness. However, the direct utilization of CO_2 as a renewable carbon source represents an attractive approach for modern organic synthesis.[1]

The catalytic capture of CO_2 by propargylic substrates - alcohols or amines - leads to cyclic α-alkylidene carbonates or carbamates, which are structural motifs often found in pharmaceuticals, polymers, chiral auxiliaries, polar aprotic solvents etc.[2] Combining CO_2 capture with new C-C bond formation reactions can provide direct access to complex products that otherwise require multi-step syntheses.[3]

Our efforts to develop new carboxylative C-C cross-coupling reactions for the preparation of cyclic carbonates will be presented. A proposed reaction mechanism based on experimental and computational data will also be discussed.



ACKNOWLEDGEMENTS Croatian Science Foundation (IP-2019-04-8846, D. Marković); University of Rijeka (uniri-prirod-18-102 and uniri-iskusni-prirod-23-28: D. Marković, uniri-iskusni-prirod-23-235: M. Kolympadi Markovic).

REFERENCES

1. Q. Liu, L. Wu, R. Jackstell, M. Beller, *Nat. Commun.* **2015**, *6*, 5933.
2. F. Vranješević, M. Kolympadi Markovic, D. Matulja, G. Ambrožić, J. Á. Sordo, S. Laclef, V. Vrček, D. Marković, *Catalysts* **2022**, *12*, 547.
3. S. Sun, B. Wang, N. Gu, J.-T. Yu, J. Cheng, *Org. Lett.* **2017**, *19*, 1088.

SL11

CALORIMETRIC CHARACTERIZATION OF THE "GOLDEN RAIN EXPERIMENT" IN "DROUGHT SEASON"

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In recent years, the study of solid-state reactions has gained significant attention over solution-based reactions due to their high yields, simple scale-up, and minimal solvent use.[1] While considerable research has been conducted on the kinetics of mechanochemical reactions,[2] thermodynamic studies are rather scarce. Lack of calorimetric data related to solid-state reactions can be largely ascribed to the challenges posed by heat introduced by the milling process.[3] Most commonly, thermodynamic characterization of reactions between solids has relied on indirect methods using Hess's law,[4] with direct isothermal measurements primarily conducted at elevated temperatures in metallurgy.[5] Recently, direct heat measurements of solid-state reactions at room temperature with gentle mechanical agitation have been successfully performed, providing data which were in good agreement with the literature.[6]

Building on this work, we investigated a solid-state equivalent of the golden rain experiment—salt metathesis reaction between lead(II) nitrate and potassium iodide—using isothermal calorimetry at 25°C with gentle mechanical agitation. Several experimental challenges were identified and methods for their mitigation were proposed. Experiments under various wetting conditions demonstrated the impact of liquid addition on reaction progress providing valuable insights into its role in mechanochemical reactions.

Inspiration: *The Alchemist Discovering Phosphorus*, a painting by Joseph Wright of Derby

REFERENCES

1. J.-L. Do, T. Friščić, *ACS Cent. Sci.* **2017**, *3*, 13.

2. T. Friščić, I. Halasz, P. J. Beldon, A. M. Belenguer, F. Adams, S. A. J. Kimber, V. Honkimäki, R. E. Dinnebier, *Nature Chem* **2013**, *5*, 66.

3. K. Užarević, N. Ferdelji, T. Mrla, P. A. Julien, B. Halasz, T. Friščić, I. Halasz, *Chem. Sci.* **2018**, *9*, 2525.

4. V. Stilinović, G. Horvat, T. Hrenar, V. Nemec, D. Cinčić, *Chem. Eur. J.* **2017**, *23*, 5244.

5. R. Ferro, G. Borzone, G. Cacciamani, R. Raggio, *Thermochim. Acta* **2000**, *347*, 103.

6. M. Cvetnić, R. Šplajt, E. Topić, M. Rubčić, N. Bregović, *Phys. Chem. Chem. Phys.* **2024**, *26*, 67.

SL12

TUNING CHIRALITY IN FUNCTIONAL ASSEMBLIES: FROM LIQUID CRYSTALS TO SUPRAMOLECULAR STRUCTURES IN WATER

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Chirality, *i.e.* the geometric property of an object not being superimposable on its mirror image, is an important research topic in a wide range of areas, especially in soft materials due to their huge potential for applications in diverse fields.[1] Liquid crystals (LC) are intermediate between solids and liquids, being fluids that retain some degree of ordering of their constituent parts.[2] The most common LC phases are nematics and smectics, the former being widely exploited in display technology owing to its electro-optic characteristics. The introduction of chirality into LCs results in various chiral LC phases with unique properties. Our research is focused on the synthesis and characterization of mesogenic properties of the chiral LC dimers containing 3-aryl-3- hydroxypropanoate core unit as a source of chirality (Figure 1). This building block allows variations in the material design leading to different molecular topologies and thus different self-organization. Moreover, it allowed for the synthesis of both racemic and enantiomerically pure forms, enabling a comparison of the LC phases generated by these two forms. The results contributed to general understanding of how intrinsic chirality, located in the spacer of LC dimers, influences the overall chirality in mesophases. Additionally, substituting terminal aliphatic chains with highly polar oligo(ethylene glycol) (OEG) chains would result in an amphiphilic molecule capable of self-assembling in water, consequently leading to supramolecular structures. These assemblies hold significant potential in developing systems for the efficient catalysis of organic reactions in water across a wide concentration range—an area with rapidly growing interest and promising applications in replacing organic solvents with water for environmentally friendly organic reactions.[3]

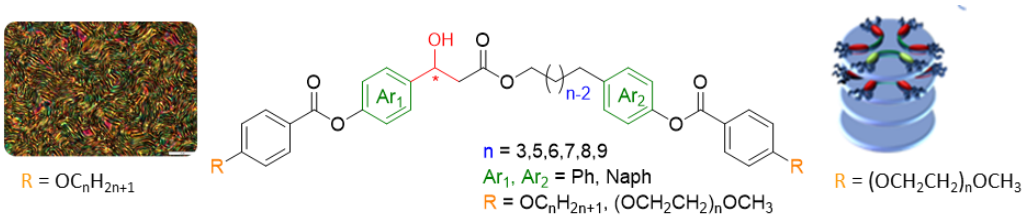

Figure 1. General structure of target dimers.

ACKNOWLEDGEMENTS This work was financially supported by STARTNOW project (NPOO.C3.2.R2-I1.06.0042) funded by the NexGenerationEU. The authors acknowledge the Croatian Science Foundation [grant no. IP-2017-04-7978 and DOK-2020-01] for financial support.

REFERENCES

1. H.K. Bisoyi, Q. Li, *Chem. Rev*. **2022**, *122* 4887–4926.
2. P. J. Collings, *Introduction to Liquid Crystals,* Taylor & Francis, London, **1997**.
3. B. H. Lipshutz, S. Ghorai, *Green Chem.* **2014**, *16* 3660–3679.

SL13

TEACHING CHEMISTRY IN THE NEW BACHELOR "REGENERATIVE MEDICINE AND TECHNOLOGY"

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Regenerative Medicine (RM) is an emerging field at the crossroads of science, technology, medicine, and entrepreneurship, aiming to replace, mimic, or recreate human cells to restore diseased or damaged tissues and organs. Recognizing the labor market's demand for multidisciplinary expertise, Maastricht University has launched the groundbreaking undergraduate program "Regenerative Medicine and Technology".[1]

This program is designed to train a new generation of researchers and engineers who can adapt to various RM domains and contribute to the development, evaluation, and commercialization of innovative medical therapies, products, and devices. The curriculum trains students in skills necessary to cure diseases, moving beyond mere symptom treatment, thus not only enhancing patient lives but also fostering a sustainable healthcare system and economy.

Chemistry is a cornerstone of this multidisciplinary program, providing students with the essential knowledge and skills to understand and manipulate biochemical processes vital for tissue growth. It also plays a crucial role in designing, preparing, and characterizing novel biomaterials that can direct cell behavior and facilitate regeneration. The program integrates chemistry with biology, engineering, medicine, and entrepreneurship to offer a comprehensive education. In this approach we employ problem- and research-based learning principles, encouraging students to think and create beyond single disciplines.

As a young program, we are committed to continually improving our curriculum and teaching methods. We actively seek perspectives from the international higher education community and welcome collaborations on multi- and transdisciplinary projects. In so doing we aspire to innovate education and contribute to a more sustainable future.

ACKNOWLEDGEMENTS

The Faculty of Health, Medicine and Life Sciences at the Maastricht University and especially the MERLN Technology-Inspired Institute for Regenerative Medicine are acknowledged for the opportunity to lead the design, development and implementation of the new Bachelor program Regenerative Medicine and Technology as well as all the support during this project.

REFERENCES

1. Bachelor Regenerative Medicine and Technology. https://curriculum.maastrichtuniversity.nl/education/bachelor/bachelor-regenerative-medicine-and-technology (accessed in August 2024)

SL14

THERMAL CONTROL OF MILLING REACTORS FOR ADVANCING PREPARATIVE MECHANOCHEMISTRY

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Mechanochemistry and thermal energy are inherently related and hard to separate. During milling, mechanical energy is partially absorbed by the milled material and milling reactor, and the remaining energy is released as heat. It is often postulated that mechanochemical reactivity results primarily from these secondary thermochemical effects.

This talk will present the new advances in mechanochemical reactivity accomplished by equipping mechanochemical processors with thermal controllers, for conducting the milling reactions at sub-ambient or elevated temperatures.[1,2] While the experimental setups are simple and easy to establish in laboratories, this external control of the bulk reaction mixture proved to have many benefits compared to conventional mechanical processing.[3] It leads to a dramatic increase in reaction rate and yield, the overall reduction in spent energy, the change of the reaction mechanisms, controllable synthesis of various products from the same reaction mixtures, and increased reaction selectivity. Due to its simplicity and advantages, combining temperature control and milling may soon become unavoidable for every synthetic laboratory.

ACKNOWLEDGEMENTS The presented research would not be possible without Tomislav Mrla, engineering team at the Workshop for Fine Mechanics and Optics of RBI, and young researchers who invested many working hours in tuning the new reactors and investigating various chemical systems. The research is supported by Croatian Science Foundation, IP-2020-02-4702.

REFERENCES

1. N. Cindro, M. Tireli, B. Karadeniz, T. Mrla, K. Užarević, Investigations of Thermally Controlled Mechanochemical Milling Reactions, *ACS Sust. Chem. Eng*. **2019**, *7*, 16301-16309.

2. T. Stolar, S. Grubešić, N. Cindro, E. Meštrović, K. Užarević, J. G. Hernandez, Mechanochemical Prebiotic Peptide Bond Formation, *Angew. Chem. Int. Ed*. **2021**, *60*, 12727-12731.

3. I. Brekalo, V. Martinez, B. Karadeniz, P. Orešković, D. Drapanauskaite, H. Vriesema, R. Stenekes, M. Etter, I. Dejanović, J. Baltrusaitis, K. Užarević, Scale-Up of Agrochemical Urea-Gypsum Cocrystal Synthesis Using Thermally Controlled Mechanochemistry, *ACS Sust. Chem. Eng.* **2022,** *10*, 6743-6754.

SL15

FISHING IN THE ACETONITRILE SEA: (THIO)UREA-CALIX[4]ARENES AS ANION BINDERS

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Thermodynamic and structural understanding of the anion-binding processes is vital for the development and improvement of many areas of their application: sensing, extraction, catalysis, biochemical transmembrane transport etc.[1] In this talk, the investigation of anion-binding properties of three new (thio)urea-calix[4]arene derivatives (Figure 1) will be presented.[2,3] The multimethod approach (NMR, ITC, UV) providing comprehensive thermodynamic insight into the binding processes will be described. A point that is not often (at least not fully) covered in similar investigations is a possibility of deprotonation of the receptor containing hydrogen bond donor.[4] The importance of considering this reaction in the data-handling procedures will be addressed. The studied receptors form anion complexes of various stoichiometries, with 1:1 species stability generally following the basicity of anions. Thiourea and urea analogues have similar affinities for anions, except for $H_2PO_4^-$ and $HP_2O_7^{3-}$, which bind more strongly to thiourea calixarene. Fumarate and hydrogen pyrophosphate anions bridge two tetra(thio)ureido-host molecules in solution. The possible trickiness in the studies aimed to unravel the thermodynamic equilibria in solution will be demonstrated using the example of maleate anion binding.

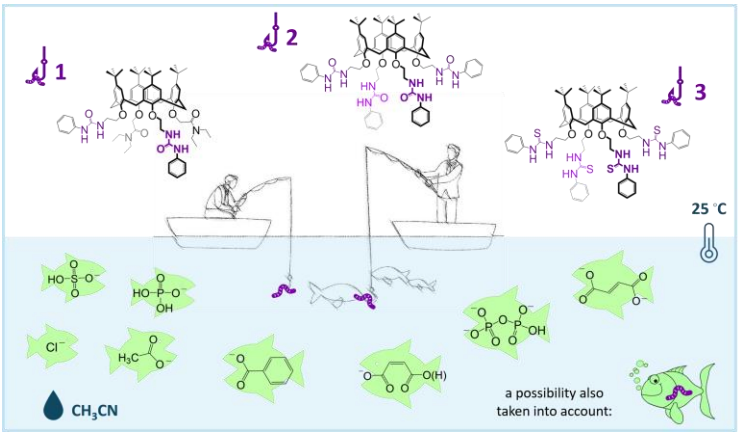

Figure 1. Structures of the investigated calixarenes and anions.

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REFERENCES

1. D. A. McNaughton, W. G. Ryder, A. M. Gilchrist, P. Wang, M. Fares, X. Wu, P. A. Gale, *Chem* **2023**, *9*, 3045–3112.

2. M. Cvetnić, N. Cindro, E. Topić, N. Bregović, V. Tomišić, *ChemPlusChem* **2024**, e202400130.

3. M. Cvetnić, N. Cindro, N. Bregović, and V. Tomišić, *ACS Phys. Chem. Au* **2024**, DOI: 10.1021/acsphyschemau.4c00077

4. D. Barišić, N. Cindro, M. J. Kulcsár, M. Tireli, K. Užarević, N. Bregović, V. Tomišić, *Chem. - Eur. J.* **2019**, *25*, 4695–4706.

SL16

DESIGNER AMPHIPHILES – TOWARD LYOTROPIC LIQUID CRYSTAL SYSTEMS FOR ORGANIC SYNTHESIS

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Recently, in the effort to make synthesis on industrial scale greener and less polluting, solvent choices have been tightened with water as one of the most prominent solvents, which still has many limitations[1,2]. Micellar systems are a promising solution to the limitations of water as a medium for organic synthesis, specifically, organic assemblies designed with a non-polar, non-aqueous interior. As promising as micelles are for organic synthesis, they have their own limitations. On the low end of concentration spectrum, there is a critical micellar concentration, under which micelles can not be formed, and on the high end, micellar systems either precipitate out of the solution, or form lyotropic liquid crystalline phases (LLC). LLC concentration range in the field of catalysis has been completely overlooked so far due to the increasing complexity of the system[3], but in our eyes, it is a field that promises lot and is worth to research further.

This research focuses on designing an amphiphilic molecule (Figure 1a), which will assemble in aqueous media forming nanotubules (Figure 1b)[4]. Furthermore, the design will enable the formation of LLC phases in high concentration range. A series of amphiphilic compounds has been synthesised and their characterization is in process. Most of them are showing supramolecular organisation, and some of them were proven to form micelles. Newly synthesised compounds are showing lyotropic LC phases, which are yet to be fully characterized. After complete analysis of these systems, development of their application for specific organic reactions in water is the next step forward.

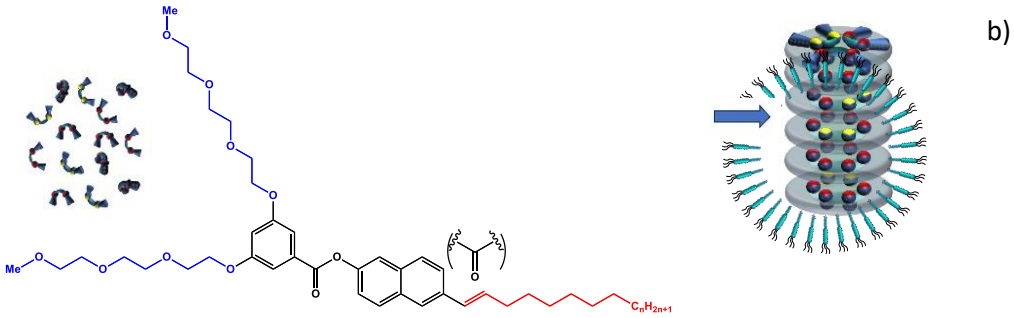

Figure 1. a) general amphiphile structure; b) supramolecular organization of amphiphiles

ACKNOWLEDGEMENTS This work was financially supported by STARTNOW project (NPOO.C3.2.R2-I1.06.0042) funded by the NexGenerationEU.

REFERENCES

1. P. Anastas, N. Eghbali, *Chem. Soc. Rev.* **2010**, 39, 301.
2. D. J. C. Constable, A. D. Curzons, V. L. Cunningham, *Green Chem.* **2002**., 4, 521.
3. B. H. Lipshutz, Curr. Opin. Green Sustain. Chem., **2018**, 11, 1–8.
4. T. Chattopadhyay, M. Kogiso, M. Asakawa, T. Shimizu, M. Aoyagi; Catal. Commun., 12, **2010**., 9–13.

SL17

DEVELOPMENT OF QuEChERS /HPLC TECHNIQUE FOR THE ANALYSIS OF VETERINARY DRUG RESIDUES IN BEEF SAMPLES

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The QuEChERS technique involved liquid-liquid extraction by partitioning with acetonitrile, followed by clean-up with a mixture of magnesium sulphate and a primary secondary amine. The extract obtained was then analyzed using HPLC. The figures of merit of the analytical methodology were determined using optimized parameters and the calibration curve was linear over the tested concentration range. The linearity ranged from 5 – 500 µg/kg for all the drug residues and correlation coefficients (r2) were greater than 0.99. The limit of detection (LOD) ranged from 1.45 – 5.02 µg/kg while the limit of quantification (LOQ) ranged from 4.68 – 6.72 µg/kg. The inter-day and intra-day precision for beef samples ranged from 1.94 – 19.03 % and 2.78 - 9.04%, respectively, and the average recoveries ranged from 79.48 ¬– 107.48 %. The selectivity was determined by a blank matrix containing external standards and a sample spiked with target analyte and it indicated a good selectivity with no interference.

POSTER PRESENTATIONS

P1

MIXED METAL OXIDES AS A HETEROGENEOUS CATALYST FOR A SMART PRODUCTION OF HIGH-QUALITY BIODIESEL FROM WASTE COOKING OIL

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Biodiesel is an eco-friendly alternative to conventional fossil fuels, derived from renewable sources such as vegetable oils, animal fats, and recycled cooking oils. As a sustainable energy option, biodiesel offers significant advantages over traditional diesel, including lower greenhouse gas emissions, biodegradability, and reduced dependence on finite petroleum resources. In the context of rising global energy consumption and increasing concerns about climate change, biodiesel has emerged as a promising solution to meet energy demands while minimizing environmental impact. With its ability to be used in existing diesel engines without modification, biodiesel provides a practical pathway for transitioning to cleaner energy sources. As countries worldwide seek to diversify their energy portfolios and reduce carbon footprints, biodiesel production plays a crucial role in promoting energy security, sustainability, and resilience in the face of fluctuating oil markets and geopolitical uncertainties.[1-5]

This study explores the catalytic potential of mixed metal oxides (Fe_2O_3-MgO) synthesized through a biogenic approach using pomegranate extract. The resulting catalysts, Fe_2O_3-MgO, demonstrate exceptional performance in biodiesel production. Detailed characterization through FTIR, XRD, XPS, nitrogen sorption, pore size distribution, TGA, and SEM reveals their unique composition and structure. In the realm of biodiesel production, the Fe_2O_3-MgO catalyst exhibits remarkable efficiency, achieving a high yield of 90%. This efficiency is attained under optimized conditions, including a methanol-to-waste cooked oil molar ratio of 15, a 5-hour reaction time, and a 2% catalyst dosage for the transesterification process. The use of waste-cooked oil as a feedstock not only reduces the overall cost of production but also contributes to waste management and environmental sustainability. The catalyst's high activity can be attributed to its enhanced surface area and unique structural properties, which facilitate greater interaction between reactants and active sites. Furthermore, the catalyst demonstrates impressive reusability, maintaining its activity over multiple cycles, thereby reducing the need for frequent replacement and lowering operational costs.

This highlights its practical applicability in large-scale biodiesel production, offering a promising route toward sustainable and economically viable biofuel alternatives.

REFERENCES

1. F. Ma, M. A. Hanna, *Bioresour. Technol.* **1999**, *70*, 1.
2. H. M. Hassan, M. S. Alhumaimess, I. H. Alsohaimi, A. A. Essawy, A. A., M. F. Hussein, H. M. Alshammari, O. F. Aldosari, *ACS Omega* **2020**, *5*, 27811.
3. N. A. Ibrahim, U. Rashid, B. Hazmi, B. R. Moser, F. A. Alharthi, S. L. Rokhum, C. Ngamcharussrivichai, *Fuel* **2022**, *317*, 123525.
4. C. G. Lopresto, *Int. J. Environ. Sci. Technol.* **2024**, 1-22.
5. T. A. Elnasr, A. T. Al-Enezi, M. F. Hussein, H. Bielal, M. S. Alhumaimess, Y. A. El-Ossaily, I.H. Alsohaimi, *Sustainable Chem. Pharm.* **2024**, *37*, 101426.

P2

FULLY INKJET PRINTED GRAPHENE-PRUSSIAN BLUE PLATFORM FOR BIOSENSING APPLICATIONS

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Inkjet printing is emerging as an important additive manufacturing method for sensor fabrication, offering scalable, non-contact deposition compatible with sensitive substrates and substances, as well as digital patterning facilitating production compared to state-of-the-art contact methods, such as screen printing.[1,2] Of particular interest is deposition of nanomaterial-based inks.[3] Graphene based inks offer good electrical conductivity, chemical stability and mechanical flexibility, but require the use of stabilizers for stable ink formulations, necessitating post-printing treatment to make the use of graphene inks feasible. Photothermal treatment methods, such as intense pulsed light (IPL) sintering, offer fast and scalable post-printing treatment that is friendly to thermally sensitive substrates.[1] Detection of hydrogen peroxide (H_2O_2) is of particular interest in the biosensing field, especially with oxidase based biosensors. By lowering the operating potential to around 0 V *vs*. Ag/AgCl, Prussian Blue offers improved selectivity by eliminating interfering signals that could hinder accurate detection at higher potentials required for uncatalyzed detection of H_2O_2, and by selectively reducing H_2O_2 formed in the enzymatic reaction with the analyte.[3] Prussian Blue nanoparticles (PBNPs) can also be synthesized and inkjet printed, as demonstrated previously.[3] This work presents a fully inkjet printed graphene-Prussian Blue platform capable of H_2O_2 detection. Post-printing treatment of graphene printed on polyimide was optimized with the use of thermal and photothermal (IPL) sintering methods. PBNPs were synthesized as previously described.[3] Prussian Blue mediator layer was deposited *via* chemical deposition, by drop casting the PBNP ink and finally, by inkjet printing the PBNP ink. Amount of deposited Prussian Blue was optimized to achieve a compromise between the resistive effects of the layer and the analytical performance of the platform. The fully inkjet printed platform was covered with chitosan and utilized for chronoamperometric detection of H_2O_2, achieving a wider linear range (0.1–5 mM, with improved stability even in 10 mM H_2O_2) and improved linearity (R^2 = 0.99909) compared to platforms with non-printed mediator layer, at the expense of lower sensitivity (22.6 µA mM^{-1} cm^{-2}). Finally, the platform was equipped with a drop cast lactate oxidase-chitosan-PVC sensing layer and employed for chronoamperometric detection of lactate, with promising results for wearable lactate sensing in physiologically relevant concentration range in sweat (3–50 mM, R^2= 0.99735, sensitivity -0.188 µA mM^{-1} cm^{-2}).

ACKNOWLEDGEMENTS This work was funded by the Croatian Science Foundation under grant UIP-2020-02-9139.

REFERENCES

1. E. B. Secor, B. Y. Ahn, T. Z. Gao, J. A. Lewis, M. C. Hersam, *Adv. Mater*. **2015**, *27*, 6683.
2. A. D. Ambaye, K. K. Kefeni, S. Mishra, E. Nxumalo, B. Ntsendwana, *Talanta* **2021**, *225*, 121951.
3. S. Cinti, F. Arduini, D. Moscone, G. Palleschi, A. J. Killard, *Sensors* **2014**, *14*, 14222.

P3

NUCLEOFUGALITY OF PHENYLSULFINATE IN ETHANOL AND AQUEOUS ETHANOL

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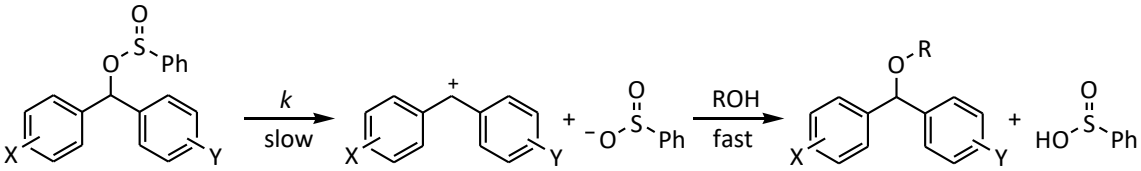
In order to determine the nucleofugality (i.e., the heterolytic reactivity) of the phenylsulfinate leaving group, substituted benzhydryl phenylsulfinates were synthesized and rate constants for the solvolysis of these substrates in neat ethanol and 80 % and 60 % ethanol-water mixtures were measured. As in the case of dozens leaving groups so far, the leaving group ability of phenylsulfinate in ethanol and mixtures was determined in terms of the N_f nucleofugality parameter according to three-parameter LFER Equation (1) established by Mayr and coworkers.[1]

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

The parameters in Equation (1) are: the nucleofuge-specific parameters N_f (the negative intercept on the abscissa of a log k/E_f correlation line) and s_f (the slope of the correlation line), and the electrofugality parameter E_f – an independent variable that quantifies the heterolytic reactivity of a certain electrofuge. Accordingly, nucleofugality parameters of phenylsulfinate in 100 %, 80 % and 60 % ethanol have been determined from corresponding log k/E_f plots, where E_f refers to electrofugalities of reference benzhydryl electrofuges. The N_f nucleofugality scale currently covers a reactivity range of 15 orders of magnitude and includes leaving groups of diverse structures and functionalities.[1–4] Determined nucleofugality parameters of phenylsulfinate allow comparison of heterolytic reactivity of this leaving group with reactivities of others. In addition, employing nucleofuge-specific parameters (N_f and s_f) of phenylsulfinate and previously determined E_f values of corresponding electrofuges,[1,5] rate constants and half-lives for solvolyses of various phenylsulfinates in a given solvent at 25 °C can be predicted according to Equation (1). In such manner, it is possible to predict resistance to solvolytic decomposition of various substrates bearing the phenylsulfinate leaving group.



Scheme 1. Solvolysis of substituted benzhydryl phenylsulfinates

ACKNOWLEDGEMENTS The authors thank the University of Zagreb for financial support of this research.

REFERENCES

1. N. Streidl, B. Denegri, O. Kronja, H. Mayr, *Acc. Chem. Res.* **2010**, *43*, 1537.
2. M. Matić, M. Katić, B. Denegri, O. Kronja, *J. Org. Chem*. **2017**, *82*, 7820.
3. M. Matić, B. Denegri, *Org. Biomol. Chem.* **2018**, *16*, 4665.
4. M. Matić, B. Denegri, I. Tarandek, L. Turković, *Int. J. Chem. Kinet.* **2022**, *54*, 561.
5. B. Denegri, A. R. Ofial, S. Jurić, A. Streiter, O. Kronja, H. Mayr, *Chem. Eur. J.* **2006**, *12*, 1657.

P4

MECHANOCHEMICAL CHLORIDE-TEMPLATED MACROCYCLIZATION OF OLIGOPEPTIDES

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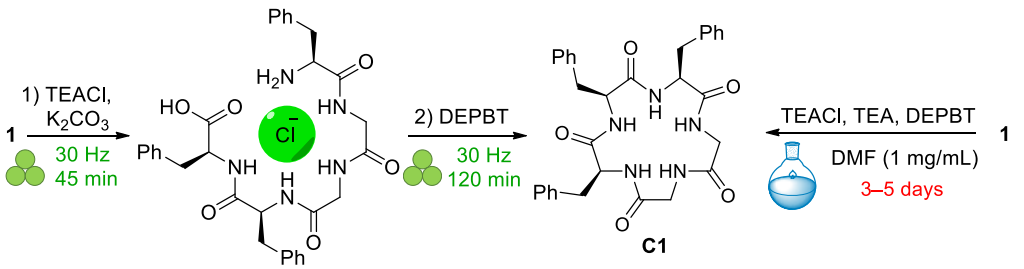
Cyclic peptides have become compounds of great interest in the last few decades due to higher biological potency compared to their linear analogues, making them attractive targets in drug development.[1] The head-to-tail macrocyclization step requires the use of templating agents to induce conformational reorganization of the linear precursor which brings the *N*- and *C*-termini in close spatial proximity.[2] Our previous work has shown that not only cations, but also anions can bind to linear and cyclic peptides and can assist the macrocyclization step.[3] This and other solution-based methods have three main drawbacks: high dilution, long reaction times and low solubility of linear peptides in organic solvents. To circumvent these problems, we have developed a mechanochemical approach in which the linear pentapeptide **1** or hexapeptide **2** is reacted with tetraethylammonium chloride in the first step and afterwards the coupling reagent is added to afford cyclic peptides **C1** and **C2** with reaction times reduced from days to a few hours. A scale-up cyclization procedure for **1** was also conducted in a planetary ball-mill. To gain insight into the role of the chloride salt, IR spectroscopy experiments and molecular dynamics simulations of the peptide-chloride complexes were performed.



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REFERENCES

1. H. Zhang, S. Chen, *RSC Chem. Biol.* **2022**, *3*, 18.
2. V. Martí-Centelles, M. D. Pandey, M. I. Burguete, S. V. Luis, *Chem. Rev.* **2015**, *115*, 8736.
3. N. Vidović, G. Horvat, D. Riva, T. Rinkovec, N. Cindro, V. Tomišić, G. Speranza, *Org. Lett.* **2020**, *22*, 2129.

P5

MAKING A HAND CENTRIFUGE LEADS TO A BETTER UNDERSTANDING OF THE EDUCATIONAL OUTCOMES OF CHEMISTRY CLASSES

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Chemistry as a natural science is a part of the compulsory teaching curriculum in primary schools. Learning and teaching chemistry is based on the acquisition of knowledge and skills through the development of cognitive processes of perception, scientific communication and reasoning.[1] The basic teaching activity, which includes all the mentioned cognitive processes, is a chemical experiment. Observing the educational outcomes of chemistry in primary school based on chemical concepts, it is evident that the acquisition of knowledge and skills can be improved by comprehensively involving students in the teaching process. The goal of the work was to connect all components of the teaching process and educational outcomes by making a hand centrifuge, respecting the level of cognitive abilities of elementary school students.[2] The added value of such work is the achievement of connections with other subjects and cross-curricular topics, especially with the subject of technical culture by applying knowledge about structure, type, and physical and chemical properties necessary for the use of different materials and the development of technologies. By summarizing the learning and teaching goals achieved with this way of working, the students' increased curiosity in their work, the development of a positive attitude and interest in chemistry, a better understanding of the basic concepts of chemistry, and the development of independence, responsibility and creativity, which was recognized through the students' presentation at the exhibition of innovations in Zagreb.

REFERENCES

1. Curriculum of the subject of chemistry for elementary schools and high schools, Ministry of Science and of Education, January **2019**.

2. Chemistry textbook for the seventh grade of primary school, M. Mamić, D. Mrvoš-Sermek, V. Peradinović, N. Ribarić, ALFA d.d., Zagreb, **2022**, pp. 77–95.

3. Expected and desired learning outcomes: competence approach; Buljubasic-Kuzmanović, V.; IN: Previšić, V., Šoljan, N. N., Hrvatić, N. (ed.), Pedagogy towards lifelong education and to the knowledge society (**2007**). Holy Week: Kratis, 110–118.

P6

EXPLORING ENZYMATIC PATHWAYS FOR DEGRADATION OF ECO-FRIENDLY 3-AMIDOQUINUCLIDINE QACs

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Quaternary ammonium compounds (QACs) are a class of small organic molecules known for their broad-spectrum antibacterial activity. For over a decade, QACs have been widely employed as active ingredients in topical antiseptic formulations, as well as key components in surface disinfectants, particularly in healthcare facilities. The extensive and sustained use of these products, especially following the recent pandemic outbreak, has led to the accumulation of conventional commercial QACs in wastewater and sludge, resulting in environmental saturation with these compounds.[1] The exposure of environmental bacterial species to subMIC concentrations of QACs, along with their inherent chemical stability, plays a crucial role in activating bacterial resistance mechanisms. To mitigate the threat posed by resistant bacteria, novel „soft“ QAC derivatives are often functionalized with hydrolysable groups, enabling the controlled degradation of these structures. This approach aims to prevent bacterial adaptation and the subsequent activation of resistance mechanisms. We have previously synthesized “soft” quinuclidine QACs, functionalized with an amido group at the C-3 position of heterocyclic core.[2] Based on the nature and position of the amide functionality, we have shown that these bioactive "soft" QACs are potential substrates for trypsin, the most abundant serine protease. Although the structure-activity relationships need to be further explored, these QACs pave the way for the synthesis of new environmentally friendly derivatives with improved biological activity and a lower environmental footprint, making them a promising alternative to commercially available QACs.

REFERENCES

1. W. A. Arbold et al., *Environmental Science & Technology*, **2023**, *57*, 20.
2. Odžak et al., *Pharmaceuticals*, **2023**, *16*, 2.

PROTECTION-FREE STRATEGY FOR ALKYLATION OF INDOLES

P7

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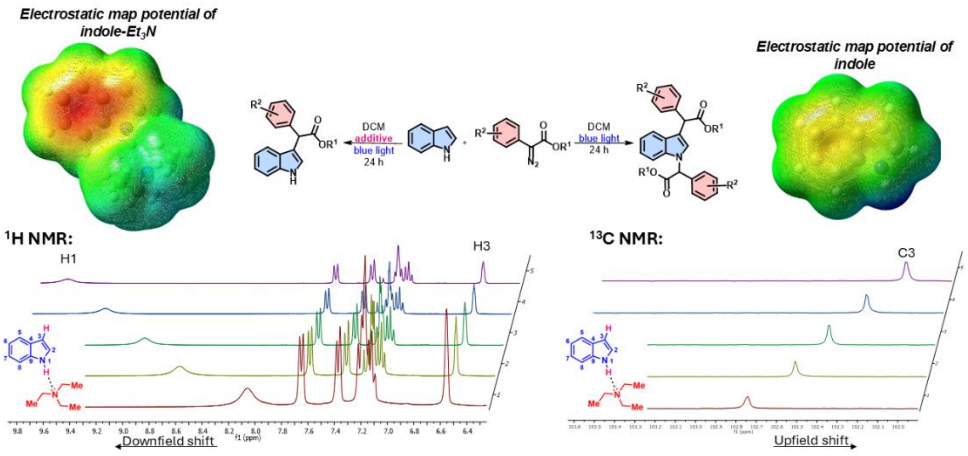
The competitive nucleophilicity between C3 and N-H positions[1] in indole molecule represents a synthetic problem when chemoselectivity is an issue. To circumvent this problem, it is necessary to introduce protecting groups that direct functionalization to the specific location. Research has shown that electron-donating groups attached to the nitrogen atom increase the nucleophilicity of the C3 position, promoting C3 alkylation. In contrast, electron-withdrawing groups tend to favor cyclopropanation.[2] Protection involves forming a new covalent bond between the protecting group and the target molecule, which adds two additional steps to the synthetic route. As a result, this increases material consumption and reduces the overall yield. This study suggests an alternative strategy to overcome these limitations using hydrogen bonding as a masked protecting group. The nucleophilicity of different positions on the indole ring was evaluated using ^{1}H, ^{13}C NMR spectroscopy and DFT calculations. The interaction of indole with specific additives (hydrogen bond acceptors) influences the change in NMR chemical shifts, which reflect the electronic environment and nucleophilicity of the atoms. For example, NMR spectra showed a downfield shift in the N-H proton signal and an upfield shift in the C3 carbon signal in the presence of triethylamine (Et_3N). Alongside with DFT calculations this indicates an increase in the nucleophilicity of C3 position. This suggests that certain additives could promote regio- and chemoselective alkylation. To test this hypothesis, a model reaction of blue light-promoted alkylation with aryldiazoacetates was conducted. Although prior attempts to functionalize unprotected indole under similar conditions were unsuccessful,[2] our results demonstrated both C-H and N-H insertion withouth an additive and the exclusive formation of C3-monosubstituted indole when an additive was used.



REFERENCES

1. N. Chadha, O. Silakari, *Eur. J. Med. Chem.,* **2017**, *134*, 159.
2. X. Zhang, C. Du, H. Zhang, X. Li, Y. Wang, J. Niu, M. Song, *Synth.,* **2018**, *50*, 889.

P8

MODELING OF HYDROGEN PRODUCTION PROCESS BY PEM WATER ELECTROLYSIS

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Production of hydrogen using renewable energy sources represents a crucial step forward in achieving the goals of the hydrogen economy and in the successful implementation of hydrogen as an alternative fuel of the future. Its efficient production is essential for it to compete in the fossil fuel market, which is nearing the end of its “shelf life.” One of the possible, effective methods for hydrogen production is water electrolysis using a PEM (proton exchange membrane) electrolyzer. The introductory section of this poster provides a brief theoretical overview of hydrogen and its classification based on production methods. The electrolysis process is presented, basic types of electrolyzers are described with a focus on the PEM electrolyzer, and fundamental thermodynamic laws that describe changes in the state of reactants during electrolysis are discussed. The construction of the electrolyzer, required components, and their characteristics, as well as the overall system enabling the electrolyzer's operation and proper storage of products, are outlined. Furthermore, a mathematical model for the task-defined electrolyzer is developed to better describe and predict the system's behavior and output parameters. A brief review is given of some of the assumptions introduced to simplify calculations and their impact on the overall calculation. One possible construction solution of the electrolyzer is modeled, and finally, a simulation for the designed electrolyzer is created in the Matlab software package, which, with specified parameters, calculates and graphically represents the desired output parameters, comparing the results with the data provided by the electrolyzer manufacturer.

P9

SYNTHESIS AND HHDH-CATALYZED KINETIC RESOLUTION OF PROPARGYLIC EPOXIDES

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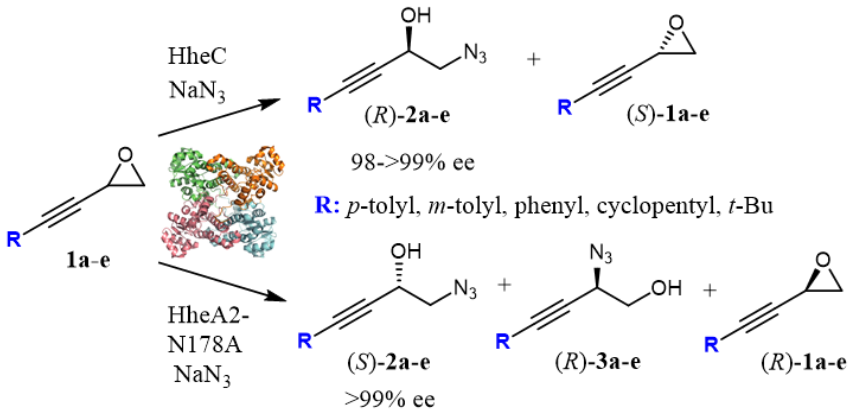
The versatile reactivity of propargylic epoxides and alcohols, due to the presence of a triple bond, is used in the synthesis of various organic compounds and building blocks.[1] However, there are not many known methods for the preparation of optically pure propargylic epoxides and alcohols, and the existing ones often require specific reagents.[1] Halohydrin dehalogenases (HHDHs) can be used to obtain enantiomerically pure compounds from racemic epoxides.[2] These important biocatalysts facilitate epoxide ring-opening reactions with unnatural nucleophiles such as azides. Here we report the biocatalytic transformation of propargylic epoxides using HHDHs. Six propargylic epoxides with different substituents were synthesized. Kinetic resolution reactions catalyzed by HHDHs in the presence of azide were performed. Two enzymes with opposite stereoselectivities, HheC and HheA2-N178A were used and yielded azido alcohols (98 - >99% *ee*, *E*-value >200) and epoxides (29 - 88% *ee*). The best performing *p*-tolyl propargylic epoxide derivative was used in a sequence of two enzymatic reactions to obtain both enantiomers of the β-azido alcohol and the (*R*)-enantiomer of the α-azido alcohol, each in >99% *ee*, through complete conversion of the starting epoxide.[3] The obtained azido alcohols were used in the click reactions with terminal acetylenes to obtain optically pure triazolyl propargylic alcohols.



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REFERENCES

1. R. Abonia, D. Insuasty, K. K. Laali, *Molecules* **2023**, *28*, 3379-3440.

2. Z. Findrik Blažević, N. Milčić, M. Sudar, M. Majerić Elenkov, *Adv. Synth. Catal.* **2021**, *363*, 388-410.

3. R. J. Kolman, P. Švaco, M. Majerić Elenkov, I. Dokli, *Adv. Synth. Catal.* **2024**, doi: 10.1002/adsc.202400734.

P10

DIASTEREOSELECTIVE DOUBLE GRIGNARD REACTION ON RIBONOLACTONES

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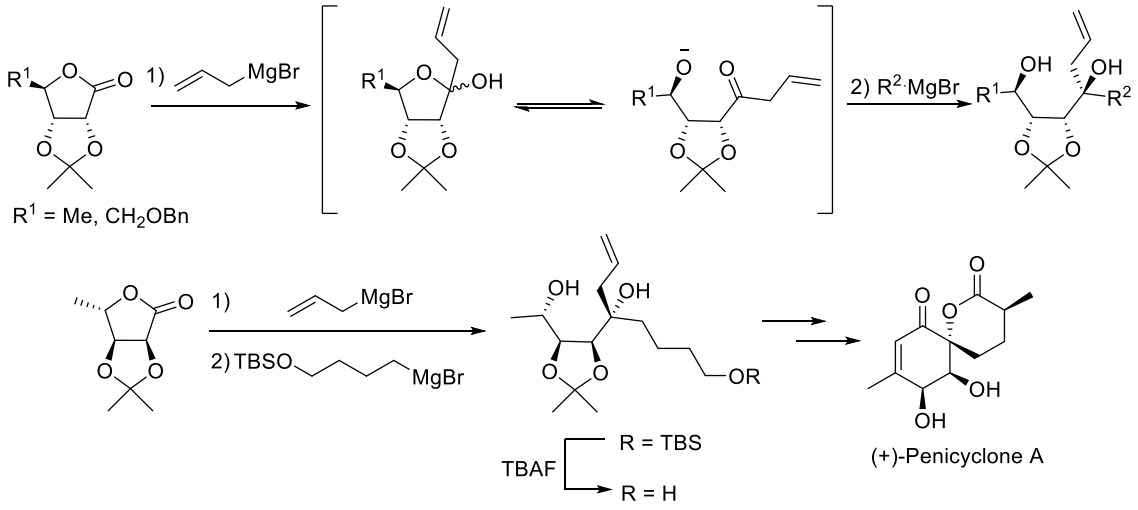
It is generally known that esters and lactones react with Grignard reagents to form tertiary alcohols. However, specific substrates have been shown to yield mono addition products with organometallic reagents.[1] We envisioned that a double Grignard reaction with two different reagents might be possible when using sugar-derived lactones as substrates. Chelation control during the second nucleophilic attack would then lead to the diastereoselective formation of chiral tertiary alcohols. Two ribonolactone derivatives were reacted with allylmagnesium bromide at low temperature in the first step, followed by addition of the second Grignard reagent. Reverse addition was also examined, but the main products were diallyl adducts of the starting material, most likely due to the high reactivity of allylic magnesium halides.[2] This strategy was employed in the total synthesis of the natural polyketide (−)-Penicyclone A[3] and its enantiomer. Further work is underway to explore the use of other organometallic species in the second step to achieve the addition of less reactive Grignard reagents in the first step.



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REFERENCES

1. T. Yamazaki, T. Terajima, T. Kawasaki-Taskasuka, *Tetrahedron* **2008**, *64*, 2419.
2. N. D. Bartolo, K. A. Woerpel, *J. Org. Chem.* **2018**, *83*, 10197.
3. G. Talajić, E. Topić, J. Meštrović, N. Cindro, *J. Org. Chem.* **2022**, *87*, 16054.

P11

STRUCTURAL DETERMINATION OF SULFATED GLUCURONOSYL GLYCOSPHINGOLIPIDS BY ADVANCED MASS SPECTROMETRY

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Glycosphingolipids (GSLs) are essential cell membrane components of eukaryotic cells playing important roles in many biological and pathological processes. Therefore, they are useful targets for development of novel approaches for diagnosis and therapeutic treatment of human diseases.[1] Sulfated glucuronosyl glycosphingolipids (sulfo-GlcA-GSLs) are known to be implicated in induction of certain autoimmune neurological diseases which emphasizes the need for detailed and careful composition and structure characterization of these species present in tissues and body fluids, particularly in order to structurally identify epitopes that might induce production of auto-antibodies. Advanced mass spectrometry has become irreplaceable methodology in glycolipidomics, allowing a high resolution and mass accuracy detection of GSL species and identification of even minor biologically relevant structures.[2]

The nanoelectrospray ionization quadrupole time-of-flight mass spectrometry (nano-ESI-QTOF MS) method for detection and structural identification of sulfo-GlcA-GSLs was optimized in the negative ion mode using chemically synthesized 3-sulfoglucuronosyl neolactohexaosyl ceramide, VI^3-GlcA(3-sulfo)-nLc$_6$Cer (d18:1/18:0), the neolactotetraosyl analogue IV^3-GlcA(3-sulfo)-nLc$_4$Cer, and their non-sulfated counterparts. The optimized conditions ensured fine signal intensity of the molecular ions detected in MS1 at femtomole sample consumption, efficient ion isolation and subsequent fragmentation in MS/MS experiment resulting in structural information-rich fragmentation patterns from which the key structurally diagnostic ions were specified. The method was then applied to characterize the composition of complex native mixture of sulfo-GlcA-GSLs isolated from bovine *cauda equina* and to determine structures of detected species by sequencing analysis. As the data revealed, the native mixture contained an unexpectedly large number of individual molecular species differing due to both a high structural diversity of the ceramide portions and the presence of isomeric forms of particular glycan moieties. The found molecular structures belong to three major molecular classes: sulfated GlcA-nLc$_4$Cer with the dominant glyco-isoform IV^3-GlcA(3-sulfo)-nLc$_4$Cer; analogous GlcA-nLc$_4$Cer; and sulfo-nLc$_4$Cer. Besides detailed compositional characterization of the analyzed samples, the quality of collected structural data enabled identification of novel sulfated and glucuronosylated species including glyco-isomers occurring in the mammalian nervous system.

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REFERENCES

1. Z. Guo, *J. Carbohydr. Chem.* **2022**, *41*, 63.

2. Ž. Vukelić, A. D. Zamfir, L. Bindila, M. Froesch, J. Peter-Katalinic, S. Usuki, R. K. Yu, *J. Am. Soc. Mass Spectrom.* **2005**, *16*, 571.

P12

SYNTHESIS AND BIOLOGICAL ACTIVITY OF ACRYLONITRILE DERIVED BENZOXAZOLES

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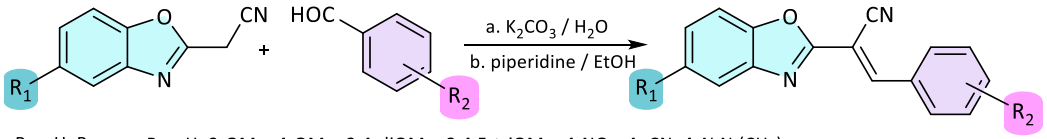
Benzoxazole ring is a well-known attractive scaffold in medicinal chemistry due to the wide range of biological and pharmacological properties of its derivatives and among the most important are antitumor, anticancer, antiviral or antimicrobial. In addition, it can be used as a starting building block for the synthesis of various biologically active complex molecules.[1,2] Herein we present the synthesis and biological evaluation of acrylonitrile derived benzoxazoles prepared by aldol condensation from differently substituted benzaldehydes and 2-cyanomethylbenzoxazoles. Synthesis of targeted compounds was carried out by aldol condensation in water with the addition of the base Na_2CO_3 (a) or by aldol condensation in ethanol with the addition of a catalytic amount of piperidine (b).[3,4] The structures of the newly prepared compounds were confirmed by means of ^{1}H- and ^{13}C-NMR spectroscopy and well as MS spectrometry. Antiproliferative activity *in vitro* was evaluated on several human cancer cells while the antibacterial activity *in vitro* was tested on a panel of some Gram-positive and Gram-negative bacterial strains. Additionally, for the most active compounds their interaction with *ct*-DNA was evaluated by several spectroscopic methods.

KEY WORDS: acrylonitrile, antiproliferative and antibacterial activity, benzoxazoles, *ct*-DNA



R_1 = H, Br R_2 = H; 2-OMe; 4-OMe; 2,4-diOMe; 3,4,5-triOMe; 4-NO_2; 4- CN; 4-*N*,*N*-$(CH_3)_2$; 4-*N*,*N*-$(CH_2CH_3)_2$; 2-CH_3 , 4-*N*-(CH_2CH_3)-*N*-(CH_2CH_2CN); 4-*N*,*N*-(CH_2CH_2Cl); 4-*N*-(CH_3)-*N*-(CH_2CH_2OH); 4-OH; 3,4-diOH; 3,4,5-triOH

Figure 1. Synthesis of acrylonitrile derived benzoxazoles.

ACKNOWLEDGEMENTS The Croatian Science Foundation funded this work (HRZZ-IP-2020-02-8090).

REFERENCES

1. A. Abdullahi, K. Y. Yeong, *Med. Chem. Res.* **2024**, *33*, 406.

2. S. Soni, N. Sahiba, S. Teli, P. Teli, L. K. Agarwal, S. Agarwal, *RSC Adv.* **2023**, *13*, 24093.

3. C. Youssef, H. B. Ammar, M. Belhouchet, K. Beydoun, R. B. Salem, H. Doucet, P. H. Dixneuf , *J. Heterocyclic Chem.* **2011**, *48*, 1126.

4. I. Boček Pavlinac, L. Persoons, D. Daelemans, K. Starčević, R. Vianello, M. Hranjec, *Int. J. Biol. Macromol.* **2024**, *266*, 131239.

P13

DECIPHERING THE MOLECULAR PUZZLE: EXPLORING THE MECHANISMS UNDERLYING CHELATOR ACTIONS ON METALLO β-LACTAMASES

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β-lactam antibiotics (such as penicillins and carbapenems) are among the most commonly prescribed antibiotics worldwide due to their broad-spectrum efficacy against various bacterial infections.[1] β-lactamases are enzymes that inactivate β-lactam antibiotics via hydrolysis.[2] Two types are known: serine β-lactamases (SBLs) with a serine active site and metallo β-lactamases (MBLs) with a zinc active site.[3] Strategies to counteract β-lactamase-mediated resistance include developing novel β-lactam antibiotics resistant to hydrolysis and creating β-lactamase inhibitors that restore the effectiveness of co-administered antibiotics.[4] Many SBL inhibitors are available for combination therapy against resistant infections, but few MBL inhibitors are in clinical trials, and none are commercially available.[1,5] Our research group has extensively studied the zinc chelator NOTA[9] as an MBL inhibitor, showing promising activity.[6-9] This study aims to investigate the mechanism of action of NOTA on zinc ions in the New Delhi MBL (NDM-1) using computational techniques to inform the design of more effective inhibitors. NOTA was prepared and docked into a suitable binding site of NDM-1 (PDB ID: 3SPU). The enzyme and ligand were further prepared with MCPB.py and underwent classical molecular dynamics (MD) simulations using Amber24. NOTA was found to coordinate with one of the zinc ions via its carboxylate oxygen, extracting it from the active site. Further *in silico* testing will adjust the force field of the zinc ions and repeat simulations with a dimeric NDM-1. Adaptive steered MD and parallel cascade selection MD will also be performed to assess the energy profile of NOTA-zinc interactions. This study lays the groundwork for future therapeutic strategies targeting MBLs.

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REFERENCES

1. G. Bahr, L. J. González, A. J. Vila, *Chem. Rev.* **2021**, *121*, 7957.
2. K. H. Tan X, K. Baugh, Y. Huang, N. Kadiyala, *Infect. Drug Resist.* **2021**, *14*, 125.
3. M. W. Crowder, J. Spencer, A. J. Vila, *Acc. Chem. Res.* **2006**, *39*, 721.
4. L.-C. Ju, Z. Cheng, W. Fast, R. A. Bonomo, M. W. Crowder, *Trends Pharmacol. Sci.* **2018**, *39*, 635.
5. D. Berman, S. J. Chandy, O. Cansdell, *Lancet Global Health*, **2022**, *10*, e293.
6. M. Shungube, A. K. Hlophe, L. Girdhari, *RSC Adv.* **2023**, *13*, 18991.
7. N. Reddy, L. Girdhari, M. Shungube, *Antibiotics* **2023**, *12*, 633.
8. B. K. Peters, N. Reddy, M. Shungube, L. Girdhari, *ACS Infect. Dis.* **2023**, *9*, 486.
9. A. M. Somboro, D. Tiwari, L. A. Bester, *J. Antimicrob. Chemother.* **2015**, *70*, 1594.

P14

BASE-MEDIATED SYNTHESIS OF SULTONE-SPIROOXINDOLES FROM 3-HYDROXYOXINDOLES AND 2-(HETERO)ARYLETHENESULFONYL FLUORIDES

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Sulfur-containing spirooxindoles are recognized for their significant biological activity[1,2] yet accessing these compounds with diverse heteroatoms in the spirocyclic core has remained challenging.[3] The development of SuFEx click chemistry by Nobel Laureate Prof. Barry Sharpless[4] has resulted in simpler and more efficient access to sulfur-heterocycles, most notably the synthesis of sultones.[5,6] Sultones, which are cyclic esters of hydroxysulfonic acids, have shown promising biological activity.[7] A method to access a spirooxindole which contains a valuable sultone cycle within the spirocyclic core has yet to be reported. This study introduces a facile inorganic base-mediated method, utilizing the green solvent acetone to synthesize novel sultone-containing spirooxindoles via a tandem Michael addition reaction and SuFEx click reaction. The use of green solvents proved essential in suppressing side reactions, leading to the successful synthesis of 21 novel sultone-spirooxindoles in yields ranging from 28% to 91%. Additionally, an organocatalyzed asymmetric variant of the reaction was explored, laying the groundwork for the future development of asymmetric sultone-containing spirooxindoles.

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REFERENCES

1. D. Cheng, Y. Ishihara, B. Tan, C. F. III Barbas, *ACS Catal.* **2014**, *4*, 743.

2. V. V. Vintonyak, K. Warburg, H. Kruse, S. Grimme, K. Hübel, D. Rauh, H. Waldmann, *Angew. Chem., Int. Ed.* **2010**, *49*, 5902.

3. M. Feng, B. Tang, S. H. Liang, X. Jiang, *Curr. Top. Med. Chem.* **2016**, *16*, 1200.

4. J. Dong, L. Krasnova, M. G. Finn, K. B. Sharpless, *Angew. Chem., Int. Ed.* **2014**, *53*, 9430.

5. A. Ungureanu, A. Levens, L. Candish, D. W. Lupton, *Angew. Chem.* **2015**, *127*, 11946.

6 X. Chen, G.-F. Zha, G. A. L. Bare, J. Leng, S.-M. Wang, H.-L. Qin, *Adv. Synth. Catal.* **2017**, *359*, 3254.

7. Y. Xu, Z. Zhang, J. Shi, X. Liu, W. Tang, *Arabian J. Chem.* **2021**, *14*, 103037.

SURFACTANT FREE MICROEMULSION COMPOSED OF HEXANOL, ETHANOL AND WATER

P15

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Microemulsions are thermodynamically stable, optically transparent mixtures of at least two immiscible liquids (usually one polar and one non-polar) and an amphiphilic compound, often a surfactant, which are referred to as surfactant-based microemulsions (SBMEs). However, the use of surfactants can introduce issues such as environmental concerns, increased costs, and potential toxicity.[1] To address these challenges, researchers have been exploring the development of surfactant-free microemulsions (SFMEs), which can provide similar benefits without the negative aspects associated with surfactants. These SFMEs are typically composed of two immiscible liquids and an amphi-solvent. Ternary system we studied consists of hexanol, water, and ethanol. The phase behavior of this system reveals both a single-phase microemulsion region and a multiphase region. Conductometric measurements were used to identify microregions within the single-phase area, while dynamic light scattering (DLS) confirmed the presence of structures with varying hydrodynamic radii near the binodal curve. Although SFMEs remain thermodynamically stable for extended periods, they eventually degrade over time. Nonetheless, they offer advantages such as reduced toxicity, lower production costs, and easier purification of nanoparticles.[2]

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REFERENCES

1. X. Zhong, M. Song, J. Chai, X. Cui, J. Wang, *Journal of Molecular Liquids* **2019**, *300*.
2. W. Hou, J. Xu, *Curr. Opin. Colloid Interface Sci.* **2016**, *25*, 67.

P16

ADAPTIVE TITRANS ADDITION FOR TITRATIONS INVOLVING EQUILIBRIA DESCRIBED BY SCATCHARD EQUATION

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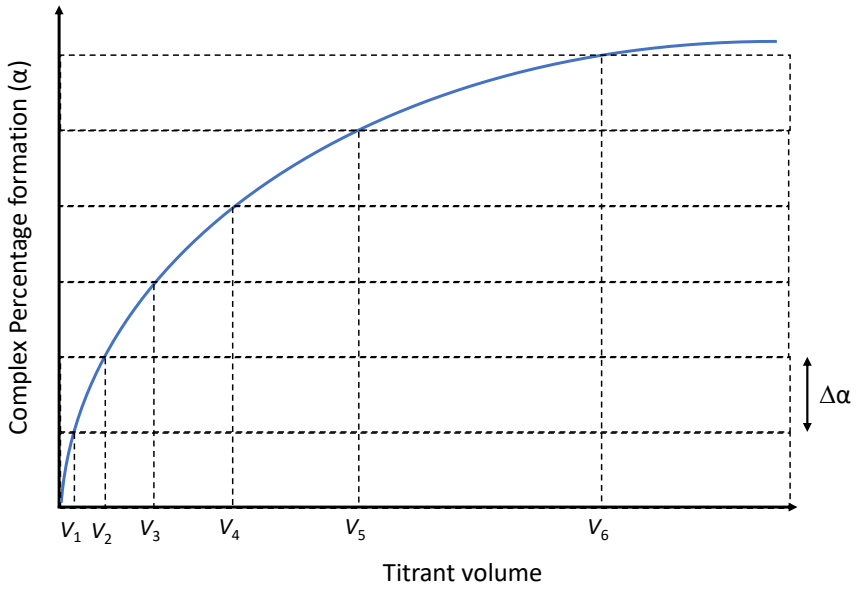
Titrations experiments are routinely used for stability constant determinations of supramolecular complexes in solution due to the commercially available instruments, the ability to gather large amount of data for analysis and the simplicity of the practical part of the experiment. The volumes of the titrant solution are primarily chosen to cover a specific range of titrant concentrations in cuvette after mixing, with little to some attention to the change of the complex distribution with the titrant concentration. Here we report adaptive titrant addition procedure that selects the titrant volumes with respect to the constant change in the percentage formation of the complexes that have multiple independent binding sites. Such equilibria are usually described by models based on Scatchard equation involving two parameters: stability constant and the number of independent binding sites on the host molecule.[1] The chemometric analysis of the simulated data with and without variable titrant volume addition is performed and the results are compared with respect to the parameter values and uncertainties.[2]



REFERENCES

1. G. Scatchard, *Ann. N. Y. Acad. Sci.* **1949**, *51*, 660.
2. J. Tellinghuisen, *J. Phys. Chem. B* **2007**, *111*, 11531.

P17

PROTON-COUPLED ELECTRON TRANSFER REACTIONS OF FLAVONOIDS QUERCETIN AND CATECHIN

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Flavonoids, quercetin and catechin, are attractive bioactive molecules due to their wide range of properties, including anticancer, anti-inflammatory, antiviral, anti-aging, and many others.[1] At least part of these activities is associated with an antioxidative mechanism, which involves electron transfer, often coupled with proton transfer. However, experimental evidence of the reaction mechanism is still limited.[2-4]

In this study, the mechanism of electron and proton transfer in reactions between flavonoid (quercetin or catechin) and DPPH radical in dioxane:water (99:1 or 95:5 *v*/*v*) solvent mixture is investigated through experimental kinetic analysis and computational chemistry methods. The reaction rate constants, kinetic isotope effects, and thermochemical analysis indicate a concerted proton-coupled electron transfer mechanism. The potential involvement of hydrogen tunneling is examined by analyzing isotopic differences in activation parameters A_H/A_D and ΔEa(D-H).

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REFERENCES

1. S.-M. Tang, X.-T. Deng, J. Zhou, Q.-P. Li, X.-X. Ge, L. Miao, *Biomed. Pharmacother.* **2020**, *121*, 109604.
2. K. U. Ingold, D. A. Pratt, *Chem. Rev.* **2014**, *114*, 9022.
3. J. Torić, A. Karković Marković, S. Mustać, A. Pulitika, C. Jakobušić Brala, V. Pilepić, *Int. J. Mol. Sci.* **2024**, *25*, 6341.
4. M. C. Foti, C. Rocco, Z. Jin, R. Amorati, *New J. Chem.* **2024**, *48*, 16047.

P18

ENHANCING ELECTROCHEMICAL PERFORMANCE OF POLY-(3-HEXYLTHIOPHENE): A COMPARISON OF ELECTROSPUN FIBERS AND FILMS

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Nanofibers are attractive nanostructures due to high and tuneable surface to volume ratio, however they were relatively rarely obtained from conducting polymers. In this work conducting polymer nanofibers were successfully prepared from regiorandom poly(3-hexylthiophene).[1] Significant improvements in electrochemical properties were observed during the electrochemical doping process conducted in the aqueous phase, which also resulted in changes to optical properties and water contact angle-effects not seen in polymer films. Additionally, pronounced and irreversible structural changes, such as increased crystallinity from the incorporation of doping ions, were confirmed through optical and X-ray crystallographic studies. These modifications led to decreased resistance and enhanced electrochemical performance of the nanofiber mat. This effect was found to be unique to nanofibers and attributed to their high surface-to-volume ratio. Thus, it was demonstrated for the first time that the electrochemical doping process of polythiophene is dependent on the polymer format, making it an attractive method for improving the electrochemical properties of polymers in nanofiber form.

REFERENCES

1. A. Jelińska, J. Kalisz, D. Pociecha, K. Maksymiuk, A. Michalska, *Electroanalysis* **2024**, *36*, e202300287.

THERMAL AND STRUCTURAL CHARACTERIZATION OF SELECTED BIOPOLYMERS AFTER IRRADIATION

P19

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We have investigated commercial polymers derived from natural sources, specifically poly(hydroxybutyrate) (PHB), poly(hydroxybutyrate-valerate) (PHBV), and poly(lactic acid) (PLA). These biopolymers are fully or partially biodegradable and offer a more environmentally friendly alternative to traditional packaging materials like polyolefins. The study involves irradiating these polymers with a 25 kGy dose using a Co^{60} gamma source at the Ruđer Bošković Institute. This dose is typically used for sterilization and allows researchers to study how radiation affects the polymers. It is well known that irradiation can alter sensitive materials such as polymers, either causing them to degrade or cross-link, depending on their chemical structure. The outcome of irradiation depends on conditions such as the presence of additives and other factors. Generally, biopolymers are observed to degrade at higher irradiation doses[1].

Incorporating gamma radiation in the sterilization process can extend the lifecycle of these materials, allowing them to be reused and recycled without harmful environmental impact associated with the chemical treatment used in recycling. To assess thermal stability, the biopolymers PHB, PHBV, and PLA are tested using differential scanning calorimetry (DSC). This helps researchers understand changes in melting temperature T_m, crystallization T_c, melting enthalpy ΔH_m crystallization enthalpy ΔH_c, and degree of crystallinity w_c, before and after irradiation. These measurements also reveal changes in glass transition temperature for PLA and show that the crystallization and melting behaviour of biopolymers depend on heating and cooling rates.

Chemical changes, such as the formation of new functional groups in polymers due to radiation, are analysed using FTIR-ATR spectroscopy (Fourier transform infrared spectroscopy with attenuated total reflection). This technique observed changes in the absorbance of specific bands for PHB, PHBV, and PLA at specific dose[2]. We have also examined the supramolecular structure of these polymers through optical microscopy. Any changes in the semi-crystalline structure caused by radiation of the polymer will be monitored by X-ray diffraction (XRD) on the powder samples[2,3]. The ultimate goal of this research is to explore the full potential for reusing biodegradable polymers after collection and sterilization, thereby reducing plastic waste in the environment.

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REFERENCES

1. H. Yang et al., *Polymer International,* **2004**, *53*, 1677.
2. L. M. Oliviera et al., *Polymer Degradation and Stability*, **2006**, *91*, 2157.
3. M. Vidotto et al., *Radiation Physics and Chemistry*, **2021,** 109 456.

P20

SHAKING THINGS UP: A SOLID-STATE APPROACH TO THE COREY-FUCHS REACTION

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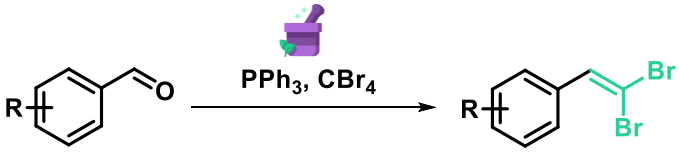
Dihaloalkenes are among the most important precursors used in organic synthesis, and one of the methods for their synthesis is the first step of Corey-Fuchs reaction.[1] It involves a transformation of an aldehyde using triphenylphosphine and tetrahalomethane.[2] These compounds play a vital role in the synthesis of various heterocycles, carboxylic acids, esters and thioamidestioamides. [3]

Despite its utility, this reaction has several drawbacks, e.g., the use of large volumes of solvents, low temperatures and various reaction times ranging from 15 minutes to several hours.[1,2] In the search for an environmentally friendly method, we decided to investigate whether mechanochemistry could be applied to the synthesis of dibromoalkenes using Corey-Fuchs protocol. Mechanochemistry is the study of chemical reactions initiated or driven by mechanical force rather than traditional heat or light energy.[4]

This poster discusses the results obtained so far during the investigation of the mechanochemical variant of the reaction.



The general route for the solid-state synthesis of dibromoalkenes and alkynes.

REFERENCES

1. E. J. Corey, P. L. Fuchs, Tetrahedron Lett. **1972**, *13*, 3769.

2. R. M. Denton, J. An, B. Adeniran, A. J. Blake, W. Lewis, A. M. Poulton, *J. Org. Chem.,* **2011**, *76*, 6749.

3. a) L. Tao,W. Yang, W. Zhao, *ChemistrySelect* **2021**, *6*, 8532. b) J. Vankar, A. Gupta, J. P. Jadav, S. H. Nanjegowda, G. N. Gururaja, *Org. Biomol. Chem.* **2021**, *19*, 2473. b) S. Biswas, B. Van Steijvoort, M. Waeterschoot, N. R. Bheemireddy, G. Evano, B. U. W. Maes, *Angew. Chem. Int. Ed.* **2021**, *60*, 21988.

4. A. D. McNaught, A. Wilkinson, *IUPAC. Compendium of Chemical Terminology*, 2 Ed., Blackwell Scientific Publications, **1997**, Oxford, England.

SOLUTION IS REACTION WITHOUT SOLVENT

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Mechanochemical synthesis has become a widely adopted, eco-friendly alternative to traditional solution synthesis.[1,2] There are advantages of this approach, including avoidance of solvents, reduced chemical consumption, simplified setup, and shorter reaction times, often resulting in higher yields. In this study, a series of compounds, primarily aromatic isothiocyanates and thioureas, were synthesized using the ball milling technique.[3] A comparison of reaction results between solution synthesis and mechanochemical synthesis was carried out. Optimization of the mechanochemical synthesis of isothiocyanates focused on factors such as reaction time, the addition of small amounts of solvent (known as liquid-assisted grinding (LAG)), and a solid grinding additive. Experimental results demonstrate that maximum yields were obtained with extended reaction times.

Keywords: mechanochemistry, synthesis, ball milling, aromatic isothiocyanates, thioureas

REFERENCES

1. D. Margetić, *Organic Mechanochemistry: A New Tool for Sustainable Synthesis*, Elsevier, Amsterdam, **2025**.
2. D. Margetić, V. Štrukil, *Mechanochemical Organic Synthesis*, Elsevier, Amsterdam, **2016**.
3. V. Štrukil, D. Margetić, M. D. Igrc, M. Eckert-Maksić, T. Friščić, *Chem. Commun.* **2012**, *48*, 9705-9707.

P22

HYDROGEN TUNNELING IN REACTION OF DOPAMINE AND DPPH RADICAL

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Dopamine is a biological catecholamine that acts as neurotransmitter in the central nervous system and also as hormone in the peripheral endocrine system. Due to its catechol moiety, dopamine has a function of endogenous antioxidant and its antiradical activity towards several types of reactive oxygen species (ROS) is already known.[1,2] The reaction of dopamine and DPPH radical was previously investigated in polar water/methanol reaction medium in which the SPLET mechanism was confirmed[3] but some computational studies pointed out the possibility of HAT/PCET mechanism in this reaction as well.[4] In this study, the same reaction was conducted in mostly nonpolar homogenous system of 1,4-dioxane:water = 95:5 *v/v* in an attempt to provide experimental evidence of HAT/PCET mechanism. The kinetic measurements of reaction rates at different temperatures and kinetic isotope effects were experimentally determined. The values of KIE significantly greater than semi-classically expected values, together with thermodynamic activation parameters, reveal the presence of hydrogen tunneling in the reaction and possible HAT/PCET mechanism. Additional evidence in support of the underlying reaction mechanism was gained by computational chemistry methods.

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REFERENCES

1. D. S. Dimić, D. A. Milenković, J. M. Dimitrić Marković, Z. S. Marković, *Mol. Phys.* **2017**, *116*, 1166.
2. T. Shimizu, Y. Nakanishi, M. Nakahara, N. Wada, Y. Moro-oka, T. Hirano, T. Konishi, S. Matsugo, *J. Clin. Biochem. Nutr.* **2010**, *47*, 181.
3. K. Jodko-Piórecka, B. Sikora, M. Kluzek, P. Przybylski, G. Litwinienko, *J. Org. Chem.* **2022**, *87*, 1791.
4. D. Dimić, D. Milenković, J. Dimitrić Marković, Z. Marković, *Phys. Chem. Chem. Phys.* **2017**, *19*, 12970.

P23

PRELIMINARY RESEARCH ON *QUERCUS PUBESCENS* BEE POLLEN: ULTRASONIC EXTRACTION AND ESTIMATION OF CYTOTOXIC POTENTIAL

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Bee pollen is a valuable bee product consisting of agglutinated flowers pollen grains, small amounts of bee salivary secretions, nectar and/or honey.[1] The composition of bee pollen strongly depends on the plant source and regional origin.[2] In this study, unifloral bee pollen of *Quercus pubescens* from the Croatian region (Otočac) was obtained and selected for preliminary research. The aim of the research was to apply ultrasonic solvent extraction as a green method and to evaluate the bioactive potential of the obtained bee pollen extract. The unifloral bee pollen was selected on the basis of its visual appearance and further ascertained by microscopic examination (palynological analysis).[3] The solvent extraction of the bioactive substances was carried out by indirect sonication of unifloral bee pollen in an ultrasonic bath at 40°C for 15 minutes with two re-extraction under the same extraction conditions. The solvent (methanol) was simply evaporated from the obtained bee pollen extract, and the dried samples were prepared for the determination of cytotoxic activity on two cancer cell lines, osteosarcoma (U2OS) and colon cancer cells (HCT116), using the MTS-based CellTiter 96® Aqueous Assay. The results were expressed as mean IC_{50} values (IC_{50} = 22.11 mg mL^{-1} for the U2OS cell line and 23.92 mg mL^{-1} for the HCT116 cell line), indicating the cytotoxic potential of the bee pollen extract. This preliminary study encourages finding solutions for further development of environmentally friendly methods for isolation of natural bioactive compounds from bee pollen from the Croatian region.

ACKNOWLEDGEMENTS This research was conducted as part of the institutional research project entitled “Research of chemical diversity and bioactive potential of natural products", funded by the Faculty of Science of the University of Split.

REFERENCES

1. A. Pascoal, S. Rodrigues, A. Teixeira, X. Feás, L. M. Estevinho, *Food Chem. Toxicol.* **2014**, *63*, 233.
2. M. Martinello, F. Mutinelli, *Antioxidants* **2021**, *10*, 71.
3. O. M. Barth *et al. Annals of Brazilian Academy of Sciences* **2010**, *82*, 893.

P24

THERMODYNAMICS OF STEROID COMPLEXATION REACTIONS WITH CYCLODEXTRINS AND CUCURBIT[7]URIL

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Cyclodextrins and cucurbiturils are well known as receptors for lipophilic guests among which steroids stand out as particularly noteworthy due to their diverse structures, low solubility, and biological significance.[1,2] Inclusion of steroids in the cavities of these macrocycles has been studied primarily by means of NMR spectroscopy[2,3] and, to a lesser extent, calorimetry.[2,3] The obtained results indicate the need for systematic investigations into the influence of the steroid structure, as well as the type and position of polar functional groups on the thermodynamic reaction parameters. The importance of investigating these reactions is further emphasized by the fact that complexation of steroids with cyclodextrins and cucurbiturils enhances their bioavailability[1,2] and is sometimes used for their removal from food products.[4]

In this work, the thermodynamics of inclusion of several steroids and bile salts in cucurbit[7]uril, β- and γ-cyclodextrin was investigated in water at 25 °C. Special emphasis was placed on the influence of steroid ring geometry on the complex stoichiometry and thermodynamic complexation parameters. The complexation reactions were enthalpically driven in the case of heptameric receptors, while the inclusion within γ-cyclodextrin was both enthalpically and entropically favorable. The number and position of hydroxyl groups in bile salts significantly affected the stability of complexes with cyclodextrins. In line with our previous findings,[5–7] the $\Delta_r G°$ for the reaction of two investigated steroids with γ-cyclodextrin was almost temperature-independent (temperature enthalpy-entropy compensation), despite the considerably negative $\Delta_r C_p°$ values.

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REFERENCES

1. É. Fenyvesi *et al.*, *Environ. Chem. Lett.* **2019**, *17*, 375–391.
2. A. I. Lazar *et al.*, *J. Am. Chem. Soc.* **2016**, *138*, 13022–13029.
3. R. Holm *et al.*, *J. Incl. Phenom. Macrocycl. Chem.* **2013**, *75*, 223–233.
4. L. Alonso *et al.*, *J. Dairy Sci.* **2009**, *92*, 863–869.
5. K. Leko *et al.*, *Chem. – Eur. J.* **2020**, *26*, 5208–5219.
6. A. Usenik *et al.*, *New J. Chem.* **2023**, *47*, 18745–18755.
7. A. Usenik *et al.*, *J. Mol. Liq.* **2023**, *388*, 122774.

P25

ECOTOXIC EFFECT OF AZITHROMYCIN IN COMBINATION WITH MICROPLASTICS AND ANTIVIRALS ON *Daphnia magna*

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The use of antibiotics and antivirals significantly improved the prevention and treatment of infectious diseases, resulting in their wide usage. Moreover, the onset of the COVID-19 pandemic increased significantly the use of antibiotics and antivirals. Accordingly, we can find them in all components of ecosystems, and their toxic effect on biota is increasingly monitored.[1] Azithromycin (AZ) is a semi-synthetic macrolide antibiotic that prevents the synthesis of bacterial proteins, thereby preventing the growth and reproduction of bacteria, while antivirals act by killing or preventing the growth of viruses.[2] Microplastics (MPs) are polluting substances that are also found in all components of the environment, with the ability to absorb antibiotics and antivirals, which in combination can be more toxic than individually. These xenobiotics can enter the food chain at all trophic levels. In the present research, the acute toxicity of AZ was investigated in five concentrations of 0.001; 0.01; 0.1; 0.25 and 0.5 mmol/L, and the results confirmed that the toxic effect of AZ increased with the concentration (EC_{50} 0.6 mmol/L). In a binary combination with different MP types (polystyrene (PS), poly(ethylene terephthalate) (PET), poly(vinyl chloride) (PVC) and polyethylene (PE)) of particle size 100 – 300 µm and concentration of 500 mg/L, results showed higher mortality for combinations AZ-PE and AZ-PET, while the ternary combination of AZ and PS with antivirals atazanavir (ATA) at concentration of 0.003 mmol/L and emtricitabine (EMT), nirmatrelvir (NIR), oselfamivir (OSE), ribavirin (RIB) and sofosbuvir (SOF) at concentration of 0.1 mmol/L showed that environmental levels of antivirals did not cause toxic effect on the test organism *Daphnia magna*.

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REFERENCES

1. Y. Li, Y. Ma, L. Yang, S. Duan, F. Zhou, J. Chen, Y. Liu, *Ecotoxicol. Environ. Saf.* **2020**, *197*, 110573.
2. Z. Banić Tomašić, *Kem. Ind.* **2011**, *60*, 12.

P26

AMPHIPHILIC MOLECULES WITH IMINE LINKAGE: TOWARDS pH-RESPONSIVE ASSEMBLIES

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Stimuli-responsive features allow for the control of functions in response to specific stimuli. Their incorporation into supramolecular systems is an increasingly popular topic with numerous potential applications, including controlled drug delivery systems, responsive hydrogels, sensors, etc.[1] In recent years, the development of micellar systems as media for organic reactions has led to several commercial compounds.[2] Despite stimuli-responsive supramolecular systems for organic reactions holding great potential, they have yet to be developed.

Amphiphilic molecules create a hydrophobic environment in the solution through non-covalent interactions of their hydrophobic parts while the hydrophilic parts provide solubility. On the inside of the structure is a hydrophobic pocket where reactions can take place. Since the system is in an aqueous medium, using an easy-to-achieve pH change as a stimulus is a logical choice.[3,4]

Within this project, a series of amphiphilic molecules bearing imine pH-responsive dynamic covalent bonds has been synthesized (Figure 1). Their properties in aqueous media and self-assembly into supramolecular structures are currently being investigated. The disassembly of these supramolecular structures will be analysed as a function of pH change. Considering the preliminary results, additional structural modifications will be made, such as varying the length and number of hydrophilic and hydrophobic chains. Finally, these systems will be employed as media for organic reactions.

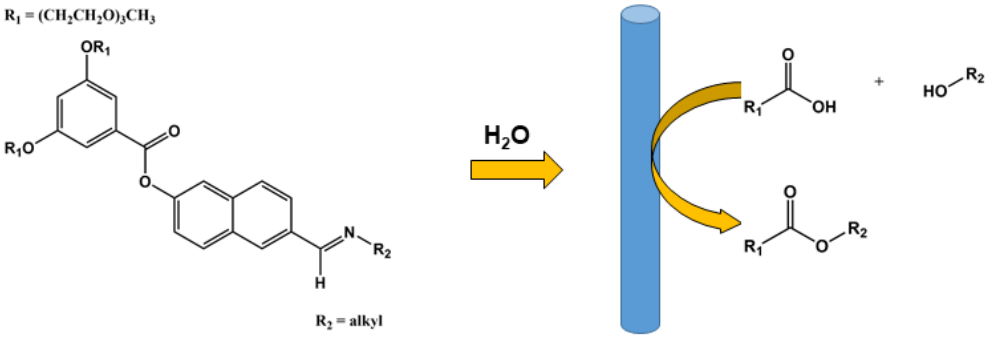

Figure 1. Objectives of the project.

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REFERENCES

1. M. Ikeda, *Polym. J.* **2019**, *51*, 371.

2. M. Cortes-Clerget, J. Yu, J. R. A. Kincaid, P. Walde, F. Gallou, B. H. Lipshutz, *Chem. Sci.* **2021**, *12*, 4237.

3. B. Parshad, S. Prasad, S. Bhatia, A. Mittal, Y. Pan, P. K. Mishra, S. K. Sharma, L. Fruk, *RSC Adv.* **2020**, *10*, 42098.

4. T. Allam, D. E. Balderston, M. K. Chahal, K. L. F. Hilton, C. K. Hind, O. B. Keers, R. J. Lilley, C. Manwani, A. Overton, P. I. A. Popoola, L. R. Thompson, L. J. White, J. R. Hiscock, *Chem. Soc. Rev.* **2023**, *52*, 6892.

P27

NAPHTHALENE DIIMIDE π-AMPHIPHILES FOR THE PREPARATION OF TUBULAR SUPRAMOLECULAR ARCHITECTURES IN WATER

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Self-assembled structures and materials have gained much attention in recent years.[1] Their properties, such as self-healing (re-assembly), adaptation and response to the external stimuli, and possible reconfiguration mimic the basic characteristics of biological systems. The self-assembly of organic molecules in aqueous media has been extensively studied due to the variety of useful structures they can form, such as tubular structures, micelles, vesicles, bilayers and others. The preparation of these organic supramolecular structures is often quite challenging and usually based on the trial-and-error approach. The implementation of selected structural motifs and their intrinsic ratio in building-block molecules (monomers), such as the ratio of hydrophobic and hydrophilic functional groups, enable the design of these systems, although just only to some extent.[1-2]

In our work, we focus on the preparation of novel organic supramolecular tubular architectures, such as nanocylinders, nanotubes and microtubes, and their subsequent modification and utilization in organocatalysis in aqueous media. The naphthalene diimide building block guides the molecular self-assembly in a linear direction through π-stacking interactions.[2,3] Thus, amphiphilic molecules bearing naphthalene diimide unit have a propensity to assemble into tubular structures in water, forming hydrophobic cavities where organic reactions can take place. In addition, water is a much greener solvent than many of the organic solvents in use today. The statement carries even greater weight when we consider the industrial scale of organic synthesis and the waste it generates, so the transition to greener industrial processes should be achieved.

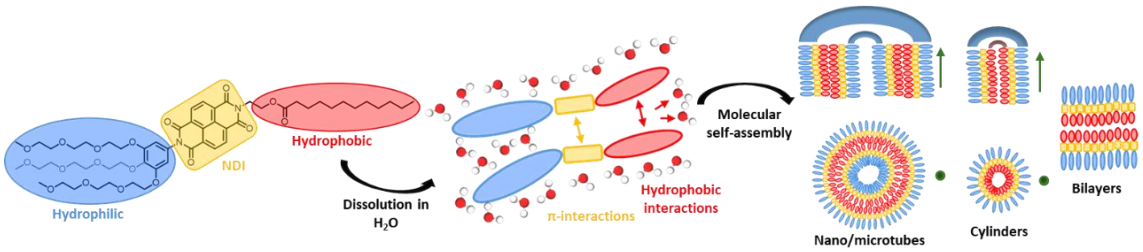

Figure 1. Interactions and self-assembly of naphthalene diimide π-amphiphiles in aqueous media.

ACKNOWLEDGEMENTS This work is financially supported by STARTNOW project (NPOO.C3.2.R2-I1.06.0042) funded by the NexGenerationEU.

REFERENCES

1. B. Parshad, S. Prasad, S. Bhatia, A. Mittal, Y. Pan, P. K. Mishra, S. K. Sharma, Lj. Fruk, *RSC Adv.* **2020**, *10*, 42098.

2. A. Sikder, Y. Xie, M. Thomas, M. J. Derry, R. K. O'Reilly, *Nanoscale* **2021**, *13*, 20111.

3. T. Choisnet, D. Canavet, M. Salle, E. Nicol, F. Niepceron, J. Jestin, O. Colombani, *Chem. Commun.* **2019**, *55*, 9519.

P28

INCLUSION OF ACETONITRILE AND METHANOL MOLECULES IN A CALIX[4]ARENE HYDROPHOBIC CAVITY

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Calixarene derivatives possessing electron-donating functional groups at the lower rim show a high affinity towards alkali and alkaline metal cations. The inclusion of solvent molecule into the calixarene hydrophobic *basket* plays an important role in determining the extent of cation complexation reactions.[1] However, the structural and thermodynamic aspects of solvent inclusion in the complexes of alkaline earth metal cations have been seldom explored in detail.

In this work, we have determined the thermodynamic reaction parameters for complexation of second-group cations by calixarene derivative **L** (Figure 1) by means of various experimental methods (UV absorption spectrometry, fluorimetry, ITC), and compared them with those corresponding to the first-group cations.[2] With this respect, the influence of solvent molecule inclusion was particularly addressed from the structural and thermodynamic points of view. The structures of the ligand-solvent and complex-solvent adducts were investigated by NMR spectroscopy, classical molecular dynamics simulations, and DFT calculations. The main structural difference between the solvent adducts of the first- and second-group cation complexes was found to be in the orientation of the solvent molecules inside the calixarene cavity (Figure 1). In the latter case, cations were additionally coordinated by the solvent -CN/-OH group, thereby significantly affecting the thermodynamic stability of the corresponding complexes.

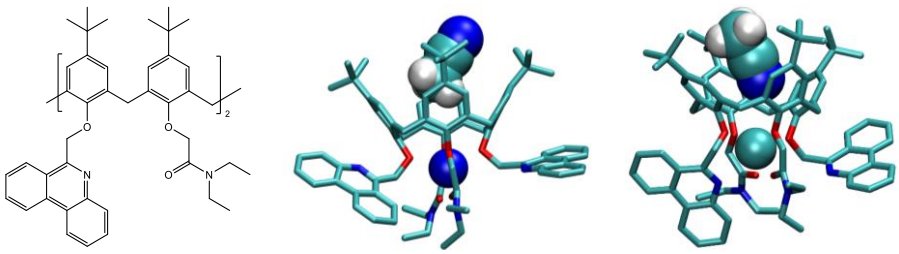

Figure 1. Structures of **L** and acetonitrile adducts of Na**L**$^{+}$ and Ca**L**$^{2+}$ obtained by MD simulations.

ACKNOWLEDGEMENTS This research was funded by Croatian Science Foundation (project MacroSol, Grant No. IP-2019-04-9560) and European Regional Development Fund (infrastructural project CIuK, Grant No. KK.01.1.1.02.0016).

REFERENCES

1. A. F. Danil de Namor, N. A. De Sueros, M. A. McKervey, G. Barrett, F. A. Neu, M. J. Schwing-Weill, *J. Chem. Soc., Chem. Commun.* **1991**, 1546.; A. F. Danil de Namor, S. Chahine, D. Kowalska, E. E. Castellano, O. E. Piro, *J. Am. Chem. Soc.* **2002**, *124*, 12824–12836.; A. S. de Araujo, O. E. Piro, E. E. Castellano, A. F. Danil de Namor, *J. Phys. Chem. A* **2008**, *112*, 11885–11894. G. Horvat, V. Stilinović, B. Kaitner, L. Frkanec, V. Tomišić, *Inorg. Chem.* **2013**, *52*, 12702–12712.; J. Požar, M. Cvetnić, A. Usenik, N. Cindro, G. Horvat, K. Leko, M. Modrušan, V. Tomišić, *Molecules* **2022**, *27*, 470.

2. K. Leko, A. Usenik, N. Cindro, M. Modrušan, J. Požar, G. Horvat, V. Stilinović, T. Hrenar, V. Tomišić, *ACS Omega* **2023**, *8*, 43074–43087.

P29

QUANTUM CHEMICAL INVESTIGATION OF STRUCTURAL AND THERMODYNAMIC PARAMETERS FOR CUCURBIT[7]URIL COMPLEXES

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Electronic and steric effects in complexes of cucurbit[7]uril (**CB7**) with benzene and phenol were investigated by extensive quantum chemical analysis. For **CB7** and all complexes simulations of *ab initio* molecular dynamics were conducted and trajectories in Cartesian coordinates were sampled for a total duration of 5 ns.[1] Molecular dynamics were propagated *on-the-fly* using the Verlet integrator in ***qcc*** and the PM7 hamiltonian implemented in MOPAC2016.[2] Trajectories were converted into the distance coordinates and complete configurational spaces were determined by tensor decomposition of trajectories together with the analysis of probability distributions in a reduced space.[3] All these generated structures for **CB7** and both complexes were optimized at the B3LYP-D3BJ/6-31G(d) level of the theory using Grimme's D3 dispersion correction and Becke-Johnson damping.[4,5] Harmonic vibrational frequencies and standard Gibbs energies of formations for all systems were also calculated. Using the Boltzmann distribution of all configurations, standard Gibbs energies of binding for benzene and phenol were estimated. The most stable complexes were those with bifurcated hydrogen bonds and had negative standard Gibbs binding energies. A comprehensive structural analysis of all calculated conformations (for **CB7**) and configurations (for complexes) along with standard Gibbs binding energies will be presented.

ACKNOWLEDGEMENTS

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REFERENCES

1. T. Hrenar, ***qcc***, Quantum Chemistry Code, rev. 0.6826, **2024**.

2. MOPAC2016, J. J. P. Stewart, Stewart Computational Chemistry, Colorado Springs, CO, USA, **2016**, http://OpenMOPAC.net

3. T. Hrenar, ***moonee***, Code for Manipulation and Analysis of Multi- and Univariate Big Data, rev. 0.68268, **2024**.

4. S. Grimme, J. Antony, S. Ehrlich and H. Krieg, J. Chem. Phys. **2010**, *132*, 154104.

5. Gaussian 16, Revision A.03, M. J. Frisch et al., Gaussian, Inc., Wallingford CT, **2016**.

P30

APPLICATION OF FLAVANONES AND ZYMOSAN A INTERACTIONS STUDIED IN DIFFERENT SOLUTIONS

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Flavanones belong to the large group of plant metabolites called polyphenols. They are found predominantly in citrus fruits like oranges, grapefruit, lemons, and limes.[1] Since citrus fruits are frequently used in the diet, the bioactive effects of flavanone compounds are constantly being under study. Flavanones showed ability to interact with food components like dietary fiber in gastrointestinal tract where different pH values prevail. Since chemical structure of flavanones change at different pH values, it can affect their bioavailability. Therefore, dietary fiber like zymosan A from yeast can potentially carry them through gastrointestinal tract and protect their structure in different pH values.[2] Interaction between flavanones and dietary fiber can be studied through adsorption process. The aim of this work was to study interactions between flavanone and zymosan A in solution with different pH values (water, pH 3, pH 7) through the adsorption process. The spectrophotometric Folin-Ciocalteu method was validated in different solution and used for monitoring the flavanone concentration in the adsorption process. Adsorption was performed at 37 °C for 3 hours. Desorption process was also conducted. The results showed that flavanone adsorbed on zymosan A was influenced by the pH value of solutions. The highest adsorption capacity was at pH 7, and lower in water and pH 3. Desorption was the highest at pH 7. This study can find different applications like possible design of functional food, creating various dietary supplements containing together flavanone and zymosan A, then to increase flavanone bioaccessibility in lower parts of the gastrointestinal tract, or they can be used in bioactive materials.[3]

ACKNOWLEDGEMENTS This work was supported by the Faculty of Food Technology Osijek.

REFERENCES

1. I. Najmanová, M. Vopršalová, L. Saso, P. Mladěnka, *Crit. Rev. Food Sci. Nutr.* **2020**, *60*, 3155.
2. H. Y. Tang, Z. Fang, K. Ng, *Trends Food Sci. Technol.* **2020**, *100*, 333.
3. A. Siemińska-Kuczer, M. Szymańska-Chargot, A. Zdunek, *Food Chem.* **2022**, *373*, 131487.

P31

PYRENE-BASED AMPHIPHILES: TOWARD TUBULAR ASSEMBLIES IN WATER

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The rapid growth of the human population increasingly affects the environment with chemical and pharmaceutical industries playing a key role. Chemists are under growing pressure to develop greener processes[1], as majority of waste in chemical production comes from toxic organic solvents.[2] Recently, significant efforts have been made to find a sustainable reaction medium, with water being the most logical choice.

Bio-inspired, organic assemblies have a great potential for performing organic reactions in aqueous media.[3] Amphiphilic molecules assemble in aqueous media to minimize the contact of hydrophobic part with polar solvent molecules, leading to the formation of stable structures like micelles, vesicles and tubules.[4] The resulting hydrophobic pocket serves as a reaction site which holds reactants in a confined space and prevents the formation of side products.

Up to this point, a series of amphiphilic molecules forming spherical micelles has been prepared (Figure 1a). The objective of this project is to prepare molecules that assemble into tubular supramolecular structures in water by incorporating a pyrene moiety within molecular structure (Figure 1b). Large aromatic systems typically assemble in one direction due to strong π-π interactions. Given that tubular structures have higher surface-to-volume ratio compared to spherical micelles, the aim is to compare the outcomes of organic reactions performed in both spherical and tubular supramolecular systems (Figure 1c).

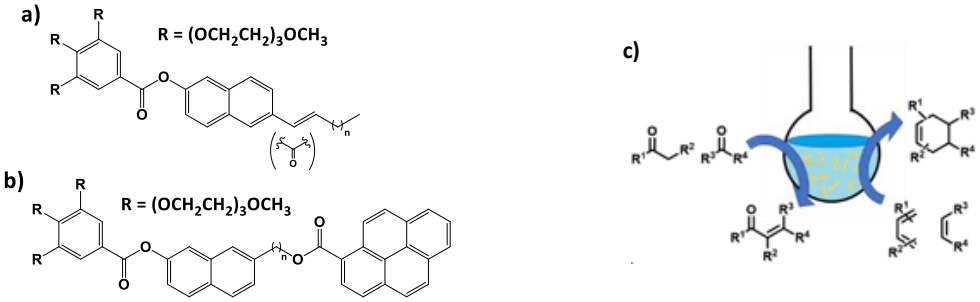

Figure 1. a) Amphiphilic molecules forming spherical micelles, b) Amphiphilic molecules for tubular structure formation, c) Organic reactions performed in spherical / tubular systems.

ACKNOWLEDGEMENTS This work was financially supported by STARTNOW project (NPOO.C3.2.R2-I1.06.0042) funded by the NexGenerationEU.

REFERENCES

1. P. Anastas, N. Eghbali, *Chem. Soc. Rev.* **2010**, *39*, 301.
2. D. J. C. Constable, A. D. Curzons, V. L. Cunningham, *Green Chem.* **2002**, *4*, 521.
3. M.O. Guler, S. I. Stupp, *J. Am. Chem. Soc.* **2007**, 129.
4. B. Parshad, S. Parsad, S. Bhatia, A. Mittal, Y. Pan, P. K. Mishra. S. K. Sharma, L. Fruk, *RSC Adv.* **2020**, 10.

P32

FIBRES WITH GREEN SYNTHESIZED Cu NANOPARTICLES MODIFIED AFTER ELECTROSPINNING

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Copper is one of the most widely recognized antimicrobial metals linked to multiple antimicrobial mechanisms such as: plasma membrane permeabilization, membrane lipid peroxidation, alteration of proteins, inhibition of protein assembly and activity, or denaturation of nucleic acids. Moreover, copper in a form of nanomaterials shows grater antimicrobial activity so is an emerging class of nano-antimicrobials providing complimentary effects and characteristics, as compared to widely used silver or zinc oxide nanoparticles. Green synthesis of copper nanoparticles was performed with ascorbic acid under mild process conditions. Reaction kinetic was determined by UV-VIS spectrometry.

Metal nanoparticle-loaded yarns produced by electrospinning can be used in a number of biomedical and textile applications such as medical devices, burn or wound dressings, healthcare materials (including disposables), personal care products, veterinary, military and bio-defense items, protective suits or clothing. This work therefore presents application of Cu nanoparticles in functionalization of the surface of medical material by deep coating method. Electrospun polycaprolactone biocompatible yarns were modified by using sol-gel procedure during which the Cu nanoparticles were incorporated within the coating. The materials were characterized before and after the modification by FTIR, UV-VIS, and SEM. The results proved efficient formation of a novel antimicrobial coating homogeneously distributed on the surface of the yarns. Additionally, antimicrobial tests of Cu nanoparticles proved the antimicrobial property of Cu nanoparticles in coating, enabling future application of novel medical material.

ACKNOWLEDGEMENTS This work was financially fully supported by the Croatian Science Foundation, project IP-2019-04-1381 entitled „Antibacterial coating for biodegradable medicine materials ABBAMEDICA“, project leader professor Iva Rezić Meštrović PhD PhD.

REFERENCES

1. I. Rezić, M. Somogyi Škoc, *Polymers* **2024**, *16*, 2320.
2. I. Rezić, E. Meštrović, *Coatings* **2023**, *13,* 1830.
3. I. Rezić, *Polymers* **2022**, *14*, 4961.

P33

THE EFFECT OF RING SIZE AND AMINO ACID TYPE ON CYCLOPEPTIDE ANION BINDING AFFINITIES

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During the past few decades there has been a growing interest in research of cyclopeptides as anion receptors. These compounds, besides their metabolic stability and bioavailability, exhibit enhanced binding affinity towards substrates compared to their more flexible linear analogs[1,2] which make them perfect candidates for antibiotics and membrane transport carriers. In this work the stability constants as well as reaction enthalpies and entropies of monovalent anion complexation by cyclohexaphenylalanine in acetonitrile and methanol were determined by means of ^{1}H NMR spectroscopy and microcalorimetry. Molecular dynamics simulations of the free receptor and its complexes were also performed to get an insight into their structures and to more deeply comprehend the factors governing the complexation equilibria. The obtained results were compared to those corresponding to pentaphenylalanine and penta- and hexaleucine analogs from our previous research[1,3] in order to elucidate the effect of ring size and amino acid type on the cyclopeptide affinity towards selected anions.

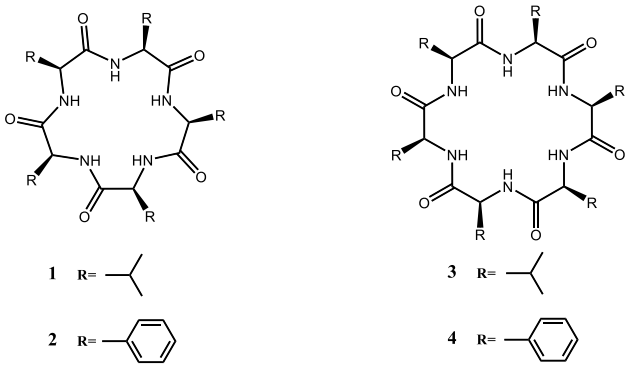

Figure 1. Structures of studied homocyclopeptides.

ACKNOWLEDGEMENTS This work was supported by the Croatian Science Foundation under project IP-2019-04-9560 (Macrosol) and European Regional Development Fund (project CIuK, KK.01.1.1.02.0016).

REFERENCES

1. I. Petters, M. Modrušan, N. Vidović, I. Crnolatac, N. Cindro, I. Piantanida, G. Speranza, G. Horvat, V. Tomišić, *Molecules* **2022**, *27*, 3918.

2. M. Modrušan, L. Glazer, L. Otmačić, I. Crnolatac, N. Cindro, N. Vidović, I. Piantanida, G. Speranza, G. Horvat, V. Tomišić, *Int. J. Mol. Sci.* **2024**, *25*, 5235.

3. G. Horvat, S. Tarana, N. Vidović, N. Cindro, G. Speranza, V. Tomišić, *J. Mol. Liq.* **2021**, *340*, 116848.

P34

CHARACTERIZATION OF HYDROXYETHYL CELLULOSE IN THE REFERENCE PRODUCT

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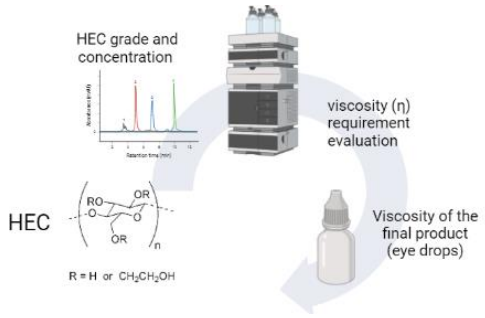
Hydroxyethyl cellulose (HEC) is a non-ionic, water-soluble polymer primarily used in ophthalmic products as a viscosity enhancer and thickening agent. Commercially available HEC comes in different grades, that differ mainly on the chain length (from 90 to 1300 kDa).[1] This has a direct impact on the HEC solution viscosity. The viscosity of a product is considered as a critical quality attribute (CQA). The specific grade (determined as the viscosity of HEC solution) and concentration of HEC are regarded as critical material attributes (CMA), aligning with the principles of quality by design (QbD).[2]

The aim of this research was to determine the grade (polymer length) and concentration of HEC present in the reference product (RP), during development of a generic product. The goal was to verify the equivalence with the RP, particularly regarding the viscosity as product's CQA. The grade and concentration of HEC in the RP were determined by Size Exclusion Liquid Chromatography (SEC-LC) with Refractive Index Detection (RID) using multiple probes and standards. Once the HEC's grade was confirmed, viscosity of 1% solution was evaluated as its CMA. During complex development, viscosity of the selected grade HEC solution was evaluated, and a stricter range of viscosity for the HEC solution was selected to ensure a final product of desired characteristics. Other factors during the manufacturing process besides grade and concentration of HEC influence final product viscosity.[3]

In conclusion, during development of a generic product, analytical characterization of HEC is critical to obtain a generic product equivalent to the RP. In this study, the selected grade and concentration of HEC were confirmed, which was also verified by formulation tests that were previously mentioned.[3] It is important to keep in mind that a complementary approach is necessary when developing complex formulations.



REFERENCES

1. Ashland, *Formulating elegant liquid and semisolid drug product*, brochure, Ashland, **2018**.
2. European Medicines Agency, *Draft guideline on quality and equivalence of topical products*, **2018**.
3. I. Poropat, K. Dubaić, M. Jurčević, D. Jureša, L. Munjas Jurkić, L. Štefan, T. Tomljanović, *Utjecaj hidroksietil celuloze na viskoznost gotovog lijeka (kapi za oko)* in A. Jukić, V. Ocelić Bulatović, D. Kučić Grgić, *20th Ružička Days 2024 'Today science – tomorrow industry' - book of Abstracts,* **2024** p. 96.

IN SEARCH FOR DESCRIPTORS IN CHIRAL Cp-CATALYSTS

P35

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Chiral cyclopentadienyl (Cp) metal complexes are an exceptional tool for inducing stereodivergent interactions between achiral molecules. Any change in the architecture of the ligand reflects on the overall stereoelectronic nature of the chiral Cp-catalyst.[1, 2] The application of these complexes for asymmetric C-H functionalization with 3d-metals has been previously shown by the synthesis of dihydroisoquinolones from *N*-chlorobenzamides with a broad range of alkenes.[3]

We propose alternative ways of constructing chiral Cp-ligands based on two main descriptors: percentage of buried volume and stereotopographic maps. We designed a synthetic route toward chiral Cp-ligands bearing additional variable substitutions on the Cp core. The structure of the DFT-optimized Cp complex with phenyl substituents, having buried volume 50.4 % is very similar to previously reported catalyst inducing high regio- and enantioselectivities.[3] (Figure 1). Interestingly, despite the similarity in the percentage of buried volume, the stereoelectronic properties of the proposed Cp-catalyst are significantly different compared to the previously studied one, thus opening the possibility for fine-tuning the stereoselectivity by varying substitution patterns.

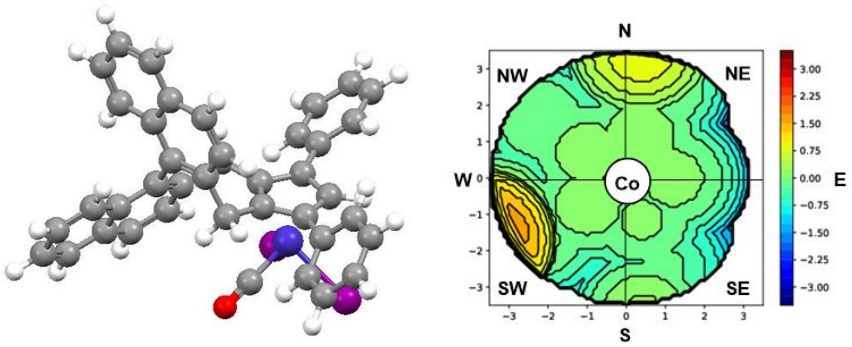

Figure 1. Optimized structure of chiral Co(III) cyclopentadienyl catalyst with phenyl substituents (left) and stereotopographic map (right). Buried volume: 50.4 %, B3LYP-D3/6-311+(2d,p) level of theory (LANL2DZ for cobalt and iodine).

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REFERENCES

1. G. Smith, B. Audic, M. D. Wodrich, C. Corminboeuf, N. Cramer, *Chem. Sci.* **2017**, *8*, 7174.

2. Y. Sun, N. Cramer, *Chem. Sci*. **2018**, *9*, 2981.

3. K. Ozols, Y.-S. Jang, *J. Am. Chem. Soc.* **2019**, *141*, 5675.

P36

NEW MONOQUATERNARY AMMONIUM SURFACTANTS AND THEIR PERMEABILITY THROUGH MODELED BIOMEMBRANE

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Quaternary ammonium surfactants (QASs) are amphiphilic molecules characterized by their unique physicochemical properties, making them highly effective in applications such as antiseptics and disinfectants. Their mode of action is often compared to that of antimicrobial peptides, which initially engage in electrostatic interactions with membrane surfaces, followed by membrane disruption and subsequent cell lysis. However, despite computational studies display interaction with membrane, still this mechanism was not fully elucidated.[1] Here, parallel artificial membrane permeability assay (PAMPA) was employed to investigate QASs potential to integrate or disrupt artificial membrane in hope to correlate their interaction with membrane with cytotoxicity potential. Therefore, a new series of mononquaternary quinuclidine surfactants were synthesized and their membrane permeability potential was analyzed in comparison to commercial standards. We show that the commercial standards have much higher potential to integrate into the artificial membrane (>90%) than the newly synthesized QASs which aligns with their higher cytotoxicity. These results suggest that the higher percentage of membrane integration could serve as a predictor of membrane disorganization in biological systems.

REFERENCES

1. S. Alkhalifa et al., *ChemBioChem*, **2019**, *21*, 10.

P37

DONOR-ACCEPTOR CHARGE-TRANSFER COMPLEXES BETWEEN *N*-SUBSTITUTED PYRIDINIUM OXIMES AND HEXACYANOFERRATE(II)

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Supramolecular materials are continuously attracting considerable attention because of the modularity of their structural components, inherent reversibility, and overall versatility. The utility of quaternary pyridinium salts (QPS) upon building supramolecular pyridinium-based metal-organic charge-transfer complexes (CTCs) stems from the noncovalent interactions from which they assemble, endowing them with great variety of dynamic properties that can be designed and controlled in both aqueous solution and solid state. Among diverse subclasses of QPSs, pyridinium oximes are already recognized as promising electron-accepting building blocks for the design of stimuli-responsive 2D- and 3D-inter-ionic CTCs with the $[Fe(CN)_6]^{4-}$ ion as an electron donor.[1,2] In addition, $[Fe(CN)_6]^{4-}$ platform, as a potential acceptor of six or more bifurcated H-bonds, is an excellent building block in creating functional H-bond networks.

Herein, we present the comparative spectroscopic study of inter-ionic CTCs formed between *N*-substituted mono-pyridinium oximes and $[Fe(CN)_6]^{4-}$ in aqueous solution and solid state. The *N*-methylpyridinium-2-oxime chloride (PAM2-Cl), *N*-methylpyridinium-3-oxime iodide (PAM3-I), *N*-methylpyridinium-4-oxime chloride (PAM4-Cl) and *N*-benzoylethylpyridinium-4-chloride (BEPA4-Cl) were employed as electron acceptors and H-bond donors. Variations in the position of oxime group and the size of substituent on the pyridinium ring allowed us to establish the intricate relationship between structural features of QPSs and structural and chromic properties of their $[Fe(CN)_6]^{4-}$-based CTCs. The crystal structure of $(PAM2)_4[Fe(CN)_6]\cdot 2H_2O$ emphasizes the role of lattice water molecules in self-assembly of such CTCs as represented in Fig. 1.

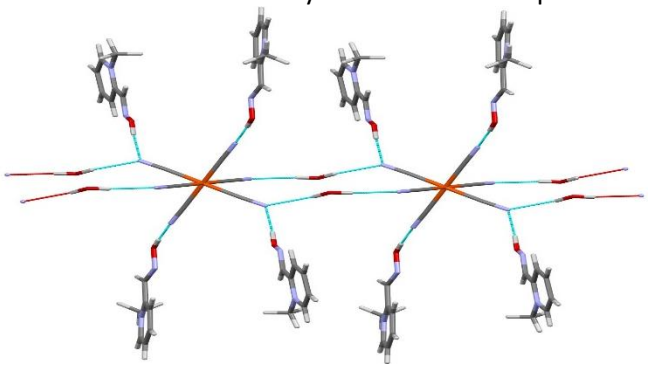

Figure 1. Hydrogen bonding pattern in the structure of $(PAM2)_4[Fe(CN)_6]\cdot 2H_2O$.

REFERENCES

1. B. Foretić, R. Vianello, D. Matković-Čalogović, D. Jadreško, I. Picek, *New J. Chem.* **2018**, *42*, 16115.

2. I. Picek, D. Matković-Čalogović, G. Dražić, G. Kapun, P. Šket, J. Popović, B. Foretić, *Molecules* **2024**, *29*, 1698.

P38

GRINDING NICKEL COMPOUNDS – MECHANOCHEMISTRY IN COMPLEXES SYNTHESIS

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The manufacture of noble metal complexes as catalysts or pre-catalysts is critical in industrial and laboratory chemical synthesis. However, the high cost and rarity of these elements have led to a shift to more affordable alternatives. Elements such as palladium, platinum, ruthenium, rhodium, and iridium slowly give way to their much more widespread neighbors from the periodic table (including iron, cobalt, and nickel). It should be noted that in synthesizing metal complexes, apart from the economic aspect, issues related to protecting the natural environment are also essential. Nowadays, most syntheses of metal complexes are based on using large amounts of solvents and high temperatures. Additionally, post-reaction mixtures frequently require multi-step purification.[1] One possible solution to this problem is to conduct synthesis solventless under mechanochemical conditions (e.g., milling).[2]

Mechanochemical synthesis of metal complexes has been gaining popularity recently. So far, there are only a small number of reports on solid-state synthesis of Iron Triad metal (Fe, Co, Ni) complexes.[3] On my poster, I would like to present the results of my current research on the synthesis of phosphine nickel(II) complexes.

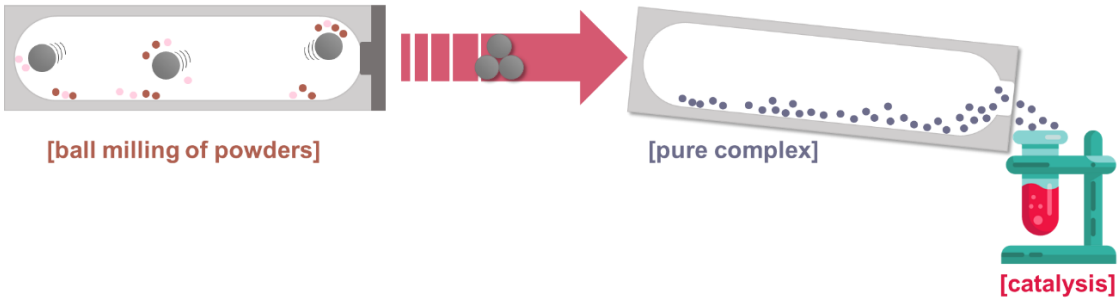

Figure 1. Graphical representation of mechanochemical synthesis of complexes.

REFERENCES

1. E. C. Constable, G. Parkin, L. Que Jr. (Eds.), *Comprehensive Coordination Chemistry*, 3rd Ed., Elsevier **2021**.

2. G. W. Wang, *Chem. Soc. Rev.* **2013**, *42,* 7668.

3. F. Leon, F. Garcia, *Metal Complexes in Mechanochemistry*, [in:] *Comprehensive Coordination Chemistry*, 3rd Ed., E. C. Constable, G. Parkin, L. Que Jr. (eds.), Elsevier **2021**.

P39

SYNTHESIS, ANTIPROLIFERATIVE ACTIVITY AND ADME PROFILING OF NOVEL RACEMIC AND OPTICALLY PURE ARYL-SUBSTITUTED PURINES AND PURINE BIOISOSTERES

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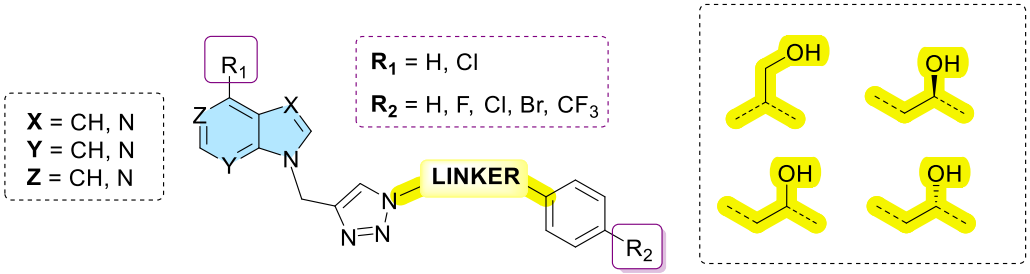
Purine-based compounds have played a central role in chemotherapy for over fifty years due to their high efficacy against rapidly proliferating cells. These compounds are commonly used to treat hematologic and solid cancers by mimicking natural nucleobases or nucleosides. In line with the proven therapeutic significance of purine bioisosteres, our previous studies demonstrated that a 7-deazapurine derivative showed significant inhibitory effects against HeLa cells (IC_{50} = 0.98 µM) and CFPAC-1 cells (IC_{50} = 0.79 µM). In addition, a benzimidazole derivative with a 1-(*p*-chlorophenyl)-1,2,3-triazole moiety showed highly selective inhibition of non-small cell lung cancer A549 cells in the nanomolar range [2,3].

Herein we present the synthesis, antiproliferative evaluation, and ADME profiling of racemic and optically pure purine bioisosteres featuring a hydroxyethyl linker with primary and secondary hydroxyl groups.



ACKNOWLEDGEMENTS: Financial support from the Croatian Science Foundation under the project No IP-2022-10-9420

REFERENCES:

1. Y. Wang, Y. Pan, Z. Lv and S. Gou, *Eur. J. Med. Chem.* **2024**, *271*, 116415.

2. A. Bistrović, P. Grbčić, A. Harej, M. Sedić, S. Kraljević-Pavelić, S. Koštrun, J. Plavec, D. Makuc, S. Raić-Malić, *J. Enzyme Inhib. Med. Chem.* **2018**, *33*, 271.

3. A. Bistrović, L. Krstulović, I. Stolić, D. Drenjančević, J. Talapko, M.C. Taylor, J.M. Kelly, M. Bajić, S. Raić-Malić, *J. Enzyme Inhib. Med. Chem.* **2018**, *33*, 1323.

P40

SYNTHESIS OF NAPHTHOL PRECURSORS FOR THE DEVELOPMENT OF INTRAMOLECULAR SPIROCYCLIZATIONS

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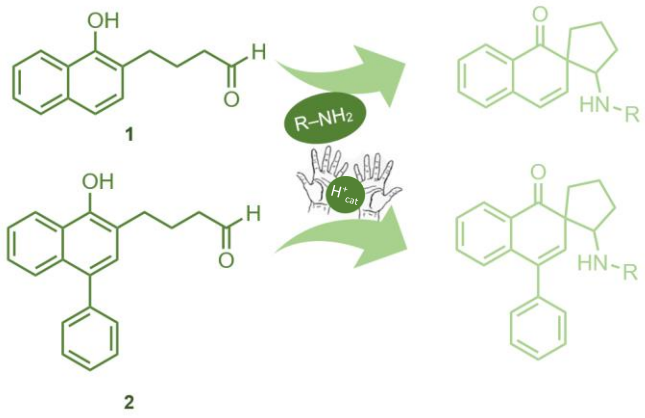
To develop organocatalytic asymmetric dearomative intramolecular spirocyclizations, this study looks into the synthesis of two precursors: 4-(1-hydroxynaphthalen-2-yl)butanal (**1**) and 4-(1-hydroxy-4-phenylnaphthalen-2-yl)butanal (**2**) [1]. Three distinct synthetic routes were tried for the synthesis of compound **1**. The initial route involved the synthesis via succinic acid ester, where the desired naphthol derivative was generated through Fries rearrangement. This approach was ultimately abandoned due to unsuccessful deprotection steps. The second route involved the elongation of substituted naphthylacetaldehyde with two carbon atoms, which also failed due to deprotonation of the undesirable carbon atom during the Wittig reaction. The desired aldehyde **1** was successfully synthesized by elongating substituted naphthaldehyde with three carbon atoms using the Wittig reaction. Compound **2** was synthesized via a three-step process. To obtain the *para*-substituted product, the first step involved a Suzuki coupling reaction of MOM-protected *para*-chloronaphthol, yielding the *para*-substituted product. The structure was elongated in the second step by adding the aliphatic chain using *n*-butyllithium and a bromopropyldioxolane. Finally, all protecting groups were removed to obtain the desired final compound **2**. The intramolecular spirocyclization with the obtained compound **1** was unsuccessful due to the free *para*-position relative to the phenol, which interfered with the reaction and led to undesired condensation. Studies of the intramolecular spirocyclization of compound **2** are currently in progress.



ACKNOWLEDGEMENTS Funded by the European Union – NextGenerationEU project ToSiAn (Total synthesis of bioactive metabolites -From deep sea microorganisms to new class of antibiotics and synthetic methodologies, NPOO.C3.2.R2-I1.06.00430) and HrZZ IP-2022-10-5184

REFERENCES

1. T. Dohi, A. Maruyama, N. Takenaga, K. Senami, Y. Minamitsuji, H. Fujioka, S.B. Caemmerer, Y. Kita, *Angew. Chem., Int. Ed.* **2008**, 47, 3787.

P41

PHOTOCHROMIC THIN FILMS FOR ADVANCED OPTICAL INFORMATION STORAGE

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Information storage using photochromic materials shows great promise in the development of optical neural networks, where synaptic weights could be written directly into the material using low-intensity light pulses. The optical power necessary for switching photochromic compounds such as diarylethenes can be lower than 1 $\mu W/mm^2$, which is easily achievable using electroluminescence of avalanche-mode light-emitting diodes in conventional silicon technology. Seamless integration of thin-film photochromic materials with silicon light emitters and detectors has the potential to advance electrical and optical interconnectivity in hardware realizations of optical neural networks, thus tackling power and scalability challenges in low-light communication and computation systems.

Diarylethenes are a class of heterocyclic aryl compounds that have attracted significant attention due to their reversible photochromic properties. These molecules undergo a light-induced transformation between two forms, resulting in a color change when exposed to ultraviolet (UV) or visible light. A key advantage of diarylethenes is their excellent thermal stability; unlike other photochromic compounds, their cyclization (ring-closing) and cycloreversion (ring-opening) processes do not occur spontaneously but are strictly light-driven. This makes diarylethenes highly reliable for optoelectronic applications. Some of them can complete open/close cycle over 10^4 times,[1] which makes them very useful in advanced technologies, including optical data storage, molecular devices, and smart materials.

In this work, the focus was on the preparation of photochromic thin films using the spin coating method. We explored combinations of different polymers, such as polystyrene (PS) and poly(methyl methacrylate) (PMMA), with two commercially available diarylethenes: 1,2-bis(2,4-dimethyl-5-phenyl-3-thienyl)-3,3,4,4,5,5-hexafluoro-1-cyclopentene (compound **2**) and *cis*-1,2-dicyano-1,2-bis(2,4,5-trimethyl-3-thienyl)ethene (compound **3**). Characterization was focused on ultraviolet-visible (UV-ViS) spectroscopy of both liquid and thin-film samples. We gathered data on absorption spectra, the conversion rates between both isomeric forms, and the impact of different polymer matrices and solvents. We also examined how the thin-film preparation method influenced the optical properties.

ACKNOWLEDGEMENTS Funded by European Union - NextGenerationEU fund – National Recovery and Resilience Plan Development Research Grants (grant no. NPOO.C3.2 R2-I1.06.0025).

REFERENCES

1. M. Irie, *Chem. Rew.* **2000**, *100*, 5.

P42

ALKALI METAL CATION COMPLEXATION BY LOWER-RIM TERTIARY-AMIDE CALIX[4]ARENES

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Calixarenes are probably the most widely used macrocyclic scaffolds for a range of ion receptors and binders of neutral species. These macrocyclic ligands can be relatively easily functionalized at both the upper and lower rim, which allows the preparation of ligands selective for diverse classes of guests in a range of media, but very rarely in water. To overcome this obstacle, we have recently introduced a new class of water-soluble glycocalixarenes[1] designed for efficient hosting of first-group cations (Figure 1). In this work the role of triazole and glucose functionalities in the coordination reactions is explored by studying the binding of alkali metal cations with calix[4]arenes functionalized with tertiary-amide groups at the lower rim (Figure 1) in methanol, *N,N*-dimethylformamide, and acetonitrile.[2]

The obtained results reveal that all studied reactions are enthalpically controlled and the peak affinity of receptors for sodium cation is observed. The complex stabilities are the highest in acetonitrile, followed by methanol and *N,N*-dimethylformamide. The solvation of the reactants and products plays a very important role in the binding process, especially the inclusion of solvent molecules in the calixarene hydrophobic cone. Importantly, the ligand solubilities are greatly affected by the presence of glucose subunits which hardly influence the calixarene receptor properties.

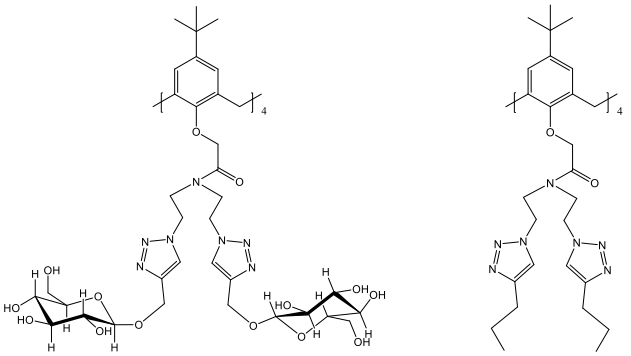

Figure 1. Structures of the investigated calixarenes.

ACKNOWLEDGEMENTS This work has been supported by Croatian Science Foundation (IP-2019-04-9560 and the European Regional Development Fund (KK.01.1.1.02.0016).

REFERENCES

1. Tomišić *et al*., *Org. Biomol. Chem*, **2018**, *16*, 904–912.
2. Požar *et al*., *Molecules,* **2022**, *27*, 470–491.

P43

THE COMPLEXATION OF ALIPHATIC GUESTS WITH CUCURBITURILS AND CYCLODEXTRINS

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The supramolecular recognition of non-polar guests by macrocyclic ligands has received much attention over the past decades.[1,2] Contrary to the endothermic micellization (classical hydrophobic effect), the complexation is, due to the removal of energetic solvent from the receptor cavities, predominantly exothermic, even completely enthalpy driven (non-classical hydrophobic effect).[1,2] Considering a particularly strong temperature dependence of hydration enthalpies for aliphatic compounds, one would expect a notable influence on the corresponding inclusion thermodynamics. Still, the complexation reactions were primarily investigated at 25 °C. With this in mind, we examined the binding of linear and (poly)cyclic aliphatic guests with size-compatible cyclodextrins and cucurbiturils by means of ITC and NMR over a 278–338 K temperature range. A pronounced $\Delta_r H°(T)$ and $\Delta_r S°(T)$ dependence due to temperature-induced disordering of the guest-hydrating water was observed for examined reactions.[3,4] This significantly affected the thermodynamics of cyclodextrin complexation reactions, however the inclusion within cucurbiturils remained predominantly enthalpy driven at all examined temperatures.[3,4] The carried out investigations also revealed that the dehydration of cucurbituril cavities is accompanied with lower entropy changes than the analogous process involving cyclodextrins.[3,4] Apart from that, the endothermic binding of larger diamondoid guests with γ-cyclodextrin at lower temperatures supports the classical hydration of these bulky guests.[4]

ACKNOWLEDGEMENTS This work has been supported by Croatian Science Foundation (IP-2019-04-9560 and UIP-2017-05-9653) and the European Regional Development Fund (KK.01.1.1.02.0016).

REFERENCES

1. M. V. Rekharsky, Y. Inoue, *Chem. Rev.* **1998**, *98*, 1875.
2. F. Biedermann, W. M. Nau, H.-J. Schneider, *Angew. Chem. Int. Ed*. **2014**, *53*, 11158.
3. Požar *et al.*, *J. Mol. Liq.* **2023**, *388*, 122774.
4. Požar *et al.*, *New J. Chem.* **2023**, *47*, 18745.

P44

IN VITRO RELEASE TESTING OF *CLINDAMYCIN PHOSPHATE + BENZOYL PEROXIDE, 10 + 50 mg/g GEL*

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In vitro release test (IVRT) is an established tool for characterizing and evaluating product performance of a semi-solid dosage form as the *in vitro* release rate can reflect the combined effect of several physical and chemical parameters, therefore is considered as suitable for equivalence evidence, in lieu of a clinical therapeutic study per *Draft guideline on quality and equivalence of topical* products.[1] In this study, the aim is to develop and validate IVRT methods for both active ingredients of *Clindamycin phosphate + benzoyl peroxide, 10 + 50 mg/g gel*, to adequately discriminate possible differences in formulations during pharmaceutical development as per EMA Draft guideline and FDA SUPAC-SS.[2]

The product is intended for treatment of *acne vulgaris* and formulated as a single-phase gel with clindamycin phosphate, (CP) dissolved within the solution, and benzoyl peroxide (BPO) in suspension, both acting on the surface of the skin. The selected test system for both IVRT of CP and BPO consists of six immersion cells Model A - Enhancer cell, used with assembly of small volume vessels and mini-paddles as stirring system modelled after the standard USP Apparatus 2. Firstly, to develop both methods, test parameters including the media composition, pH and volume, membrane material and pore size, as well as stirring speed were varied and quantified by Reversed phase - High Performance Liquid Chromatography (RP-HPLC). Secondly, the validation included proper assessment of the IVRT method attributes (drug substance solubility and stability in the media, drug substance binding to the membrane, intra-run and inter-run precision of release rates, linearity of release rate, recovery, mass balance, and dose depletion, method discrimination sensitivity, selectivity and specificity and robustness with respect to the most critical method parameters), as well as quantitative RP-HPLC methods. Results obtained with different test parameter settings clearly indicate that both drug properties and instrumental details can have a huge impact on the outcome of *in vitro* drug release studies for both active ingredients.

Thus, the selection of adequate test parameters is crucial for the success of the release experiments and, as shown in the present study, optimal test parameters/conditions need to be established and validated on a case-by-case study.

REFERENCES

1. European Medicines Agency, Committee for Medicinal Products for Human Use (CHMP), *Draft Guideline on Quality and Equivalence of Topical Products,* **2018**, *CHMP/QWP/708282/2018.*

2. U.S. Department of Health and Human Services, Food and Drug Administration, Center for Drug Evaluation and Research, *SUPAC-SS: Guidance for Industry: Nonsterile Semisolid Dosage Forms Scale-Up and Postapproval Changes: Chemistry, Manufacturing, and Controls; In Vitro Release Testing and In Vivo Bioequivalence Documentation*, **1997**, *CMC 7.*

P45

DESIGN OF MORPHOLINE-BASED UGI PRODUCTS AS BUTYRYLCHOLINESTERASE INHIBITORS

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The Ugi reaction is a versatile multicomponent reaction that can generate peptide-like molecules in a single step by condensation of carbocyclic acid, aldehyde, amine, and isocyanide. It is a valuable tool in drug discovery because it allows the synthesis of structurally diverse compounds in one step, which is crucial for exploring chemical space and identifying bioactive molecules with potential therapeutic effects.[1, 2] These compounds often show broad activity against biological targets. Some Ugi products have been investigated for their cholinesterase inhibitory activity,[3] which is particularly relevant in the treatment of neurodegenerative diseases like Alzheimer's or Parkinson's disease. In this work, we have synthesized a small library of structurally related peptidomimetics through the Ugi reaction by using aryl or alkyl carbocyclic acid and amine, morpholine-based isocyanide and formaldehyde. The structure of the prepared compounds was confirmed by 1D and 2D ^{1}H and ^{13}C NMR spectroscopy. The inhibition potential of prepared compounds on equine butyrylcholinesterase has been evaluated by the spectroscopic Ellman method. IC_{50} values of prepared compounds for butyrylcholinesterase were in the range from 10 μM to 445 μM, which makes them promising scaffolds for further development of butyrylcholinesterase inhibitors.

ACKNOWLEDGEMENTS This work was financially supported by the Croatian Science Foundation as part of the project Target-guided synthesis of cholinesterase inhibitors supported by machine learning (IP-2022-10-9525).

REFERENCES

1. Á. Cores, J. Clerigué, E. Orocio-Rodríguez, J. C. Menéndez, *Pharmaceuticals* **2022**, *15*, 1009.

2. G. Graziano, A. Stefanachi, M. Contino, R. Prieto-Díaz, A. Ligresti, P. Kumar, A. Scilimati, E. Sotelo, F. Leonetti, *Int. J. Mol. Sci.* **2023**, *24*, 6581.

3. P. Brandão, Ó. López, L. Leitzbach, H. Stark, J. G. Fernández-Bolaños, A. J. Burke, M. Pineiro, *ACS Med. Chem. Lett.* **2021**, *12*, 1718.

P46

ANTIMICROBIAL COATED BIOPOLYMERS FOR DENTAL AND MEDICAL APPLICATION

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According to some predictions, 25,000 deaths in Europe per year and costs over € 1.5 billion are the result of resistant microorganisms. In this work, therefore, new biodegradable materials were developed with an antimicrobial active coating for medical and dental applications. By developing antimicrobial biodegradable polymers that prevent the onset of infections, we tried to respond to the World Health Organization's demands, which has highlighted this problem as a major problem to the world public health in this century. Coatings with mixtures of nanoparticles were designed to inhibit or eliminate microbial growth, reducing infection risks associated with medical textiles[1] and devices, surgical implants, and dental materials. In the development of the coating with antimicrobial formulation,[2] we applied response surface methodology within the Design of experiment program for predicting the antimicrobial activity of nanoparticles in their mixtures. Thus-calculated antimicrobial mixtures were used for functionalization of the surface of biodegradable polymers by combination of sol-gel process, microencapsulation, electro-spinning and 3D printing.[3] New dental and medical antimicrobial polymers were characterized by spectroscopic (UV-VIS, ICP-MS, FTIR), chromatographic (GC, TLC) and microscopic (SEM-EDX, TEM) methods. After modification of the polymers, their new functional properties (hydrophobicity, antimicrobial efficiency, stability, zeta potential, surface pH, etc.) were examined, and the results obtained have shown that the antimicrobial surface was efficient against Methyl resistant Staphylococcus aureus after several hours of exposure, leaving a potential space for further development prior application in dental and medical purposes.

ACKNOWLEDGEMENTS This work was financially fully supported by the Croatian Science Foundation, project IP-2019-04-1381 entitled „Antibacterial coating for biodegradable medicine materials ABBAMEDICA“, project leader professor Iva Rezić Meštrović PhD PhD.

REFERENCES

1. I. Rezić, M. Somogyi Škoc, *Polymers* **2024**, *16*, 2320.
2. I. Rezić, E. Meštrović, *Coatings* **2023**, *13,* 1830.
3. I. Rezić, *Polymers* **2022**, *14*, 4961.

P47

GENERIC MEDICATED SHAMPOO DEVELOPMENT – DOES FOAMING MATTER?

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Medicated shampoos contain active pharmaceutical substances needed for the treatment of a specific scalp condition which are incorporated into a solution of surfactants with a mild effect on the hair and scalp. During generic development of topical products with a biowaiver regulatory strategy,[1] in addition to qualitative and quantitative sameness, comparable microstructure, textural properties and behavior on the application site between reference medicinal product (RMP) and development product should be demonstrated,[2] with foam stability being one of the parameters specific for shampoo evaluation. Usually, patient perception of shampoo's efficacy is related to its ability to create a large amount of foam. Although it is proven that extensive foaming is not mandatory for effective washing of hair and scalp, a stable foam ensures that needed contact time of the product at the place of application is achieved, and also the reduction of friction and removing of impurities from the scalp. By using Dynamic Foam Analyzer[3] (DFA100, Kruss), scientific analysis of liquid foam of RMP and development product is evaluated. The instrument precisely measures the foam volume during formation and decay over time as a measure of foam stability. It also measures foam structure i.e., bubble size and distribution. By analyzing foam properties, comparability with the RMP is confirmed in line with the corresponding purpose of the product – a stable foam that ensures the therapeutic effect of the product at the site of application.

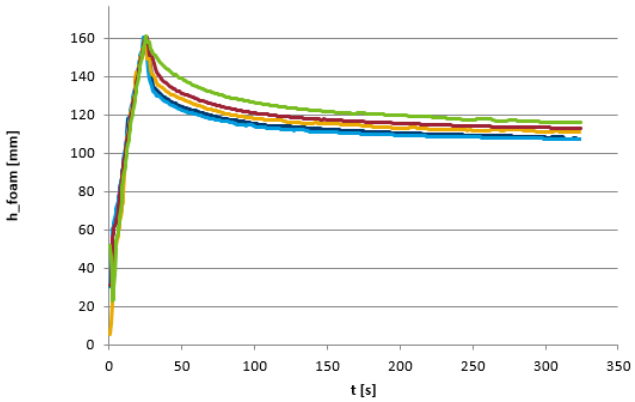

Figure 1. Decay in foam height over time between development product (green) and four different batches of reference product.

REFERENCES

1. Guideline on quality and equivalence of locally applied, locally acting cutaneous products, EMA/CHMP/QWP/708282/2018.

2. R.-K. Chang, A. Raw, R. Lionberger, L. Yu, *AAPS J.* **2013**, *15*, 41.

3. User Manual: ADVANCE for Dynamic Foam Analyzer – DFA100.

P48

MUCOADHESION OF PHARMACEUTICAL SOLUTIONS CONTAINING SODIUM HYALURONATE – INFLUENCE OF CONCENTRATION AND MOLECULAR WEIGHT OF SODIUM HYALURONATE

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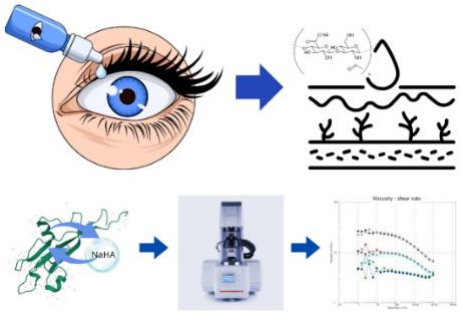
Sodium hyaluronate (NaHA) is a polymer commonly used in the eye drops to hydrate and support the regeneration of the eye.[1] It also exhibits mucoadhesive properties, meaning that it interacts with mucin, a part of the mucous membrane on the surface of the eye, which prolongs solution's retention time. Therefore, therapeutic efficiency of the drug may be improved in solutions that contain NaHA *via* better absorption and bioavailability of the drug.[2] The aim of this study was to test the influence of molecular weight (MW) of used NaHA, and its concentration on mucoadhesion, along with the influence of the solution's osmolality. Mucoadhesion was determined as relative rheological synergism, using porcine gastric mucin and by analysing rheological profiles.[3] Rheological profiles were determined for each prepared NaHA solution, mucin, and their mixture. Lower molecular weight NaHA (≈250 kDa) showed no interaction with mucin, whereas higher molecular weight NaHA (≈980 and 1420 kDa) exhibited higher solution's viscosities and interaction with mucin. However, the relationship between the determined relative rheological synergism and the MW of NaHA/viscosity of solution was not proportional. Higher concentration of NaHA, which increased the viscosity of the solution, increased interaction with mucin proportionally. Interaction with mucin increased with higher osmolality, even though higher osmolality decreased the viscosity of the solution. This confirms that more factors than just the viscosity of the solution influence its mucoadhesive properties. It can be concluded that by optimising MW and concentration of NaHa, and osmolality of the solution, desired mucoadhesion may be achieved to result in the drug product of satisfying bioavailability, which is important when developing new drugs.



REFERENCES

1. B.C.H. Ang, J.J. Sng, P.X.H. Wang, H.M. Htoon, L.H.T. Tong, *Sci. Rep.* **2017**, *7*, 9013.

2. S. Casey-Power, R. Ryan, G. Behl, P. McLoughlin, M.E. Byrne, L. Fitzhenry, *Pharmaceutics* **2022**, *14*, 1479.

3. S. Rossi, B. Vigani, M.C. Bonferoni, G. Sandri, C. Caramella, F. Ferrari, *J. Pharm. Biomed. Anal.* **2018**, *156*, 232.

SYNTHESIZING NEW DERIVATIVES OF BIOBASED SURFACTANTS

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Today, there is a growing awareness of the need to develop more sustainable alternatives to traditional industrial processes and products. The concept of green chemistry was developed by Anastas and Warner in 1998.[1] Their 12 principles enable the development of sustainable and environmentally friendly chemistry and the products we use in everyday life, one of which are surfactants. Surfactants are amphiphilic molecules with a wide range of applications. They are used in pharmaceuticals, detergents, emulsifiers, oil recovery enhancers, etc.[2] Biosurfactants are natural compounds produced by a variety of microorganisms: fungi, yeasts and bacteria. They are an environmentally friendly alternative to chemical surfactants.[3] Some of the advantages of biosurfactants compared to their chemical counterparts are their lower toxicity, better biodegradability and specificity. The global market for surfactants was worth approximately 45 billion dollars in 2023,[4] with biosurfactants accounting for only a small proportion (approximately 10%), demonstrating the need to grow this part of the market.

Sophorolipids are a type of biosurfactants that have a wide industrial application, but there is a need for structural variations to further expand the range of applications.[5] Enzymatic and chemical modifications of sophorolipids offer the possibility of synthesizing new derivatives with other functional groups that cannot be obtained by the fermentation process. In this study, the enzymatic modification of sophorolipids was investigated using a reaction engineering approach involving kinetic measurements.

ACKNOWLEDGEMENTS This research has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101000560.

REFERENCES

1. P. Anastas, J. Warner, Green chemistry: Theory and practice, Oxford University Press, England, 1998.
2. S. M. Shaban, J. Kang, D.-H. Kim, *Compos. Commun.* **2020,** *22*, 100537.
3. P. Singh, Y. Patil, V. Rale, *J. Appl. Microbiol*. **2019**, *126*, 2.
4. https://www.fortunebusinessinsights.com/surfactants-market-102385
5. K. M. J. Saerens, I. N. A. Van Bogaert, W. Soetaert, *FEMS Yeast Res.* **2015**, *15*, fov075.

P50

UNVEILING THE POTENTIAL OF WEAK INTERACTIONS ON THE CRYSTALS' RESPONSE TO MECHANICAL STIMULI

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The traditional perception of crystals being rigid, stiff and fragile started to dramatically change in the last few decades. New research has put crystals under the spotlight and brought attention to a whole new world of dynamic crystalline compounds capable of displaying a wide range of different motions stimulated by pure mechanical force, light or change in temperature.[1–6] Crystals of one-dimensional coordination polymers, equipped with ligands bearing various functional groups, provide a pathway for systematic study of this unexpected yet highly valuable phenomenon.[3–6] It was observed that a delicate structural change on a molecular level of 1D Cd(II) coordination polymers, which only slightly influences the strength and directionality of intermolecular interactions, can lead to drastic changes in displayed mechanical properties.[4–6] For example, in a family of nearly isostructural compounds, a whole range of mechanically induced flexible responses were observed, from purely elastic bending to exceptionally plastic pliability.[5,6]

In order to gain a deeper understanding of how fine structural details impact the mechanical properties of crystals, a study was conducted on six different Cd(II) coordination polymers. These compounds varied slightly in composition, including differences in bridging ligands (Cl^-, Br^-, I^-) and the choice of heterocyclic ligand (3-methylpyridine and 2-methylpirazine). The slight differences in molecular and crystal structure, as well as the morphology of crystals, have been observed to lead to significant changes in response to mechanically induced stress. Crystals of compounds with 3-methylpyridine ligand displayed 2-D isotropic elastic bending with varying degrees of flexibility, while polymers with 2-methylpirazine ligand displayed different types of mechanical response, ranging from 1-D elasticity to 1-D elastic→plastic bending. The mechanical behaviour of the crystals was found to be correlated with the structural features, bringing us closer to understanding mechanically responsive crystalline compounds and enabling the consideration of crystalline materials for their potential utilization in emerging technologies.

ACKNOWLEDGEMENTS This work has been fully supported by the Croatian Science Foundation under project "From form to function: Mechanically flexible crystalline materials with controllable responses"(IP-2019-04-1242).

REFERENCES

1. W. M. Awad et al., *Chem. Soc. Rev*. **2023**, *52,* 3098.

2. P. Naumov, D. P. Karothu, E. Ahmed, L. Catalano, P. Commins, J. Mahmoud Halabi, M. B. Al-Handawi, L. Li, *J. Am. Chem. Soc.* **2020,** *142,* 13256.

3. M. Đaković, M. Borovina, M. Pisačić, C. B. Aakeröy, B.-M. Kukovec, Ž. Soldin, I. Kodrin, *Angew. Chem. Int. Ed.* **2018**, *57*, 14801.

4. M. Pisačić, I. Biljan, I. Kodrin, N. Popov, Ž. Soldin, M. Đaković, *Chem. Mater* **2021**, *33*, 3660.

5. M. Pisačić, I. Kodrin, I. Biljan, M. Đaković, *CrystEngComm* **2021**, *23*, 7072.

6. M. Pisačić, I. Kodrin, A. Trninić, M. Đaković, *Chem. Mater.* **2022**, *34*, 2439.

P51

RARE-EARTH ELEMENTS AND CONFIGURATIONAL ENTROPY IN CERIA-ZIRCONIA: NEW INSIGHTS

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Nanocrystalline CeO_2 is applicable across various technological fields with the emphasis on catalysis due to its accessibility, cost-effectiveness, stability, and durability. Combining cerium and zirconium oxides, CeO_2-ZrO_2 system has attracted the attention in the last decades due to its mechanical, electrical and thermal properties, but also in wide variety of applications in areas such as electronics, engineering, catalysis and fuel cells.[1] When redox process occurs, Ce^{4+} transforms into Ce^{3+} and vice versa, the disturbance of the surface of CeO_2-ZrO_2 structure results in oxygen vacancies and active sites which are prior for catalytic activity. The modified aqueous citrate sol-gel method was used for the synthesis of ceria-zirconia-based solid solutions $Ce_{0.5}Zr_{0.5}O_2$ and $La_{0.1}Ce_{0.1}Pr_{0.1}Gd_{0.1}Y_{0.1}Zr_{0.5}O_2$. Solid solution powders were subjected to a reduction in high-temperature tubular furnace at 1500 °C to obtain pyrochlore phases $Ce_2Zr_2O_7$ and $(La_{0.2}Ce_{0.2}Pr_{0.2}Gd_{0.2}Y_{0.2})_2Zr_2O_7$. Re-oxidation of the reduced powders was performed to obtain κ-phases $Ce_2Zr_2O_8$ and $(La_{0.2}Ce_{0.2}Pr_{0.2}Gd_{0.2}Y_{0.2})_2Zr_2O_8$ at 600 °C in a muffle furnace. Schematic representation of the ceria-zirconia system is shown in Figure 1. In detail structural, microscopic and spectroscopic studies were performed to determine the improvement of physicochemical properties. The photoreduction activity was investigated by conducting the photocatalytic hydrogenation of CO_2.

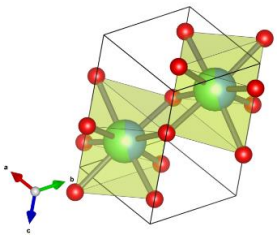

Figure 1. Crystal structure of solid solution ceria-zirconia system.

ACKNOWLEDGEMENTS This work was supported by the Croatian-Israeli Scientific Research project under the name: High-entropy oxides photoabsorbers for efficient and stable photoelectrochemical hydrogen generation.

REFERENCES

1. S. Urban, P. Dolcet, M. Möller, L. Chen, P. J. Klar, I. Djerdj, S. Gross, B. M. Smarsly, H. Over, *App. Catal., B.* **2016**, *197*, 23.

P52

CHARACTERIZATION OF ADAMANTYL THIOETHERS BY ROTATIONAL SPECTROSCOPY

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The thioether group (R–S–R´) is a common motif in the structures of bioactive molecules and is often a starting point in the formation of higher oxidation state sulfur derivatives.[1] Despite a vast number of known thioether containing derivatives, a compound class incorporating the adamantyl group remains scarcely described in the literature. However, such alkyl adamantyl thioethers could have pharmaceutical applications due to a combination of properties emerging from these functional subunits. We therefore studied the fundamental properties of a prepared series of alkyl adamantyl thioethers using a combination of high-resolution rotational spectroscopy and computational tools.[2] Here it should be noted that the studied 1,1'-diadamantyl thioether is one of the largest molecules studied to date by high-resolution rotational spectroscopy. We also compared the obtained findings with a structurally analogous 1,1'-diadamantyl ether that we explored previously[3,4] in order to assess the influence of the sulfur atom on the intermolecular cluster formation with solvents molecules, especially water (Figure 1). Investigation of such microsolvated clusters provides valuable insights into the preference of water to establish sulfur-centered hydrogen bonds with thioethers.

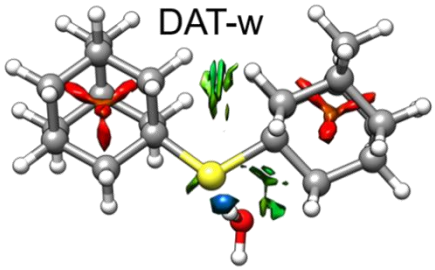

Figure 1. Structure of the monohydrated complex of 1,1'-diadamantyl thioether with depicted non-covalent interaction surfaces, blue (strong attraction *via* hydrogen bonds), green (weak dispersion interactions) and red (repulsion inside the adamantyl cages).

REFERENCES

1. E. A. Ilardi, E. Vitaku, J. T. Njardarson, *J. Med. Chem.* **2014**, *57*, 2832.

2. P. Pinacho, D. Loru, T. Šumanovac, M. Šekutor, M. Schnell, *ChemPhysChem* **2023**, *24*, e2023005.

3. M. M. Quesada Moreno, P. Pinacho, C. Pérez, M. Šekutor, P. R. Schreiner, M. Schnell, *Chem. Eur. J.* **2020**, *26*, 10817.

4. M. M. Quesada Moreno, P. Pinacho, C. Pérez, M. Šekutor, P. R. Schreiner, M. Schnell, *Chem. Eur. J.* **2021**, *27*, 6198.

P53

EVALUATING TASK-SOLVING EFFICIENCY IN CHEMISTRY AND CHEMICAL ENGINEERING USING LARGE LANGUAGE MODELS (LLMS)

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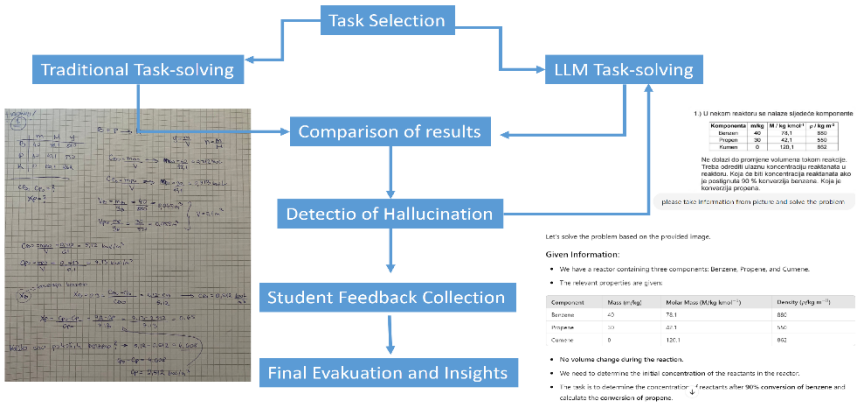
Following the highly successful application of Large Language Models (LLMs) in solving tasks in general chemistry, this study presents results on more complex problems in the fields of chemistry and chemical engineering. The performance of LLMs will be compared with traditional problem-solving methods to evaluate their effectiveness. Additionally, the study will assess the impact of LLMs on the learning process and student outcomes, comparing how these models influence understanding, engagement, and efficiency in mastering complex concepts. The research methodology was based on selecting various tasks to be solved in parallel using both classical methods and LLMs. The procedures and solutions were compared, with a focus on identifying areas where LLMs did not provide valid results. Special attention will be given to instances of hallucination—situations where the LLM generated incorrect, irrelevant, or fabricated information that does not correspond to the input data or the known scientific facts. This evaluation aims to showcase both the problem-solving capabilities of LLMs and their potential to enhance the overall educational experience in technical disciplines, while also identifying their limitations.



SYNTHETIC ROUTES TO *N*-GUANIDINYL ANTHRACENOISONDOLE

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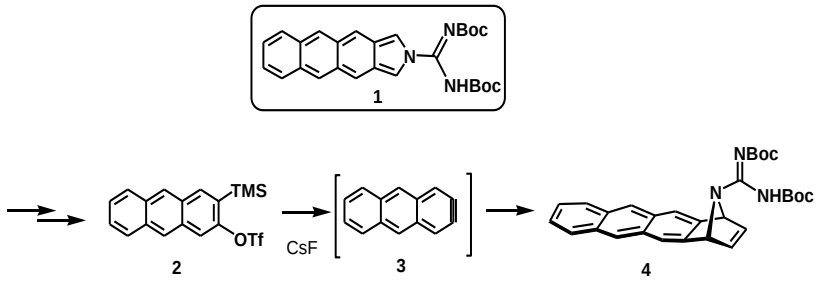
Isobenzo species, including isoindoles are reactive intermediates which undergo Diels-Alder reactions and are of synthetic interest.(1) These can be prepared from the corresponding 7-azabenzonorbornadienes **4** by Warrener's tetrazine cycloaddition/cycloreversion protocol (2,3) Whereas synthesis of 2,3-anthracene aryne **3** is known (4), the harsh reaction conditions prevented its application in the presence of guanidine substituents. Several synthetic routes to the synthesis of *N*-guanidinyl anthracenoisoindole were explored. The key advancement to successful synthesis was preparing novel, 2,3-anthryl Kobayashi aryne precursor **2**.



Keywords: organic synthesis, heteroaromatic compounds, isoindoles, arynes, cycloaddition reaction, Friedel-Crafts reaction

REFERENCES

1. L. F. Fieser, M. J. Haddadin, *J. Am. Chem. Soc.* **1964**, *86*, 2081.
2. R. N. Warrener, *J. Am. Chem. Soc.* **1971**, *93*, 2346.
3. E. Gil de Montes, A. Istrate, C. D. Navo, E. Jiménez-Moreno, E. A. Hoyt, F. Corzana, I. Robina, G. Jiménez-Osés, A. J. Moreno-Vargas, Gonçalo J. L. Bernardes, *Angew. Chem., Int Ed.* **2020**, *59*, 6196.
4. Sharp Corp., Daito Chemix Corp., Japan Patent JP2008088124, **2008**.

P55

PREPARATION OF ADAMANTYL HEXAAZA CROWN ETHERS AND THEIR ALKALI METAL COMPLEXATION

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Aza crown ethers[1] are host molecules with a wide range of possible use, including as complexation agents for metals, receptors with redox-active groups, ionophores, amphiphiles, chelating agents, *etc*. We previously explored similar cage aza crown ethers[2,3] and cryptands,[4,5] so now we expanded our focus on the up to now unknown subclass of hexaaza crown ethers (macrocycles containing six nitrogen atoms in the crown core) substituted with the adamantane-bearing side chains (Figure 1). After synthesis and characterization of target adamantyl hexaaza crown ethers **1**–**3**, we assessed their complexation abilities by performing extraction experiments using picrates of alkali metals (Li^+, Na^+, K^+, Rb^+, and Cs^+). We also supplemented the obtained experimental findings with a computational study of both the parent adamantyl hexaaza crown ethers and their strongest alkali metal complexes. In that way we could not only confirm the affinity of this class of compounds for alkali metals but also gain more insight into the conformational processes occurring as a consequence of the binding event.

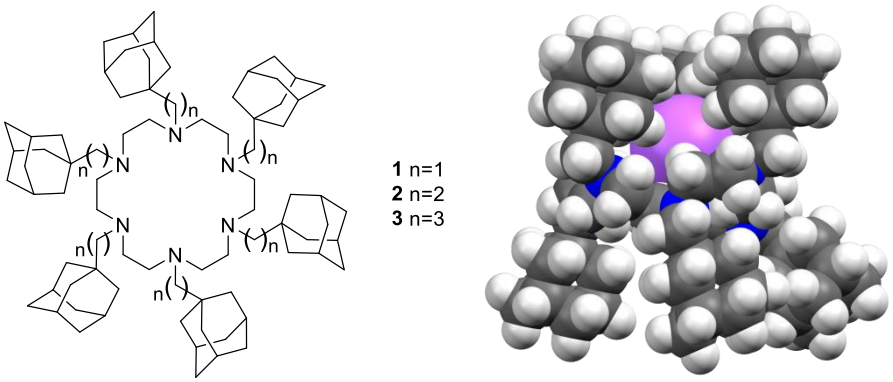

Figure 1. Structures of hexaaza crown ethers **1**–**3** and depiction of the **1**•Na^+complex.

REFERENCES

1. K. E. Krakowiak, J. S. Bradshaw, D. J. Zamecka-Krakowiak, *Chem. Rev.* **1989**, *89*, 929.

2. K. Mlinarić-Majerski, T. Šumanovac Ramljak, *Tetrahedron* **2002**, *58*, 4893.

3. T. Šumanovac Ramljak, K. Mlinarić-Majerski, B. Bertoša, *Croat. Chem. Acta* **2012**, *85*, 559.

4. A. P. Marchand, S. Alihodžić, A. S. McKim, K. A. Kumar, K. Mlinarić-Majerski, T. Šumanovac, S. G. Bott, *Tetrahedron Lett.* **1998**, *39*, 1861.

5. T. Šumanovac Ramljak, I. Despotović, B. Bertoša, K. Mlinarić-Majerski, *Tetrahedron* **2013**, *69*, 10610.

P56

SOLVENT EFFECTS ON REACTIVITY AND SELECTIVITY OF (3+2) CYCLOADDITION REACTIONS

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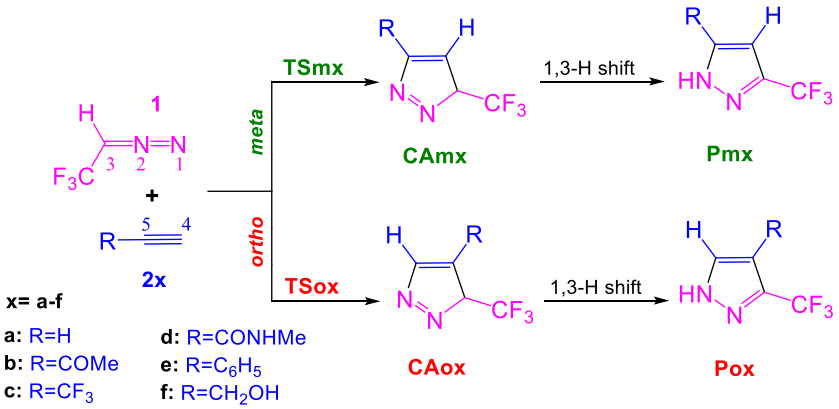
The effects of solvent on reaction rate, selectivity and chemical equilibrium have been extensively studied.[1] Solvents can significantly influence the kinetics and thermodynamics of reactions by affecting the energies of species along the reaction coordinate.[2]

Cycloaddition (CA) reactions are essential tools in synthetic organic chemistry.[3] Investigating CA reactions in the gas and solution phases through computational studies allows for a comparative analysis that can validate experimental observations and highlight the importance of solvent effects, which can be easily missed in purely experimental studies.

Quantum calculations were used to study the kinetic solvent effects on the (3+2) CAs of trifluorodiazoethane (1) with substituted terminal alkynes (2). All stationary points were fully optimized at the M06-2X/6-311G(d,p) level of theory in the gas phase. Moreover, the effects of dichloromethane as a solvent were studied using the conductor-like polarizable continuum model (CPCM) with M06-2X and B2PLYPD3 functionals. Interestingly, while the M06-2X calculations in both gas and solvent phases did not align well with the experimental observations,[4] the results from B2PLYPD3 functional completely agreed with them. These calculations indicate that the solvent slows the reaction rate and favors the formation of meta-regioisomers. Transition state investigations show that these reactions proceed through asynchronous transition states with weak or non-polar characteristics.



ACKNOWLEDGEMENTS We are grateful to the Hakim Sabzevari University for financial support.

REFERENCES

1. C. Reichard, T. Welton, *Solvents and Solvent Effects in Organic Chemistry* **2011**, 4th edition.

2. J. J. Varghese, S. H. Mushrif, *React. Chem. Eng.* **2019**, *4*, 165.

3. A. Padwa, W.H. Pearson, *Synthetic Applications of 1,3-Dipolar Cycloaddition Chemistry Toward Heterocycles and Natural Products*, John Wiley & Sons, New York, **2002**.

4. P.K. Mykhailiuk, *Chem. Rev.* **2020**, *120,* 12718.

P57

HIGH-ENTROPY OXIDES: A NEW FRONTIER IN PHOTOREDUCTION OF CO_2

Dalibor Tatar,[a] Igor Djerdj,[a] Jelena Kojčinović,[a] Stjepan Šarić,[a] Habib Ullah,[b] András Sápi,[c] Ronen Gottesman,[d] Oded Millo,[e] Doron Azulay[f]

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Herein, we investigate the potential of nanostructured high-entropy oxides (HEOs) for photocatalytic CO_2 hydrogenation, a process with significant implications for environmental sustainability and energy production.[1] Several cerium-oxide-based rare-earth HEOs with fluorite structures were prepared for UV-light driven photocatalytic CO_2 hydrogenation toward valuable fuels and petrochemical precursors. The cationic composition profoundly influences the selectivity and activity of the HEOs, where the $Ce_{0.2}Zr_{0.2}La_{0.2}Nd_{0.2}Sm_{0.2}O_{2-\delta}$ catalyst showed outstanding CO_2 activation (14.4 $mol_{CO}\ kg_{cat}^{-1}\ h^{-1}$ and 1.27 $mol_{CH3OH}\ kg_{cat}^{-1}\ h^{-1}$) and high methanol and CO selectivity (7.84% CH_3OH and 89.26% CO) under ambient conditions with 4 times better performance in comparison to pristine CeO_2. Systematic tests showed the effect of a high-entropy system compared to midentropy oxides. XPS, in situ DRIFTS, as well as DFT calculation elucidate the synergistic impact of Ce, Zr, La, Nd, and Sm, resulting in an optimal Ce^{3+}/Ce^{4+} ratio. The observed formate-routed mechanism and a surface with high affinity to CO_2 reduction offer insights into the photocatalytic enhancement. While our findings lay a solid foundation, further research is needed to optimize these catalysts and expand their applications.

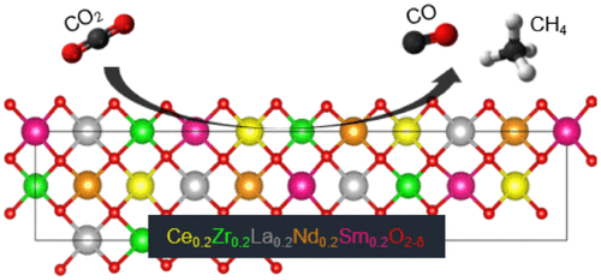

Figure 1. Graphical abstract.[1]

ACKNOWLEDGEMENTS This work was supported by the Croatian Science Foundation under the project HRZZ-PZS-2019-02-2467 and by Croatia – Israeli Scientific Research under the name: High-entropy oxides photoabsorbers for efficient and stable photoelectrochemical hydrogen generation.

REFERENCES

1. D. Tatar, H. Ullah, M Yadav, J. Kojčinović, S. Šarić, I. Szenti, T. Skalar, M. Finšgar, M. Tian, Á. Kukovecz, Z. Kónya, A. Sápi, I. Djerdj, *ACS Appl. Mater. Interfaces* **2024**, *16*, 29946.

P58

WHAT WE OBSERVE *VS.* WHAT IS HAPPENING: MOTION OF IONS IN SOLUTION UNDER THE INFLUENCE OF AN ELECTRIC FIELD

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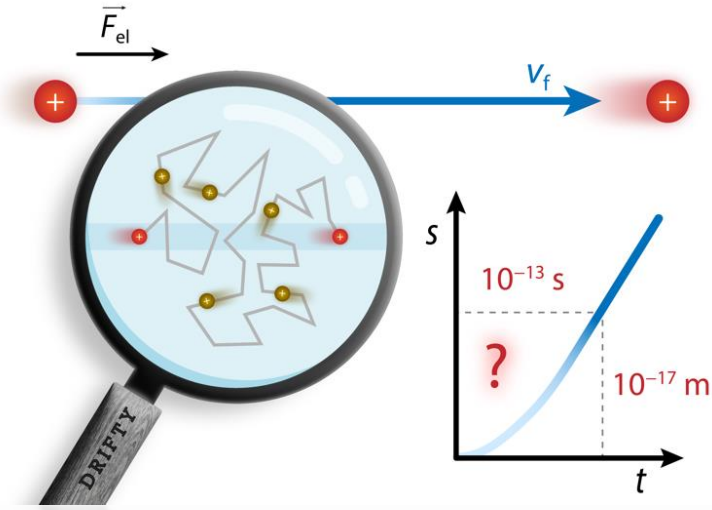
The challenge in teaching physical (electro)chemistry, particularly the motion of ions and colloidal particles under the influence of an electric field, lies in balancing macroscopic and microscopic perspectives. Traditional macroscopic approaches often lead to misunderstanding of the transport phenomena at the microscopic level.[1,2]

In this work, we introduce a strategy that includes derivation of equations used for calculation of key physical quantities related to the motion of charged particles in solution under the influence of an electric field, *i.e.* drift velocity, the time it takes and the distance the particle travels until it reaches final velocity. A simple simulation in MS Excel is also presented and available for download.[2] It provides a dynamic, visual approach to illustrating ionic motion. Integrating this method into physical chemistry courses bridges the gap between the observed and microscopic properties of the particles.

This method encourages deeper comprehension of electrolyte solution conductivity and ion transport by enabling students to visualize the processes at both the macroscopic and microscopic levels. We discuss the positive impact of this approach on students' learning experiences and overall outcomes, proposing it as an effective tool for teaching transport phenomena and relation of macro- and microscopic properties in general.



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REFERENCES

1. C. A. Vincent, *J. Chem. Educ.* **1976**, *53*, 490.

2. A. Usenik, N. Kallay, V. Tomišić, *J. Chem. Educ.* **2024**, *101*, 3805–3812.

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COPPER-MEDIATED THREE-COMPONENT COUPLING BETWEEN PROPARGYLIC ALCOHOLS, CO_2 AND ALLYL HALIDES

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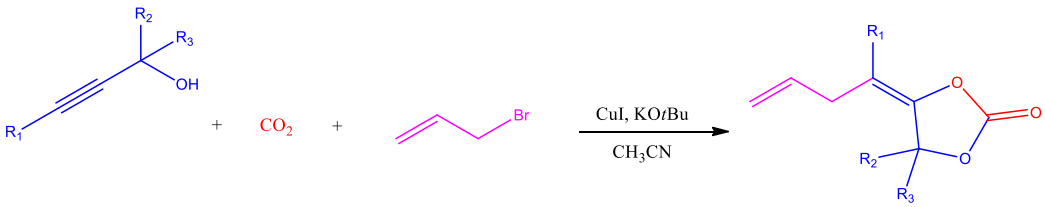
Carbon dioxide is regarded as the primary contributor to global warming caused by human activities, mainly through the burning of fossil fuels. Although CO_2 is a non-toxic, cost-effective, and abundant C1 source, it is kinetically inert and exhibits high thermal stability. The conversion of CO_2 into valuable compounds, particularly heterocycles, has garnered significant interest within the framework of sustainable chemistry.[1] One transformation that has attracted attention is the coupling of propargylic alcohols with CO_2 to form α-alkylidene cyclic carbonates, which are important for organic synthesis and pharmaceutical applications.[2] This reaction can be catalyzed by metals such as ruthenium, cobalt, palladium, silver, or copper. However, these reactions often require harsh conditions, such as strong bases or high CO_2 pressures.[3] Current methods for introducing new functional groups are limited, with only a few reports on incorporating allyl groups into these molecules.[4]
In this study, we present an efficient copper-mediated, one-pot, three-component coupling of propargylic alcohols, allyl halides, and CO_2 under atmospheric pressure. Copper was chosen over other metals due to its cost-effectiveness, stability, and ease of handling.



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REFERENCES

1. F. Vranješević, M. Kolympadi Markovic, D. Matulja, G. Ambrožić, J. Á. Sordo, S. Laclef, V. Vrček, D. Marković, *Catalysts* **2022**, *12*, 547.
2. K. Uemura, T. Kawaguchi, H. Takayama, A. Nakamura, Y. Inoue, *J. Mol. Catal. A: Chem.* **1999**, *139*, 1.
3. P. D. G. Greenwood, J. Waser, *Eur. J. Org. Chem.,* **2019**, *31-32*, 5183.
4. S. Sun, B. Wang, N. Gu, J.-T. Yu, J. Cheng, *Org. Lett.* **2017**, *19*, 1088.

P60

VISIBLE LIGHT-DRIVEN CHEMO- AND REGIOSELECTIVE ALKYLATION OF PHENOLS

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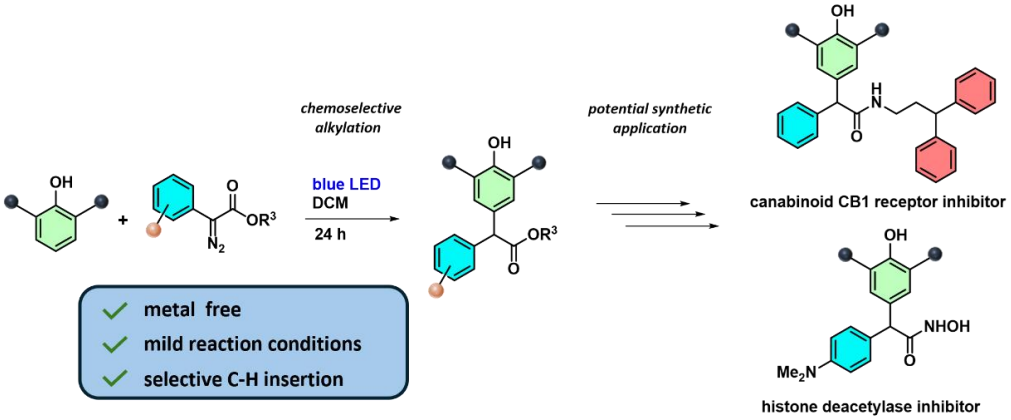
Because of the significant role of phenyl motifs in pharmaceuticals and natural products, converting readily available phenols into more structurally complex homologs is of great interest. Despite notable advances in metal carbenoid-induced C-H functionalization of arenes, the direct C-H functionalization of free phenols using diazo compounds remains particularly challenging and surprisingly uncommon. This rarity is likely because carbenoids often favour competitive O-H bond insertion over C-H functionalization.[1] Reactive diazoester carbenoid intermediates can be generated using transition metal catalysts, thermally (impractical due to harsh conditions), or in recent years photochemically using blue light which allows reactions to occur under mild conditions at room temperature without the need for catalysts, addressing issues with high energy UV-light which previously compromised chemoselectivity.[2] This research aims to develop a method for chemo- and regioselective functionalization of phenols by photoinduced C-H alkylation with diazoesters in *para*-position using blue light. This methodology is both environmentally friendly and cost-effective. The resulting *para*-C-alkylated phenol can be further transformed into molecules of great interest. One potential synthetic application includes the synthesis of histone deacetylase inhibitors, which have demonstrated significant potential as a treatment option for various cancerous and non-cancerous diseases. Another potential application is in the synthesis of cannabinoid receptor (CB1) antagonists, which have therapeutic effects against addiction, and drug abuse and help in regulating body-weight gain.[3]



REFERENCES

1 Y. Yang, B. Lu, G. Xu, X. Wang, *ACS Central Science* **2022**, *8*, 581.
2. Ł. W. Ciszewski, K. Rybicka-Jasińska, D. Gryko, *Org. Biomol. Chem.* **2019**, *17*, 432.
3. Z. Yu, B. Ma, M. Chen, H.-H. Wu, L. Liu, J. Zhang, *J. Am. Chem. Soc.* **2014**, *136*, 6904.

P61

FLEXIBLE INKJET-PRINTED 3-ELECTRODE SYSTEM FABRICATED USING INTENSE PULSED LIGHT FOR AZITHROMYCIN DETECTION

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The advancement of civilization has both positive and negative impacts. While the pharmaceutical industry has extended human lifespan, it has also significantly affected the environment. This influence is particularly evident in the spread of antibiotics in soil, water, and food. Therefore, it is crucial to monitor their concentration in specific areas. Sensors provide a simple solution for monitoring the state of the environment (SOE). Traditional instrumental methods require substantial financial resources, are time-consuming, and do not allow on-site analysis. As part of a study, an inkjet-printed, flexible sensor processed using intense pulsed light (IPL) was developed to detect azithromycin in water systems. The research included the electrochemical characterization of the inkjet-printed and intense pulsed light processed (IP-IPL) sensor. Using cyclic voltammetry at different scan rates in the presence of $[Fe(CN)_6]^{4-}$, the microscopic surface of the electrode and the heterogeneous electron transfer rate constant were estimated. The results were then compared with those of a commercial screen-printed carbon sensor and an inkjet-printed heat-treated sensor. Subsequently, all three sensors were calibrated using differential pulse voltammetry in the concentration range of azithromycin 0.05 – 10 µM, with 0.05 M $NaHCO_3$ used as a supporting electrolyte. Upon comparison, the IP-IPL sensor exhibited the widest linear range of 0.5 – 10 µM (R^2= 0.9815), with a detection limit of 0.0614 µM. Furthermore, the sensor exhibited high repeatability (RSD= 2.73%) and a satisfactory level of selectivity in the presence of NaCl, $MgSO_4$, glucose, $NaNO_3$, NH_4Cl, KI, and urea. Finally, the sensitivity of the IP-IPL sensor was tested in flow measurements using chronoamperometry, and it is 0.3139 µA/µM. The dynamic range spans from 0.5 to 10 µM, with a correlation coefficient of 0.9813. Based on the analysis that were conducted, it was determined that the IP-IPL sensor exhibited the best electrochemical and analytical properties. This may result from the formation of so-called craters after IPL treatment, which significantly contributes to the increase of the specific surface area of the electrode, which was confirmed by SEM analysis. Its satisfactory sensitivity in continuous measurements confirms its potential application in wastewater monitoring.

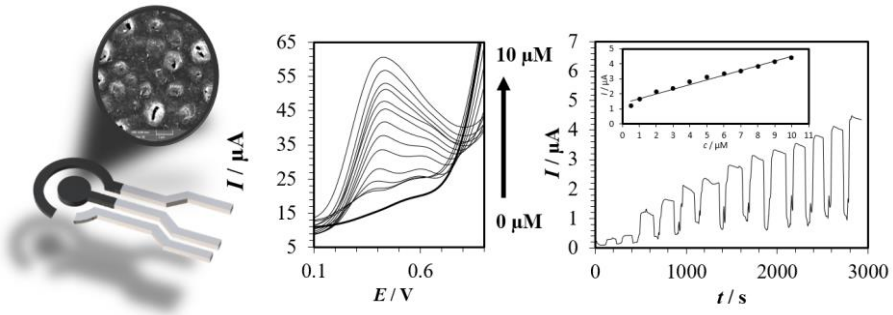

Figure 1. Results obtained using the IP-IPL sensor.

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P62

ARTIFICIAL INTELLIGENCE ALGORITHMS SIGNIFICANTLY IMPROVE MODELS OF ORAL TOXICITY OF CHEMICALS

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Recent years have shown that the development and application of algorithms for machine learning and artificial intelligence have had a major impact on chemistry. In 2024, for example, the Nobel Prize in Chemistry was awarded for the AlphaFold algorithm and the major advances in predicting the structure of proteins, which are a consequence of the successful application of artificial intelligence algorithms.[1]

In this work, the Random Forest (RF) and Transformer algorithms have been shown to be most suitable for developing and optimising models for predicting the oral toxicity of chemicals in the rat as a model organism.[2-4] Transformer is based on neural network algorithms that learn context (and thus meaning) by tracking relationships in sequential data such as the words in a sentence. We developed the models on a set of about 6000 compounds and tested them on a set of 1480 chemicals. Toxicity is expressed as log10 of the LD50 (milligrammes per kg body weight of the test animal when administered orally, resulting in death within 14 days in 50% of the animals tested). The error of the model was found to be 6-8% lower than that of the best existing models developed by the US EPA, with an error of 0.62 (log10 scale).[5]
The chemical and physical properties of the molecules in the Random Forest model are represented by electrotopological indices that take into account not only the way the atoms are connected to each other, but also the charge of the atoms. The Transformer algorithm has proven to be the best. It extracts specific chemical information relevant to toxicity from the SMILES analysis of the shape of the structure, which is treated like a word in a language. In this way, a specific structural feature (which is important for toxicity) is extracted from the SMILES structure of molecules and then used to predict toxicity. An improvement of about 10% compared to the best models of the US EPA[5] is achieved by forming an ensemble of these two models (RF and Transformer) by averaging their predictions.

ACKNOWLEDGEMENTS We would like to thank the Ministry of Science, Education and Youth of the Republic of Croatia for financial support.

REFERENCES

1. J. Jumper, et al., *Nature* **2021**, *596*, 583.
2. I. Sushko et al., *J. Comput. Aided. Mol. Des.* **2011**, *25*, 533.
3. P. Karpov, G. Godin, I. V. Tetko, *J. Cheminform.* **2020**, *12*, 17.
4. I. V. Tetko, et al. *Nat. Commun.* **2020**, *11*, 5575.
5. US EPA, https://www.epa.gov/comptox-tools/toxicity-estimation-software-tool-test, October **2024**.

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SOLVENT-FREE FORMULATION OF ANTICANCER DRUG FOR CONTROLLED RELEASE BY MECHANOCHEMICAL TREATMENT

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Dasatinib (DAS) is an anticancer drug used in the treatment of chronic myeloid and acute lymphoblastic leukemia. Due to its poor aqueous solubility, it is poorly absorbed by the gastrointestinal tract and has low bioavailability. To improve the solubility of the drug, solid dispersions of DAS in a hydrophilic polymer carrier, poly(vinyl pyrrolidone) (PVP), were prepared mechanochemically and characterized in detail by solid state analytics, which could physically explain the improved dissolution properties. This solvent-free strategy has proven significant increase in the solubility of DAS when the drug was formulated into amorphous solid dispersions (ASDs). Such *in vitro* discovery should lead to improved oral absorption and higher bioavailability of this specific drug. However, such mechanochemical treatment did not lead to a controlled release of DAS, which would be another aimed pharmaceutical property for such an antineoplastic drug. This paper will reveal our vision to use solvent-free methodology to formulate a more effective drug product with improved properties, i.e., increased solubility and controlled release profile.

Our intention here is to mechanochemically prepare ternary ASDs using an additional polymer, hydroxypropylmethylcellulose (HPMC), to modify the release profile of dasatinib. Ternary solid dispersions were prepared at different ratios using a high-energy laboratory ball mill with ZrO_2 grinding bowl and properly characterized by differential scanning calorimetry (DSC), thermogravimetric analysis (TGA) and Fourier transform infrared spectroscopy (FTIR). A decreased relative degree of crystallinity and shifts in the absorption bands for the interacting functional groups, indicating hydrogen interactions between drug and polymer(s), reveal promising properties of the ternary ASDs prepared without the use of solvents.

The prepared ASDs and the granules of excipients were used for the preparation of tablets. The tablets obtained were characterized using standardized pharmaceutical tests in accordance with the recommendations of the European Pharmacopeia. The test results showed an improvement in solubility and drug release compared to pure dasatinib, indicating a potential enhancement in the bioavailability and therapeutic efficacy of the drug product. The results presented confirm that this particular drug can be formulated mechanochemically to achieve controlled release and improve its dissolution properties.

This research demonstrates the potential of this solvent-free method to improve the bioavailability and release profile of dasatinib, which may contribute to better treatment outcomes in leukemia.

P64

STUDY OF THE LABELING AND PROPERTIES OF SOAPS USED IN NEONATAL SKIN CARE

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Objective: To assess the information on labeling and the physical and physicochemical properties of soaps used for newborns (NB).

Method: This was a quantitative and descriptive study of 17 soaps marketed in Santa Cruz, Bolivia. The labeling information (surfactants, safety tests, and pH description), as well as the physical (color and fragrance) and physicochemical (pH value) properties of the products, were analyzed, with the latter two assessed in a laboratory setting.

Results: A total of 27 types of surfactants were identified: 70.3% (n=19) were anionic, 18.5% (n=5) amphoteric, and 11.1% (n=3) non-ionic. Among the soaps, 37% (n=10) had a moderate potential for irritation. Regarding safety tests, most formulations (94.1%) indicated "dermatologically tested," while only 42% stated "ophthalmologically tested." Translucency was observed in 23.5% (n=4) of the soaps, and all formulations contained fragrance. The highest average pH value was found in traditional bar soaps (9.94 ± 0.81).

Conclusion: The formulations analyzed demonstrated a low to moderate irritation potential. Four liquid soaps and one bar soap had pH values close to that of newborn skin, indicating their suitability for maintaining skin barrier homeostasis. Although most formulations were labeled as "dermatologically tested", fewer than half indicated "ophthalmologically tested". This study offers essential insights for selecting appropriate soaps for newborns.

Keywords: skin hygiene; soaps; pH; newborn; surfactants.

REFERENCES

1. G. Stamatas, J. Nikolovski, M. C. Mack, N. Kollias, *Int. J. Cosmet. Sci.* **2011**, *33*, 17.

2. J. W. Fluhr, R. Darlenski, *Curr. Probl. Dermatol.* **2018**, *54*, 26.

3. M. O. Visscher, A. N. Carr, J. Winget, T. Huggins, C. C. Bascom, R. Isfort et al., *Pediatr. Res.* **2021**, *89*, 1208.

4. A. Cooke, C. Bedwell, M. Campbell, L. McGowan, S. J. Ersser, T. Lavender, *Midwifery* **2018**, *56*, 29.

5. T. Lavender, C. Bedwell, S. A. Roberts, A. Hart, M. A. Turner, L. Carter et al., *J. Obstet. Gynecol. Neonatal Nurs.* **2013**, *42*, 203.

6. V. Rogiers, *Skin Pharmacol. Appl. Skin Physiol*. **2001**, *14*, 117.

P65

EXTRACTIVE REMOVAL OF POLYVINYL CHLORIDE, POLYSTYRENE AND POLYETHYLENE TEREPHTHALATE FROM WATER USING DEEP EUTECTIC SOLVENT

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The problem of plastic waste, in addition to being a threat to the environment, also represents a danger to the health of living beings, given that it is introduced into the body in the form of microplastics through drinking water or food contaminated with plastic.[1] The long-term accumulation of plastic in the body causes inflammatory processes that damage cells and tissues and lead to neurological diseases.[2] Microplastics are defined as particles with dimensions less than 5 mm, and they are composed of certain polymers and additives. In the last decade, research has focused on the removal of plastic particles from water and soil, and various effective processes have been proposed, which can be mechanical (ultrafiltration[3], membranes[4]), chemical (photocatalysis, UV/H2O2[5]), physicochemical (coagulation[6], flotation[7]) and biological[8] i.e. decomposition by the action of bacteria, fungi and algae.

In this paper, extraction of microplastics from water using deep eutectic solvents (DESs) was investigated. DESs are considered environmentally friendly solvents due to their properties (non-toxic, non-flammable, non-volatile, biodegradable) and due to the possibility of repeated use as an extraction agent.[9] Polyvinyl chloride (PVC), polystyrene (PS) and polyethylene terephthalate (PET) granules were chosen as model plastic waste. The plastic particles were prepared by dissolving the granules in an organic solvent, then precipitated in ethanol. Aqueous solutions with a concentration of 1 mg/mL were prepared from such fine particles, which were submitted to extraction with DES at 25 °C for 10 minutes. By measuring the optical density, the results show the extraction efficiency of PVC, PS and PET reached 97.49 %, 94.48 % and 95.45 %, respectively. DES can be regenerated by centrifugation and separation of the extracted plastic particles.

The extraction of microplastics by DES can be proposed as a cheap and simple method for the development of green technology with a high degree of effectiveness.

REFERENCES

1. M. Ricciardi et al., *Water* **2023**, *15(9)*, 1718.
2. N. Chaukura et al., *Pollutants* **2021**, *1,* 95-118.
3. M. Enfrin et al., *Water Research* **2019**, *161,* 621-638.
4. L. Li et al., *Science of The Total Environment* **2018***, 627,* 332-340.
5. S. Kim et al., *Chemical Engineering Journal Advances* **2022**, *9,* 100213
6. G. Zhou et al., *Science of The Total Environment* **2021***, 752,* 141837
7. O. Rius-Ayra et al., *Marine Pollution Bulletin* **2021***, 167,* 112335
8. C. N. Muhonja et al., *PLoS ONE* **2018**, *13,* e0198446
9. K. Radošević et al., *Ecotoxicology and Environmental Safety* **2015**, *112,* 46-53.

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