CUTTING
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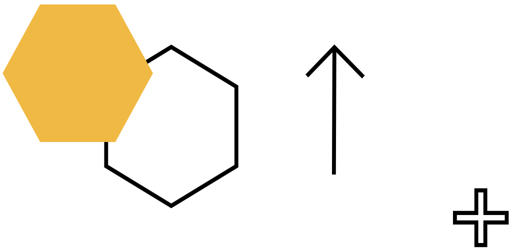
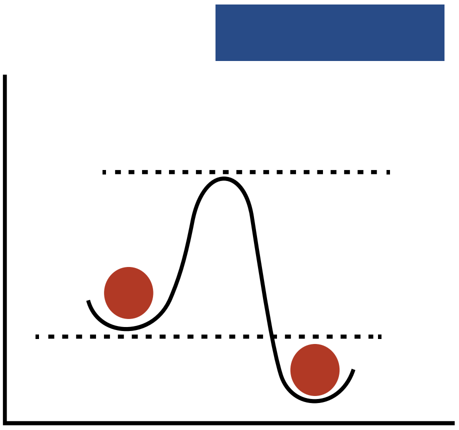
2023



CAREERS in science



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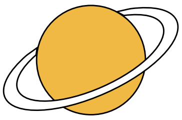
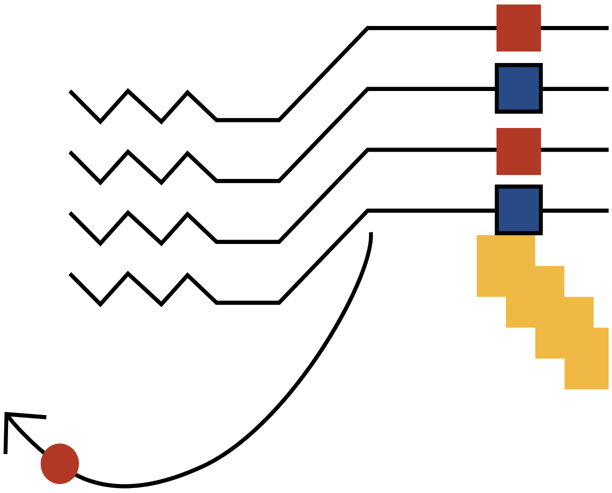
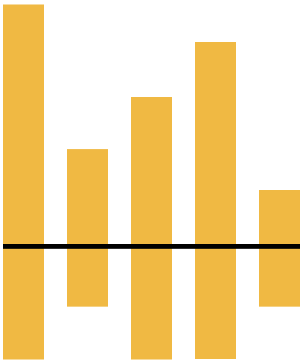
BOOK OF ABSTRACTS







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BOOK OF ABSTRACTS: Cutting Edge – Careers in Science, Scientific Conference for Young Scientists

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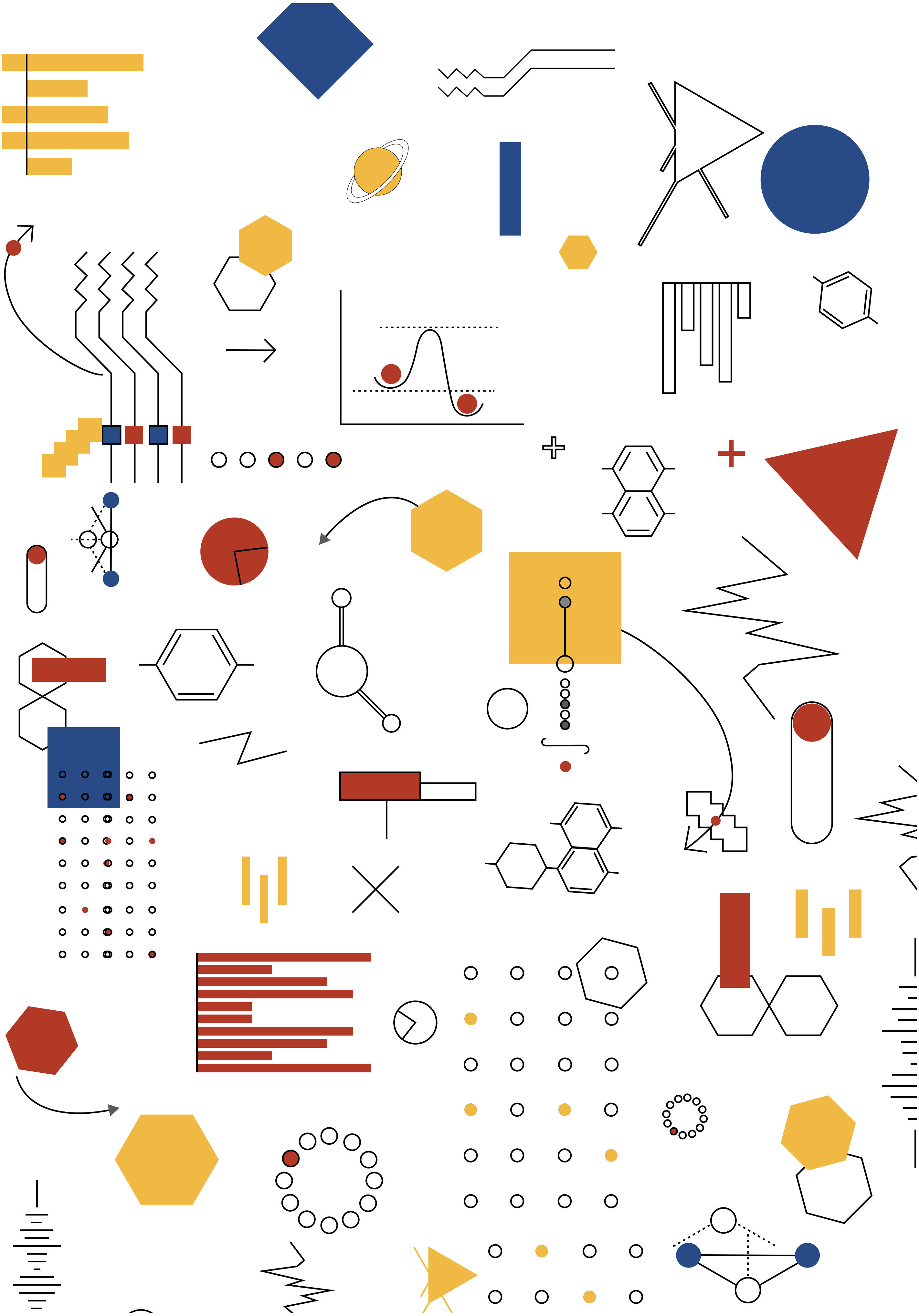


CUTTING
EDGE
2023

CAREERS in science

The 2023 Cutting Edge Conference was held on September 21, at the Faculty of Chemistry and Chemical Technology, University of Ljubljana. With the main goal of bringing together young researchers and students from different scientific fields, giving them the opportunity to present their research and providing a forum for open discussions, the conference has already celebrated its fifth anniversary.

The theme of this year's Cutting Edge conference was "*Careers in Science*". It is undeniable that many young scientists wrestle with the difficult decision of whether to enter academia or industry after completing their studies. Very often, one does not exclude the other. To this end, we invited leading scientists and researchers from various institutions to explain how to effectively turn new ideas into successful business plans, and to talk about how their careers are intertwined with both industry and academia.

The conference was attended by more than 96 participants from Slovenia and several other countries conducting research in various fields. 73 of them presented their research under three different sub-topics – Science behind the living, Materials of the future, and Technologies for the Earth and Environments.
For the first time in Cutting Edge's history, we offered a special session for secondary school students – "Young Minds". 23 participants had the opportunity to attend the conference and present the results gained in their school project.

The day before the conference, on Wednesday, September 19, the CUTTING EDGE x NOVARTIS workshop took place at the faculty, aimed at developing important career skills and development.

The conference started at 8:45 with a speech by the Dean, Prof. Dr. Andreja Žgajnar Gotvajn and the President of the Cutting-Edge Society, Dr. Matjaž Dlouhy. The opening was followed by lectures and poster sessions. The one-day conference ended with a small awards ceremony, where prizes were awarded for the best poster and the best oral presentation. Following the event, all participants were invited to a gala event at Ljubljana Castle to celebrate the fifth anniversary of the conference.

We would like to thank the members of the scientific committee: prof. dr. Marko Novinec, doc. dr. Jakob Kljun, doc. dr. Tilen Kopač, asist. dr. Ula Ruzman, asist. Uroš Zavratnik, asist. Imperl Jernej, and asist. Ema Gričar. The conference could not have been organized to this extent without the help of several students from the Faculty of Chemistry and Chemical Technology. Special thanks are extended to our collaborators and sponsors, with a particular emphasis on the Faculty of Chemistry and Chemical Technology, University of Ljubljana, for their exceptional cooperation and unwavering support.

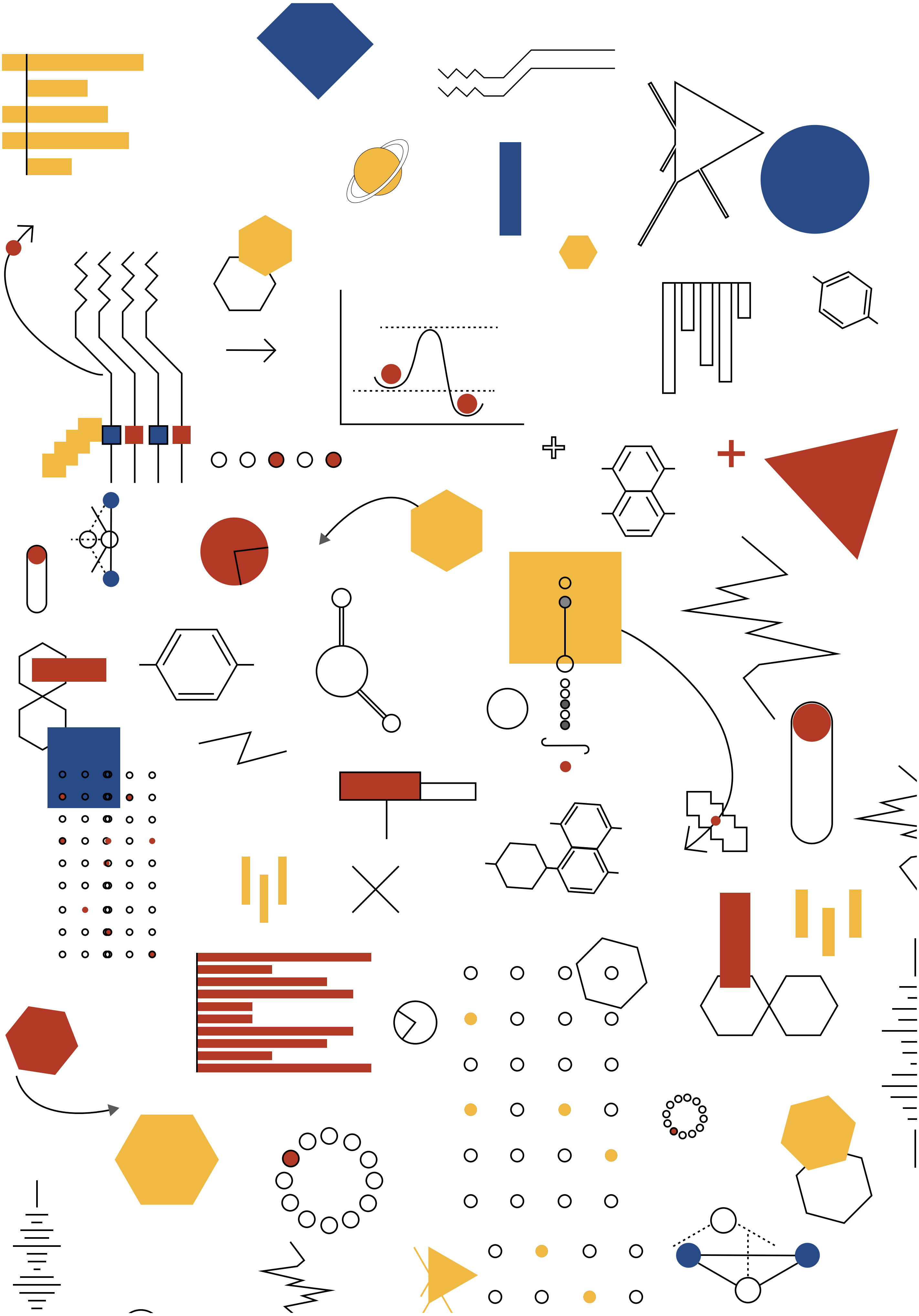
The Cutting Edge Organizing Committee is grateful to the presenters and the participants for their thought-provoking contributions. May critical thinking, a willingness to embrace multiple perspectives, and boundless curiosity always be with you.

Until next time (a hint for all eager young minds: 2025 sounds a lot like the next chocolate chip year)!

Cutting Edge Organizing Team

Conference schedule

8:00 – 8:45	**Registration and poster installment** | lobby in building X
8:45 – 9:00	**Opening ceremony** | lecture hall A
9:00 – 10:00	**Plenary session** | lecture hall A *The role of the Zero Carbon Technology Center in the transformation of the broader region into a low-carbon society* prof. dr. Robert Dominko and izr. prof. dr. Blaž Likozar from National instutite of chemistry
10:00 – 11:00	**Short presentation session I** | lecture hall A *The Invisible Power of Chemistry in Aviation* Tine Tomažič from Pipistrel *Corrosion - from theory to the practice* dr. Tadeja Kosec from Slovenian National Building and Civil Engineering Institute
11:00 – 11:45	**Coffee break with our sponsors** | lobby in building X
11:45 – 12:45	**Short presentation session II** | lecture hall A *Cutting the Edge between Academia and Industry* doc. dr. Marina Klemenčič from NOVARTIS *Startup as a vehicle to financing your research* Maj Hrovat from Juicy Marbles
12:45 – 14:00	**Lunch break** | cafeteria in building X
14:00 – 15:00	**Elevator pitch sessions** SNICKERDOODLE – Materials for the future | P1 CHOCOLATE CHIP – Science behind the living | P2 GINGERBREAD – Technologies for the earth and environment | P3
14:00 – 15:00	**Young Minds Section** Young Minds Lecture | P4 presentation by deputy dean prof. dr. Marko Novinec from FKKT UL Young Minds Presentations, happening parallel in 2 seminar rooms: GROUP 1 - seminar room 3067 (lamela 3B) GROUP 2 - seminar room 3038 (Pamela 3B)
15:00 – 16:00	**Poster session with a coffee break** | faculty hallway
16:00 – 16:15	**Closing remarks and award ceremony** | lecture hall A
20:00 – 23:00	**Gala event at the Ljubljana castle**



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Abstracts

Carbonyl functionalized imidazolates as a platform for preparation of nickel-based ZIFs

Aljaž Škrjanc,[1,2] Dominik Jankovič,[3] Anton Meden,[3] Matjaž Mazaj,[1] Erik Svensson Grape,[4] Martin Gazvoda,[3] Nataša Zabukovec Logar[1,2,*]

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Zeolitic imidazolate frameworks (ZIFs) are a subclass of metal-organic frameworks that have attracted considerable attention as potential functional materials due to their high chemical stability and ease of synthesis.[1] ZIFs are usually composed of zinc ions coordinated with imidazole linkers, with some other transition metals, such as Cu(II) and Co(II) also showing potential as ZIF-forming cations. Despite the importance of nickel in catalysis, no Ni-based ZIF with permanent porosity has yet been reported. We have found that the presence and arrangement of the carbonyl functional groups on the imidazole linker plays a crucial role in completing the preferred octahedral coordination of nickel, revealing a promising platform for the rational design of Ni-based ZIFs for a wide range of catalytic applications. Herein, we report on the synthesis of the first Ni-based ZIFs (Fig. 1) and demonstrate their high potential as heterogenous catalysts for Suzuki-Miyaura cross-coupling C-C bond forming reactions.

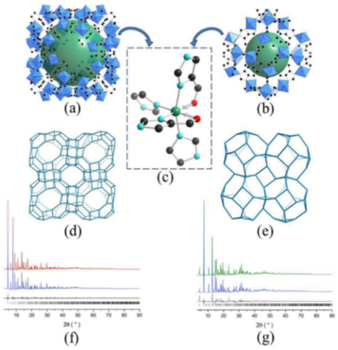

Figure 1: *Structures of the prepared materials, cage tiling and Rietveld refinement of bulk PXRD with modeled 3DED structure data.*

[1] Li, H.; Chen, W.; Liu, B.; Yang, M.; Huang, Z.; Sun, C.; Deng, C.; Cao, D.; Chen, G. A Purely Green Approach to Low-Cost Mass Production of Zeolitic Imidazolate Frameworks. *Green Energy Environ.* **2023**, 8 (3), 775–784.

Biodegradability of polybutylene adipate terephthalate microplastics in the aquatic environment

Amadeja Sajovic Žulovec,[1] Anita Jemec Kokalj,[2] Barbara Klun,[1] Gabriela Kalčikova*[,1]

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[2]Biotechnical Faculty, University of Ljubljana, Jamnikarjeva ulica 101, SI-1000 Ljubljana, Slovenia

Polymers completely revolutionized industry due to their excellent and useful properties. They are found in many applications, from simple packaging to agriculture. The latter is one of the most important inputs of plastic into soil. Currently, conventional non-degradable plastics are mostly used, but as an alternative new polymers have been investigated with specific focus on biodegradable polymers, such as polybutylene adipate terephthalate (PBAT).[1] PBAT is used for production of compostable plastic bags and as an alternative to non-biodegradable polyolefins (e.g. low density polyethylene, LDPE) used for mulching. PBAT was shown to be compostable, however its degradation in water is not widely studied.[2] In this context, the ready biodegradability of PBAT and LDPE microplastics was investigated in a closed respirometer. Results showed that both PBAT and LDPE were poorly biodegradable; PBAT degraded only up to 4% while PE did not degrade at all in 28 days (Fig. 1A). Visual inspection of microplastics by optical microscope also did not reveal any biofilm formation that could initiate biodegradation and it was concluded that both LDPE and also its alternative PBAT are not biodegradable in the aquatic environment (Fig. 1B and 1C).

Figure 1: *A) Biodegradation of PE and PBAT, B) Optical microscopy image of PBAT, C) Optical microscopy image of PE.*

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[1] Ghanbarzadeh, B.; Almasi, H. *Biodegradation – Life of Science. InTech.* **2013**.

[2] Li, S.; Ding, F.; Flury, M.; Wang, J. Dynamics of macroplastics and microplastics formed by biodegradable mulch film in an agricultural field. *Sci. Total Environ* **2023.**

Cloning and expressing SFPQ protein

Ana Pervanja,[1] Vera Župunski*,[1]

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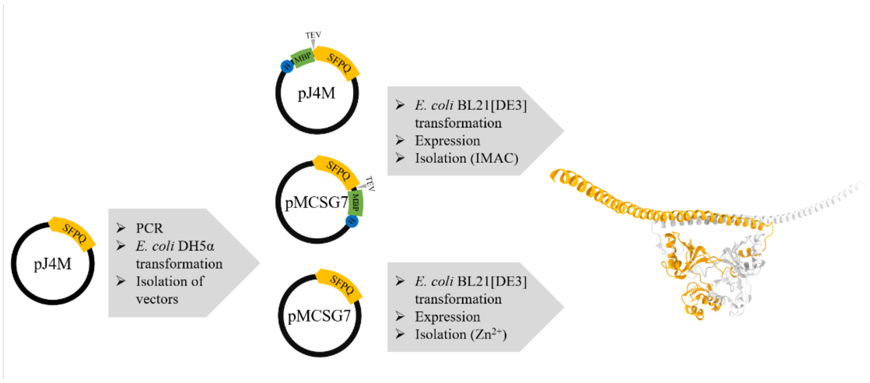
Splicing factor proline and glutamine rich (SFPQ) is a protein that interacts with protein, RNA and DNA. Because of that, it has a plethora of cell functions and is increasingly popular among neurodegenerative disease studies.[1] Our aim was to express and purify enough SFPQ to conduct experiments such as monitoring the formation of paraspeckles. Vectors pMCSG7-MBP-SFPQ and pMCSG7-SFPQ (untagged SFPQ) were prepared (**Error! Reference source not found.**). SFPQ was then expressed using pJ4M-SFPQ-MBP (prepared in the lab) and pMCSG7-MBP-SFPQ vectors. The fusion with His6 allowed the protein to be purified by immobilized metal ion affinity chromatography (IMAC). SFPQ-MBP construct was already degraded during expressing. MBP-SFPQ was expressed in sufficient amounts, but degradation occurred during the purification steps. We used the pMCSG7-SFPQ vector to express untagged SFPQ and isolate it by adding zinc chloride.[2] Proteolysis occurred upon expression and/or purification. We concluded that the cause of protein degradation is a large proportion of the disordered structure, which is more sensitive to proteases.[3] The procedures should therefore be optimized to reduce the activity of proteases.



Scheme 1: *Overview of the experiments. Structure of SFPQ homodimer is shown on the right (PDB ID: 4WIJ).*[1]

[1] Lee, M.; Sadowska, A.; Bekere, I.; Ho, D.; Gully, B. S.; Lu, Y.; Iyer, K. S.; Trewhella, J.; Fox, A. H.; Bond, C. S. The Structure of Human SFPQ Reveals a Coiled-Coil Mediated Polymer Essential for Functional Aggregation in Gene Regulation. *Nucleic Acids Res.* **2015**, 43 (7), 3826–3840.

[2] Lim, Y. W.; Lee, M. Rapid Purification Method for Human SFPQ by Implementing Zinc-Induced Polymerization. *Protein Expr. Purif.* **2020**, 171, 105626.

[3] Kalthoff, C. A Novel Strategy for the Purification of Recombinantly Expressed Unstructured Protein Domains. *J. Chromatogr. B.* **2003**, 786 (1), 247–254.

Analytical method for the determination of artemisinin in encapsulated formulations

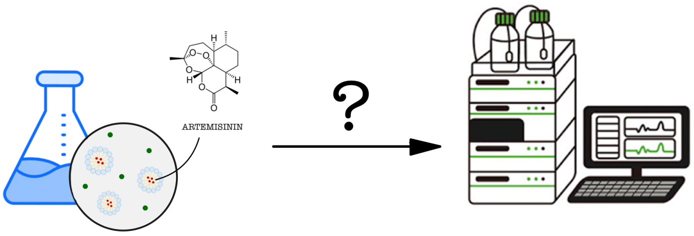
Ana Šijanec,[1] Matjaž Grčman,[1] Monika Horvat Zagorec,[1] Matevž Pompe*,[1]

[1]Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113, SI-1000 Ljubljana, Slovenia, ana.sijanec@gmail.com

Artemisinin is a medicinal substance used to combat malaria, which is obtained naturally from sweet wormwood (*Artemisia annua*). Artemisinin has been used as an antimalarial since 1972. Its proven versatility has led to increased use in the pharmaceutical and food industries in recent years. To achieve product safety and efficiency, products must be properly analyzed.[1]

The standard method for the determination of artemisinin is HPLC-UV/Vis. Due to the poor solubility of artemisinin in many solvents, the micellar formulation is often used as a drug delivery system to increase biological potency. A hydrophilic coating around the loading core allows solubilization of the hydrophobic drug and protection from degradation. Therefore, sample preparation and degradation of the micelles are crucial for the determination of artemisinin.[2,3]

To our knowledge, a method for the determination of artemisinin in micellar formulations has never been published (Scheme 1). Our method requires sample preparation by extraction with toluene and complexation of surfactants. We have also optimized the method for the determination of artemisinin using HPLC-UV/Vis. The analytical parameters of the developed method were determined as follows: Sample preparation recovery 94 % ± 1.6 %, LOD for artemisinin 0.02 mg/mL and LOQ 0.05 mg/mL.



Scheme 1: *Determination of artemisinin using HPLC-UV/Vis.*

[1] Krishna, S.; Bustamante, L.; Haynes, R. K.; Staines, H. M. Artemisinins: Their Growing Importance in Medicine. *Trends Pharmacol. Sci.* **2008**, 29 (10), 520.

[2] Mwangi, S.; Abuga, K.; Mungai, N.; Mwangi, J. A High Performance Liquid Chromatography Method for the Determination of Artemisinin in Artemisia Annua L. Leaf Extracts. *The East and Central African Journal of Pharmaceutical Sciences* **2020**, 23 (2), 48–53.

[3] Jäpelt, K. B.; Johnsen, L. G.; Christensen, J. H. Removal of Polysorbate 80 by Complexation Prior to LC-MS Analysis. *Anal. Bioanal. Chem.* **2016**, 408 (9), 2303–2307.

Copper(I) and silver(I) complexes of a bulky NHC ligand

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[2]Jožef Stefan Institute, Jamova cesta 39, SI-1000 Ljubljana, Slovenia

N-heterocyclic carbenes (NHCs) are valuable ligands in organometallic chemistry. They can significantly affect the reactivity and stability of metal complexes by tailoring their electronic and steric properties.[1] Bulky substituents around the carbene carbon atom provide significant steric hindrance, preventing side reactions and stabilizing reactive metal centers. The use of bulky NHCs revolutionized organometallic chemistry and enabled the isolation and identification of elusive metal complexes, especially low-valent transition metal atoms with low coordination numbers.[2]

Among the numerous NHC ligands, the IPr** ligand (Fig. 1) stands out for its remarkable sterically demanding nature that confers kinetic stabilization to the metal centers.[3] This ligand has a unique combination of steric properties, favorable spectroscopic features, high solubility, and a tendency to crystallize. In this study, we present an improved synthesis for this ligand that shortens reaction time while improving reaction yield. We have also successfully prepared a series of coordination compounds of copper(I) and silver(I). The structural characterization of these compounds was based on single-crystal X-ray diffraction (XRD) analysis, which allowed accurate determination of their structures.

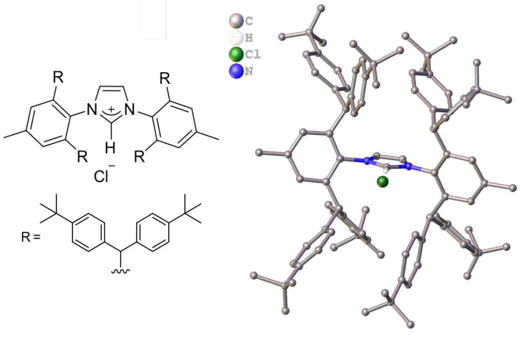

Figure 1: *Structure of IPr**HCl.*

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[1] Hopkinson, M., *et al.* An overview of *N*-heterocyclic carbenes. *Nature* **2014**, 510, 485–496.
[2] Romero, E. A., *et al.* Spectroscopic Evidence for a Monomeric Copper(I) Hydride and Crystallographic Characterization of a Monomeric Silver(I) Hydride. *Angew. Chem. Int. Ed.* **2017**, 56, 4024–4027.
[3] Weber, S. G., *et al.* Synthesis of an extremely sterically shielding *N*-heterocyclic carbene ligand. *ARKIVOC* **2012**, 3, 226–242.

An overview of consolidants for historic materials: Processes and what final characteristic to expect

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Cultural heritage is the priceless value of a place or a country. Cultural heritage objects are subject to various ageing and degradation processes that lead to a deterioration of their quality. For this reason, we resort to consolidation, which is one of the most important conservation procedures that these objects need to survive over time. Consolidation involves the use of consolidants, which are various binders dispersed in a solvent that are applied to the damaged layer of the materials to restore the lost cohesion between the particles. $Ca(OH)_2$-based consolidants are one of the most commonly used materials for consolidation due to their chemical compatibility with carbonate-containing objects. Among the most promising $Ca(OH)_2$-based consolidants are $Ca(OH)_2$ nanoparticles.[1]

Consolidation with nanoparticles is based on a carbonation reaction. During carbonation, $Ca(OH)_2$ particles react with CO_2 from the air, resulting in the formation of $CaCO_3$. This binds the loose particles and fills the cracks, solidifying the porous material. Nanoparticle consolidation has been shown to be very effective for surface consolidation. Commercial nanoparticle-based products include CaloSil® and Nanorestore®, which have been used in various studies and projects. Despite all their good properties, problems arise when deep consolidation is required.[1,2]

For this purpose, an aqueous solution of calcium acetoacetate - $Ca(OAcAc)_2$, also known as CFW (Consolidant formulation water) - was developed as part of the HEROMAT project. Calcium acetoacetate decomposes in the presence of water to calcium carbonate, carbon dioxide and acetone. The consolidation effect is achieved when CO_2 and acetone evaporate and the newly formed $CaCO_3$ particles fill the damaged substrate. CFW penetrates better into the substrate, needs to be applied less often, improves mechanical properties and has no significant effect on colour compared to nanoparticles.[3]

---

[1] Rodriguez-Navarro, C.; Ruiz-Agudo, E., Nanolimes: from synthesis to application. *Pure Appl. Chem.* **2018**, 90, 523-550.

[2] Otero, J.; Starinieri, V.; A.E., Nanolime for the consolidation of lime mortars: A comparison of three available products. *Constr. Build. Mater.* **2018**, 181, 394-407.

[3] Skrlep, L.; Pondelak, A.; Skapin, A., Method for reinforcing porous construction materials and use of calcium acetoacetate solution to this aim. EP 3004028 B1, 2017.

Microfluidic system for continuous degradation of organic pollutants

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Advanced oxidation processes (AOPs) have been the most effective method for removing synthetic organic pollutants.[1] Classic Fenton oxidation has several limitations, such as iron sludge accumulation and acidic pH range. We can overcome these limitations by using heterogeneous catalysts with immobilized iron ions, such as Fe(III)-alginate hydrogels, and environmentally friendly persulfate.[2] The redox properties of Fe(III)-alginate hydrogels can be utilized for reversible and cyclic electrochemical sol-gel transformation of alginate and persulfate activation. Electrochemical stimulation allows precise control of iron ion release, which is important, because insufficient amount of iron lowers the effectiveness of oxidation while excessive amount of iron leads to radical termination.[2,3]

In our research we determined the conditions for Fe(III)-alginate hydrogel electrodeposition and continuous electrodissolution in a microfluidic system. We used controlled release of Fe(II) ions for reaction with persulfate and generation of highly reactive sulfate radicals. We used sulfate radicals for continuous oxidation of BPA (Fig. 1). We found that optimal conditions for Fe(III)-alginate hydrogel formation are 3 mA, 200 µL/min, and 10 mM Fe(II). To optimize the generation of sulfate radicals, we used cyclic electrodissolution (3 mA, 100 µL/min) and 1 mM persulfate. We achieved 90 % degradation of BPA.

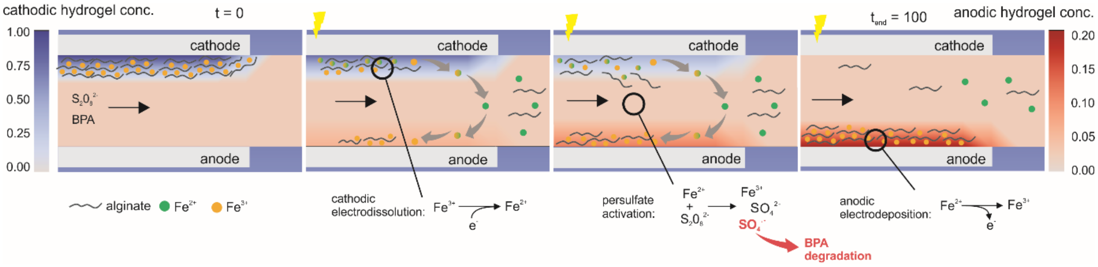

Figure 1: *Proposed mechanism of BPA degradation using cyclic sol-gel persulfate activation.*

[1] Jain, B.; Singh, A. K.; Kim, H.; Lichtfouse, E.; Sharma, V. Treatment of organic pollutants by homogeneous and heterogeneous Fenton reaction processes. *Environ. Chem. Lett.* **2018**, 16, 947–967.

[2] Kang, Y. G.; Vu, H. C.; Le T. T.; Chang Y. S. Activation of persulfate by a novel Fe(II)-immobilized chitosan/alginate composite for bisphenol A degradation. *Chem. Eng. J.* **2018**, 353, 736-745.

[3] Ambrožič, R.; Plazl, I. Development of an electrically responsive hydrogel for programmable in situ immobilization within a microfluidic device. *Soft Matter* **2021**, 17, 6751-6764.

Properties of porous carbon derived from thermal or microwave pyrolysis for oxygen reaction reduction

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This study explores the properties of porous carbon derived from polyaniline through thermal or microwave pyrolysis for oxygen reduction reaction (ORR) applications. Carbon-based catalysts, particularly nitrogen-doped carbon (N-C), are considered as promising alternatives to costly noble metal catalysts like Pt and Au.[1,2] While traditional thermal heating processes involve high energy consumption and long preparation times, microwave irradiation offers a more environmentally and economically viable synthesis for porous carbon materials. The synthesis of nitrogen-doped carbon samples includes both thermal and microwave heating techniques. The ORR activity is evaluated through cyclic voltammetry in alkaline media, employing a three-electrode setup. The results reveal comparable catalytic activity between the microwave and thermally carbonized samples (Fig. 1), with an onset potential of approximately 0.76 V vs. RHE. Moreover, a selectivity of 58±1% towards H_2O_2 is observed, highlighting the potential for decentralized H_2O_2 production. These findings have the potential to complement sustainable synthesis methods and broaden the application of microwave carbonization method in various applications including electrocatalysis, supercapacitors, and zinc–air batteries.

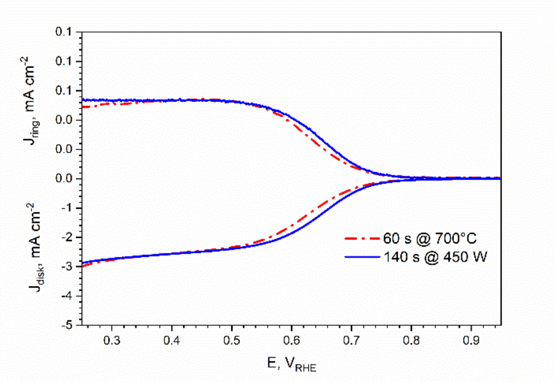

Figure 1: *The ORR results highlighted a close consistency in the catalytical activity between microwave carbonized samples (140s @ 450W) and the thermally carbonized sample (60s @ 700°C).*

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[1] Yang, S. et al. Toward the decentralized electrochemical production of H2O2: A focus on the catalysis, *ACS Catalysis* **2018**, 8(5), 4064–4081.

[2] Bouleau, L. et al. Best practices for ORR performance evaluation of metal-free porous carbon electrocatalysts, *Carbon* **2022**, 189, 349–361.

Investigating various solid-phase extraction sorbents for multicomponent analysis of organic pollutants in water

Anja Poljanšek,[1] Aleksander Kravos,*[,1] Helena Prosen[1]

[1]Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113, 1000 Ljubljana, Slovenia, aleksander.kravos@fkkt.uni-lj.si

Modern societies strongly depend on synthetic organic chemicals, such as pesticides, pharmaceuticals, industrial reagents, and personal-care products. However, these anthropogenic compounds are also continuously emitted into natural environments as undesirable emerging pollutants. Analytical chemistry, therefore, plays an important role as it performs water quality assessments and identifies emission sources. These requirements have been pushing science towards development of high-capacity, green, and versatile sample treatment procedures that would enable ultratrace LC-MS/MS analyses of variety of pollutants with different physico-chemical properties in just one single-run.[1]

SPE methods are known to be very effective in extracting a broad range of different pollutants from water samples. However, to achieve that, selection of the most suitable SPE sorbent must be done. As so, we performed comprehensive screening of five different types of reverse-phase sorbents, namely, C18, C8, polystyrene-divinylbenzene (PS-DVB), hydrophilic-lipophilic balanced (HLB), and graphitized carbon black (GCB). Extractions were done on 15 selected pollutants present in 20−100 µg/L concentration range and using UHPLC-DAD instrumental method. In summary, results suggest that HLB sorbents provide the best compromise in extraction of all 7 polar, 6 semi-polar, and 2 non-polar compounds, revealing their high multiplexing capacity (see Fig. 1). These results are useful for further method development of HLB-based SPE followed by LC-MS/MS analytical procedure.

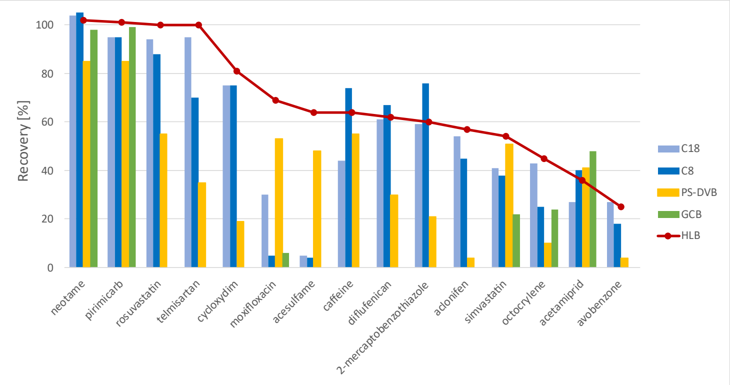

Figure 1: *Comparison of recoveries of different types of reverse-phase sorbents per analytes.*

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[1] Loos, R.; Tavazzi, S.; Paracchini, B.; Canuti, E.; Weissteiner, C., Analysis of polar organic contaminants in surface water of the northern Adriatic Sea by solid-phase extraction followed by ultrahigh-pressure liquid chromatography–QTRAP® MS using a hybrid triple-quadrupole linear ion trap instrument. *Analytical and Bioanalytical Chemistry.* ***2013***, 405, 5875–5885.

Treatment wetland as a source of water and nutrients for agriculture

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Treatment wetlands (TW) are wastewater (WW) treatment plants that mimic natural wetlands and their processes that enable pollutant removal. Treated water can be used for irrigation in agriculture while the remaining nutrients can substitute part of mineral fertilizers thus contributing to resource recovery. In this study, we changed the operation mode of TW to adjust the nitrogen discharge according to the seasonal dynamics of agricultural use – during growth season, the nutrients remained in the outflow while during winter denitrification was promoted to remove total nitrogen as fertigation is not needed.

The experiment was carried out on a pilot TW in Ajdovščina, Slovenia. The TW had vertical flow (VF) and treated 5 m^3 of primary treated municipal WW per day. In summer period, the operation of the TW was classic, while during winter, 50 % of treated water was recycled back to the inflow, thus the nitrified effluent was recycled to anaerobic inflow chamber with high organic carbon which was expected to simulate denitrification.[1] Selected WW parameters were monitored in the sedimentation tank, inflow and outflow from the TW.

TW enabled the efficient removal of COD and BOD in summer and winter. TW enabled efficient removal of TN in summer and winter (Figure 1). The average treatment efficiency was slightly lower in winter despite the recycle. Denitrification was not enhanced due to high aeration of wastewater in the TW and lower temperatures that increased oxygen solubility.

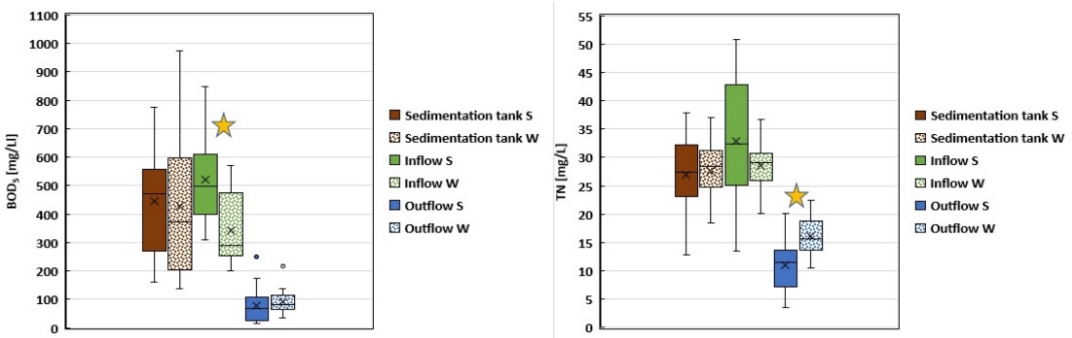

Figure 1: *Removal of BOD5 and total nitrogen during summer (S) and winter (W) period.*

[1]C. A. Arias, D. Istenič, O. Stein, X. Zhai, R. Kilian, I. Vera-Purto, H. Brix: Effects of effluent recycle on treatment performance in a vertical flow constructed wetland. *Ecological Engineering*, **2022**, 180: 106675.

The effect of charge-density on the distribution of counter-ions in aqueous solutions of ionenes - computer simulation

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Ionenes are polyelectrolytes consisting of alkyl chains of various lengths of methylene groups between which positively charged quaternary nitrogen atoms are located. By increasing the number of methylene groups between consecutive nitrogens charge density of the ionene decreases.[1,2] The term ion-specific effects refers to changes in properties of polyelectrolyte solutions depending on the type of halide counter-ion present.[3] In our work we used all-atom molecular dynamics (MD) computer simulation (OPLS forcefield) to study the difference in F^- and Br^- counter-ion binding to 3,3- and 6,6- ionenes in aqueous solutions. From nitrogen (ionene) – counter-ion radial distribution function (RDF) (Fig1) one can conclude that Br^- has larger probability to be located next to the ionene than F^-. The results are consistent with experimental data [4] and can be explained through counter-ion hydration. F^- ions have tighter hydration shell compared to Br^-, which by losing some of the water molecules from the first hydration shell can come closer to the polyion.

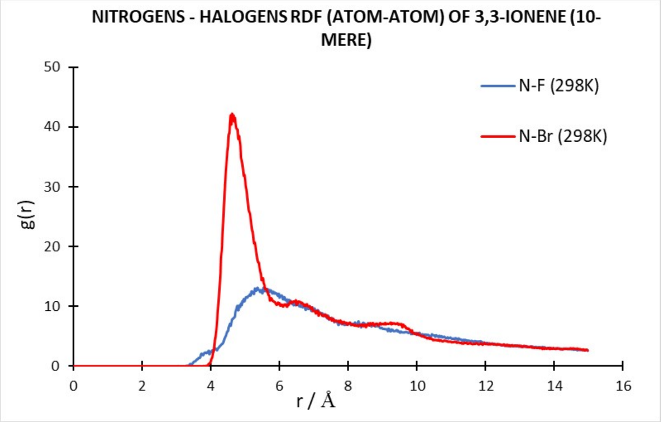

Figure 1: *Nitrogens– counter-ions RDF obtained from all-atom MD simulations.*

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[1]M. Druchok, V. Vlachy, K.A. Dill, *J. Chem. Phys.* **2009**, 130, 134903.

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Superhydrophobic coating for aluminium alloy 2024-T3 and glass

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The objective of the study was to develop a superhydrophobic coating for application on glass and aluminum alloy 2024-T3. To achieve a superhydrophobic surface with low surface energy and roughness, SiO_2 nanoparticles synthesized via the Stöber method were used, and their surface was subsequently modified with alkyl silane (AS) or perfluoroalkyl silane (FAS). The adhesion of particles to the glass and alloy surfaces was enhanced by applying a hybrid sol-gel coating composed of tetraethyl orthosilicate (TEOS), methyl methacrylate (MMA), and 3-methacryloxypropyltrimethoxysilane (MAPTMS).[1,2]

The nanoparticles and coatings were assessed after deposition using scanning electron microscopy (SEM) combined with energy dispersive spectrometry to analyze surface topography, composition, and coating thickness. Corrosion resistance was evaluated through electrochemical impedance spectroscopy in a 0.1 M NaCl solution.

The SiO_2 nanoparticles prepared had an approximate size of ~60 nm. The maximum water contact angles on the aluminum surface coated with SiO_2+AS or SiO_2+FAS particles were 135° and 151°, respectively. Moreover, the ~2 μm thick coating exhibited effective protection against corrosion when exposed to the testing medium.

This coating preparation method also presents potential business opportunities in various industries such as transportation, construction, photovoltaic system protection, and medicine.

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The effect of sample preparation on analytical evaluation of plasmid DNA

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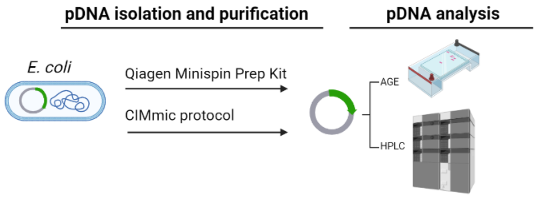
In the past decades, interest in plasmid DNA (pDNA) has increased. Due to its rapid synthesis and production in large quantities, it is considered one of the promising APIs (active pharmaceutical ingredients) in gene therapy and genetic immunization. The growing demand for more efficient production of other ATMP (advanced therapy medical products), which require pDNA as a starting material, has also stimulated bioprocess development, it's in-process and product control.[1] There are two main steps in sample preparation prior pDNA analysis. First is pDNA isolation and the second is pDNA purification. There are various methods for pDNA isolation, however by far most widely used is alkaline lysis to isolate pDNA from cell culture. After isolation, purification steps are added to achieve higher purity and concentration of isolated pDNA. The aim of pDNA purification is to separate protein, RNA, and genomic DNA from the plasmid which is performed by different combinations of enzymatic degradation (RNase), filtration, centrifugation, and selective precipitation. New fast, efficient, and economically feasible methods are being developed to achieve higher purity of the sample and thus more accurate and precise results.[2]

Our aim was to compare different protocols for pDNA isolation and purification from *E. coli* cells, with the goal of obtaining accurate concentration of all isoforms of isolated pDNA. Since the sample preparation and size of the plasmid can affect the obtained quantity and quality of the plasmid, we tested two different sample preparation protocols using three different sizes of plasmid DNA. Agarose gel electrophoresis (AGE) and HPLC analysis on CIMac pDNA column were used to determine the concentration of plasmid and ratio of different plasmid isoforms.



***Scheme 1**: Isolation and purification of plasmid DNA from E. coli cells using two different sample preparation protocols. Three samples of biomass containing different sizes of plasmid were used. Isolation recovery was quantitatively and qualitatively evaluated by HPLC (CIMac pDNA) and AGE. Created with BioRender.*

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Plasters with the addition of coal with a new decorative value

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During the closure of coal regions across Europe, coal itself will fade into obscurity, even though it once served as the primary heating fuel for a significant portion of households. The attachment to coal and coal mines can still be felt today within the local communities where coal mines were or are located. As part of a student project, we presented coal in a new function and aimed to introduce it to younger generations in this way. The main goal of the project was to create plaster with the addition of coal as a modern and aesthetically appealing building material.

More than 17 different mixtures were prepared in which the properties of both fresh and hardened mixtures, as well as mineralogical characteristics, were tested. The recipes were based on volume proportions. Thus, the reference mixture consists of Ag:A:C=3:2:1. The aggregate (Ag) used was dolomitic aggregate with a fraction of 0/2, and the binding materials used were hydrated lime powder (A) and cement (C) CEM I 24.5N or white cement CEM I 52.5 R.

We used Late Triassic dolomite, whose mineral composition, according to the results of powder X-ray diffraction analysis (XRD), indicates that dolomite minerals make up approximately 97% of the rock, with calcite minerals accounting for about 3%. The bulk density is 2847 kg/m3, and the water absorption is 0.48%. The fraction of the aggregate used was 0/2. Lignite coal was used, which belongs to the younger coal category with a younger age, estimated to be around 2 million years based on the findings of plant remains and mammoth skeletons.The test results showed that coal affects the properties of both fresh and hardened mixtures.

Bulk density, porosity, and spread were determined for all fresh mixtures in accordance with standards (SIST EN 1015-6, SIST EN 1015-7:1999, SIST EN 1015-3:2001). The spread of mixtures on the shaking table averaged between 130 mm and 150 mm, with porosity around 5%. The bulk density of the reference mixture (without coal) was 2200 kg/m^3, while mixtures with coal had a lower bulk density, averaging around 2060 kg/m3.

During further sample processing (grinding), coal particles detached from the matrix. This issue was resolved by reinforcing the matrix, achieved by increasing the cement content, ultimately resulting in mixtures with a high cement content. Electron microscopy confirmed the weakened bond between coal particles and the cement matrix.

Despite all the challenges, we have prepared a mixture that can be used in practice as decorative plaster, enabling the development of its artistic potential.

[1]Abaqus. 2018. “Abaqus Manuals.” Dassoult Systems, Providence, RI.

Mechanochemical syntheses of several transition metal polycyanometallates

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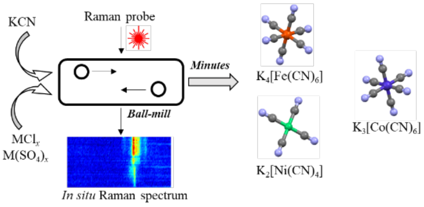
Cyanometallates are among the oldest coordination compounds known to be artificially produced, with mentions dating back to 1704. Due to their fundamental importance to chemical knowledge, a wide variety of polycyanometallates was synthetized thereafter. Moreover, many of them as well as their derivatives have shown interesting applicative properties. However, the synthesis of polycyanometallate complexes, namely their alkali-metal salts can be a hazardous chemical task, involving usage of excess of cyanide, high temperatures and overall lengthy synthesis procedures.[1]

In an attempt to simplify the synthesis of alkali-metal polycyanometallates, we have utilized mechanochemical synthesis.[2,3] In all cases, reactions were fast and in the case of $K_4[Fe(CN)_6]$ and $K_3[Co(CN)_6]$ highly selective. In the nickel system a new phase was observed among the obtained mixture of $Ni(CN)_2$ and $K_2[Ni(CN)_4]$ phases, while air-unstable $K_4[Mn(CN)_6]$ was obtained rapidly and easily under ambient conditions. To expand the knowledge of the solid-state reactivity of transition metal polycyanometallates, mechanochemical reactions were followed by *in situ* Raman spectroscopy (Scheme 1).



Scheme 1: *Raman spectroscopy for real-time and in situ monitoring of mechanochemical synthesis of some transition polycyanometallates.*

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Dispersion modeling of odor emissions from wastewater treatment plant

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Odor emissions from wastewater treatment plants (WWTP) are becoming a significant source of environmental nuisance and often result in complaints by the local population. In this work, the potential odor impact of a large WWTP in Slovakia was evaluated using dispersion modeling. The odor emissions from respective sources were calculated with Dutch emission factors,[1] considering the characteristics of the sewer system, area of the tanks and average pollution load. Consequently, the Gaussian dispersion model AERMOD was used to estimate the odor impact as 98-percentile and yearly average concentrations.

The calculation and modeling were performed for two scenarios – current and future situation. The future situation envisages the removal of sludge fields for waste from sewer cleaning; therefore, eliminating potentially large source of odor. By implementing this measure, the overall odor emission was reduced by 8,2 %. However, according to the odor dispersion, the odor impact as 98-percentile posed on nearby area remained almost constant. Additionally, the odor impact values significantly exceeded the Dutch odor limits and could potentially cause severe annoyance.[2] That suggests that further reduction measures should be applied to reduce the odor emissions and increase the quality of life of the local population.

This work represents a preliminary analysis of odor distribution at the WWTP and is expected to be followed by an on-site odor emission measurement to confirm the findings of this study.

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Transformations of pyrazolo[1,2-a]pyrazole derivatives

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The use of photochemical reactions in organic synthesis has gained popularity, but it often requires external photocatalysts because organic molecules have limited ability to absorb visible light.[1] These photocatalysts are mostly metal-based, which can be expensive and challenging to prepare, hindering their widespread use in industrial settings.[2] Additionally, the purification processes for recycling these catalysts are often laborious, posing environmental and economic concerns.[3] Consequently, there is a crucial need to develop new visible-light transformations that eliminate the reliance on external photocatalysts.

This study introduces innovative visible-light induced transformations of various pyrazolo[1,2-a]pyrazole derivatives without the need for external photocatalysts. These derivatives hold significant biological importance but have limited known photochemical transformations of their core structure.[2] By employing different reaction conditions, the pyrazolo[1,2-a]pyrazoles yield a diverse array of final products. Notably, the synthesis of products containing sterically hindered structures, which are conventionally challenging to obtain due to unfavorable entropic factors and transannular interactions, was successfully achieved. Our method demonstrates compatibility with various functional groups and does not depend on external photocatalysts, providing a cost-effective and environmentally friendly approach to synthesizing these potentially valuable compounds.

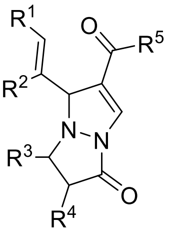

***Figure 1:** Starting pyrazolo[1,2-a]pyrazole derivatives.*

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[2]Petek, N., et al., Visible-Light Driven Selective C–N Bond Scission in anti-Bimane-Like Derivatives. *Org. Lett.* **2021**, 23, 5294–5298.

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Stability testing of Pt-nanoalloy electrocatalysts using high temperature accelerated degradation tests

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Proton exchange membrane fuel cells (PEMFCs) are one of the most promising technologies for establishing a carbon-neutral society. However, the biggest obstacle for their massive adoption is still unsolved electrocatalyst issues.[1] Here, high-temperature accelerated degradation tests (HT-ADTs) performed in an in-house designed high-temperature disc electrode (HT-DE) setup, enabling stability testing of Pt-nanoalloy electrocatalyst at the close-to-real operational conditions,[1,2] will be presented. The electrochemical properties are evaluated by measuring the ORR-polarisation curve and CO-electrooxidation cyclovoltammograms (CVs) in a typical thin-film rotating disc electrode (TF-RDE) setup. On the other hand, HT-ADTs, performed in the HT-DE setup, consist of several thousand cycles in a specific potential window. This allows determination of difference of electrochemically active surface area as well as specific activity of the electrocatalyst before and after ADT.[1,2]

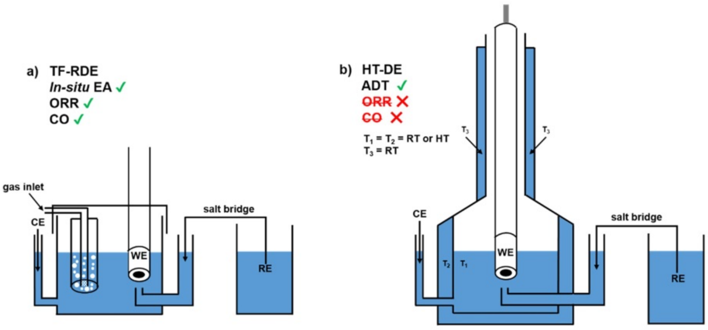

Figure 1: *a) TF-RDE setup b) HT-DE setup.1,2.*

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Natural Disinfection: The Promise of Essential Oils

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Essential oils are highly aromatic compounds extracted from plants that have a strong scent.[1] In this study, we extracted essential oils from three different plant species – rosemary, lavender, and sweet wormwood - from the NE and SW regions of Slovenia. We also extracted essential oil from rosemary grown in coastal areas. The extracted oils were characterized using infrared spectroscopy. To evaluate their biological activity, we used a modified version of the Kirby-Bauer disc diffusion method. Our results showed that the composition of the essential oils varied depending on the region where the plants were grown and that the isolated essential oils had an inhibitory effect on the growth of certain bacteria, even better than five commercial hand sanitizers tested (Fig 1). This study highlights the importance of considering the geographical location of plants when extracting essential oils, as it can impact their composition and biological activity.

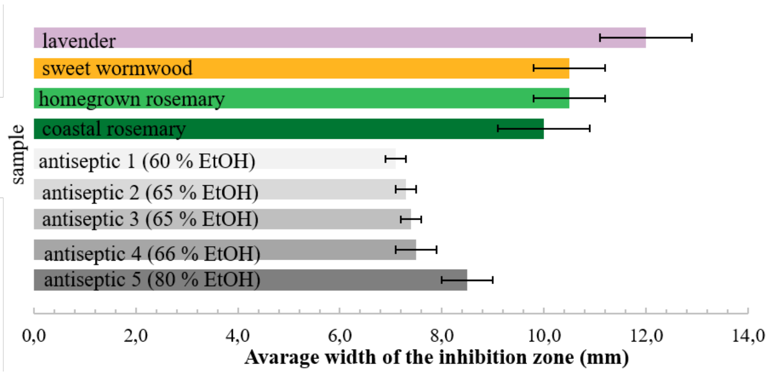

Figure 1: *Comparison between five hand sanitizers and lavender oil.*

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Characterisation of hydrogels based on cellulose derivatives

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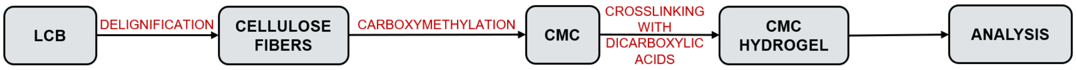
Hydrogels are three-dimensional macromolecular networks capable of absorbing and releasing large amounts of water in a reversible manner in response to certain environmental stimuli.[1] They can be divided into those made of natural polymers and those made of synthetic polymers. Among the main natural hydrogels, cellulose-based hydrogels are very popular because they are made from lignocellulosic biomass (LCB). Cellulose is a material that is difficult to modify. Therefore, cellulose derivatives such as carboxymethylcellulose (CMC), hydroxyethylcellulose, and hydroxypropylcellulose are usually used as starting materials for cellulose-based materials.[2] In the preparation of hydrogels, the linear cellulose polymer chains need to be crosslinked, and dicarboxylic acids are interesting crosslinkers. Less commonly used crosslinking reagents include divinyl sulfone and epichlorohydrin. Determining the structure of cellulose-based hydrogels and where the cellulose chains are bound is a difficult task because of their insolubility. Solid-state NMR spectroscopy is an interesting tool for structure determination and would allow estimation of the fraction of cross-linked and free functional groups,[3] the degree of cross-linking and the degree of modification of cellulose fibers.

In our study, we focus on the use of dicarboxylic acids to crosslink carboxymethylcellulose with the aim of developing hydrogels. The hydrogels were prepared using citric acid as crosslinking agent and varying the degree of crosslinking. We will present the results of the study on the absorption properties of cellulose-based hydrogels by thermal analysis and determination of structural properties by NMR spectroscopy (Scheme 1).



***Scheme 2:** Path from cellulose to cellulose-based hydrogels and determination of their properties.*

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Fluorescence-enabled glycan analysis: HPLC method with solid-phase extraction for robust characterization

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Glycans play crucial roles in various biological processes, including cell signaling, immune response, and protein functionality. Their structural diversity and complexity make their analysis challenging yet essential for understanding their functional implications in biology. Due to their natural lack of light-emitting properties, derivatization with fluorophores is necessary to enable their detection and analysis. Fluorescence detection offers several advantages in glycan analysis, including enhanced sensitivity and the ability to detect low concentrations of analytes. In this study, we aim to develop an analytical HPLC method for glycans with fluorescence detection, enabling efficient characterization and quantification of these biomolecules. Additionally, we employ the principles of Quality by Design (QbD) to ensure robustness and reliability in the analytical method development process[1].

The application of QbD principles in analytical method development allows for a systematic and comprehensive approach to achieve desired analytical performance. The QbD framework enables a proactive approach to method development, encompassing risk assessment, experimental design, and multivariate analysis. This approach ensures method robustness, minimizes variability, and enhances method understanding, ultimately leading to reliable and reproducible glycan analysis[2].

In the laboratory, we employed solid-phase extraction (SPE) techniques to clean up and enrich the glycan samples, eliminating interfering substances and reducing matrix effects. By carefully selecting appropriate SPE sorbents and optimizing extraction conditions, we achieved efficient removal of excess fluorescence marker used for detection. This step is crucial as high levels of fluorescence background can compromise the sensitivity and accuracy of glycan quantification. Furthermore, we implemented the QbD principles throughout the entire method development process, enabling a thorough characterization of critical method parameters, risk assessment, and identification of critical process parameters (CPPs) and critical quality attributes (CQAs).

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Unexpected protein complex formation during recombinant expression of stem bromelain in Escherichia coli

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Stem bromelain, a cysteine protease with a molecular weight of 22.3 k_Da, is predominantly found in the stems of the pineapple plant (*Ananas comosus*), and it has recently attracted considerable attention due to its diverse biotechnological applications.[1,2] Bromelain is currently the subject of active research as a promising candidate for the treatment of gastric and colorectal cancer, as it showcases potent anti-inflammatory properties and demonstrates the remarkable capability to cross the intestinal membrane without degradation, while retaining its biological properties.[3] In our study, we aimed to express and purify the recombinant stem bromelain protein using modified *Escherichia coli* bacterial cells. We achieved high-level expression using an *E. coli* expression system, the resultant protein mixture was then purified using glutathione S-transferase affinity chromatography. When the purified fraction was analyzed by size exclusion chromatography (SEC), we were surprised to find that in addition to the expected molecular weight for bromelain pro-peptide (38 kDa), a large fraction with molecular weight of over 669 kDa was observed (Fig. 1). The result suggests that an unexpected complex formation occurred in the process. Further studies are needed to unravel the nature of the co-purified protein complex and to elucidate the factors responsible for the co-purification with the target protein.

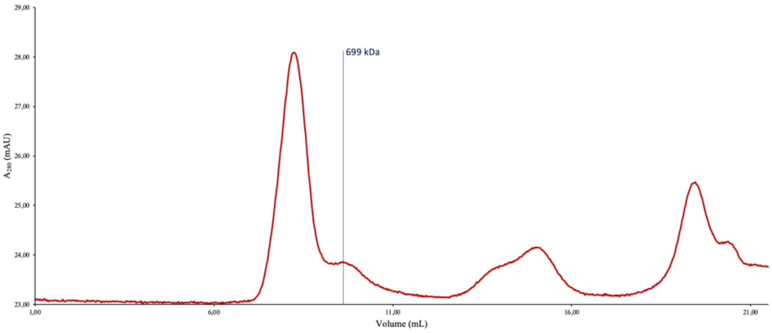

***Figure 1:** Size exclusion chromatogram obtained by utilizing Superdex 200 Increase 10/300 GL.*

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Design and Characterization of Novel Fluorescent Probes for Imaging of Amyloid β Plaques in Alzheimer's Disease

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Fluorescent dyes play an important role in the optical vizualization of amyloid β (Aβ) plaques, which are a major feature of Alzheimer's disease (AD).[1,2] In this research, a series of new fluorescent probes were synthesized to investigate their structure, optical properties, and binding affinity to Aβ. The probes were designed using central π-system scaffolds with electron-donating (EDG) and electron-withdrawing groups (EWG) serving as end caps. By incorporating different functional groups, we were able to tweak the optical properties and binding affinity to Aβ *in vitro*, *in cellulo* and on brain slices from deceased AD patients (see Figure 1). The probes showed selective binding to Aβ fibrils, and their interactions with Aβ were proposed by docking studies and molecular dynamics simulations. These results provide valuable insight into the potential use of these probes as diagnostic tools for AD.

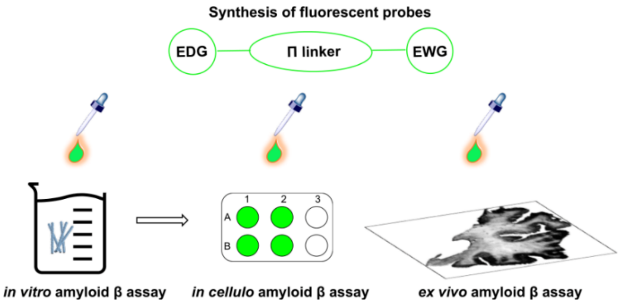

Figure 1: *Simplified structure of fluorescent probes together with executed biochemical assays.*

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Antimicrobial activity of spider webs

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The scope of our research was the antimicrobial properties of spider webs and whether spider silk, in combination with LB, M9, and FR, is suitable substrate for microbial growth. There are 50.356 species of spiders in the world, each synthesizing their webs with different building blocks that thrive in different environments. Silk is produced in the spinning glands and ducts. Spiders have three pairs of spinning glands that can (but not necessarily) move independently of the back pair of legs. Each gland is connected to one spinning duct through a special canal. Sticky substances (used to catch prey) are attached to the duct and are then pulled out by the spider's own weight. Spider silk is made up of proteins that contain many nonpolar and hydrophobic amino acids and no tryptophan. If the C and N ends didn't bond, microbes wouldn't be able to cling to spider webs. Consequently, the web would not be maintained and repaired. Different microorganisms are found on spider webs, each utilizing their habitat in different ecological niches. Through the process of collecting spider silk webs and isolating them on different growth media and DNK extractions, we have discovered that various microorganisms do live on spider webs.

" Spider eggs consist of energy-rich molecules and water, which makes them an ideal substrate for pathogenic and non-pathogenic microorganisms, which is why spiders deposit them in a silk sheath to protect them from chemical and mechanical influences from the environment. Since silk is mainly composed of protein and small amounts of carbohydrates in the form of glycosylated proteins in the thin outer shells, it is hypothesized that bacteria and fungi can use it as a source of nutrients. It is assumed that spiders deposit antimicrobial molecules on the silk, which act as protection for eggs and captured prey from pathogenic organisms."

“The key conclusions of our research is that the most microorganisms grew on the LB culture medium, because this culture medium also contains the most nutrients and the least number of them grew on the FR culture medium, which is also expected, since it is the culture medium with the fewest nutrients. Since the least number of microorganisms grew on the FR medium, we could assume, that the spider web is a similar substrate to the FR medium.”

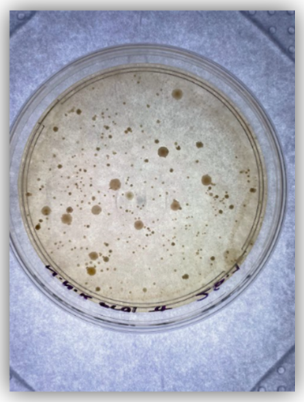

Figure 1: Luria–Bertani medium with different type of colonies.

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Formation and characterization of S. epidermidis biofilm in silicone tubular bioreactor

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According to the National Institutes of Health, up to 80 % of microbial infections are due to biofilm formation, with catheter associated urinary tract infections being among the most common hospital-acquired infections.[1] Bacterial biofilms are complex structures of bacteria connected by a self-produced polymeric matrix (EPS), mainly composed of polysaccharides, secreted proteins, and extracellular DNAs.[2] Within the biofilm, bacteria adapt to harsh living conditions by reducing their metabolism and altering their gene expression, resulting in biofilm infections that are usually chronic and impervious to both the immune system and antibiotics. To study biofilm formation in silicone catheters, *Staphylococcus epidermidis* bacteria were used, grown in a continuously operating mixing - tubular bioreactor system[3] under defined conditions, at constant temperature, linear velocity, and bacterial physiological state during supply, determined by chemostat dilution rate.

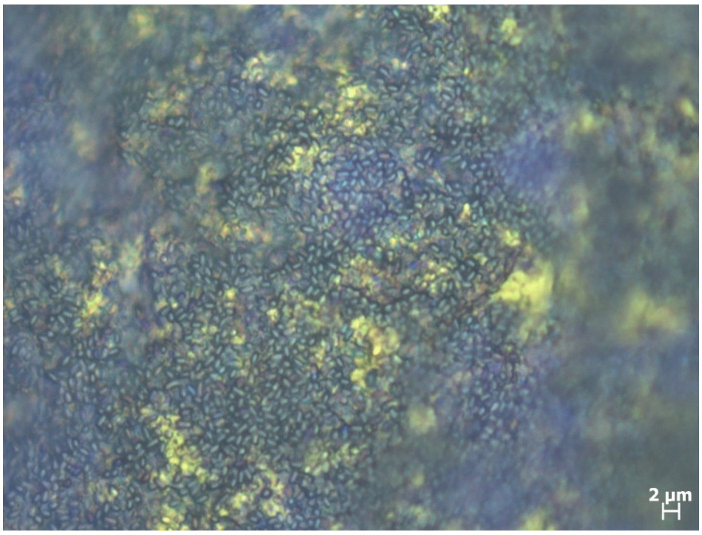

***Figure 1**: Bacterial biofilm formation on silicone tubular bioreactor after 24 h of continuous SM buffer flow, with crystal violet staining.*

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How sizable can dipolar interactions be in crystal structures?

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Interactions between permanent molecular dipoles are among the important intermolecular interactions. Due to their long range, dipolar interactions in crystal structures can be much stronger than the interaction between two standalone dipoles. Depending on the mutual orientation of dipoles, dipolar interaction can be repulsive or attractive. With the aid of the point-dipole approximation,[1] we evaluated dipole–dipole interactions for various model periodic structures, ranging from ordered 1D chains of dipoles to 2D planar and 3D rearrangements of dipoles. We show that for such periodic dipole arrangements, dipolar interactions can be up to about ten times stronger than between two standalone dipoles (Fig. 1). This implies that for an adequate estimation of dipolar interactions in crystal structures, the use of periodic-boundary conditions is necessary.

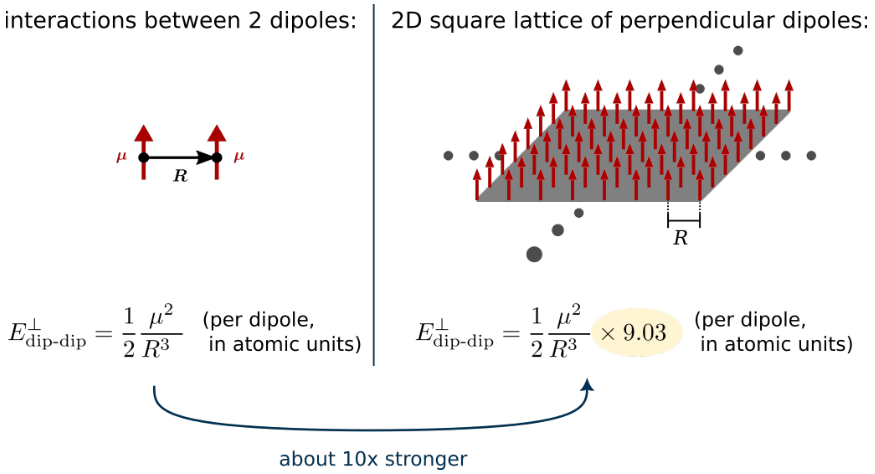

Figure 1: *Left: two point-dipoles oriented perpendicular to the connecting vector* **R**. *Right: a square lattice of point-dipoles oriented perpendicular to a 2D plane. For the square lattice of dipoles, dipolar interactions are about ten times stronger than between two standalone dipoles.*

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Can Venous Thrombosis be Diagnosed by Anyone?

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[2]LKH Südsteiermark - Standort Wagna, Pelzmannstraße 18, AT-8435 Wagna, Austria
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Ultrasound is used to diagnose venous thrombosis in compression ultrasonography, in which the examiner presses on the vein with a probe (Fig. 1). The examiner diagnoses venous thrombosis if he fails to completely close the vein. However, if he cannot flatten it even though there is no clot in it, he may make a false positive diagnosis.[1]

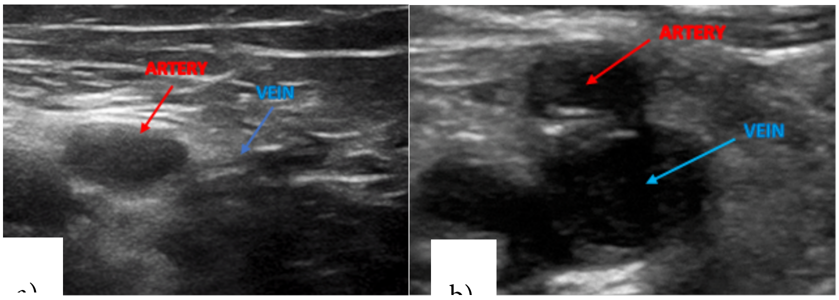

Figure 1: *a) No venous thrombosis, b) Venous thrombosis is present.*

In clinical practice, one of the causes of a false-positive diagnosis is insufficient pressure on the vein with the ultrasound probe. We investigated the extent to which upgrading the ultrasound probe with a dynamometer that measures the pressure applied by the probe to the vein would reduce the effects of inadequate force application. We designed an experiment in which we compared the correctness of the procedure of two groups of investigators. The first group used a conventional ultrasound probe, whereas the second group used a probe that was upgraded with a dynamometer. It had been previously calibrated to the force required for complete closure of the vein. The results show that upgrading the ultrasound probe significantly improves the correctness of the procedure. In addition, we monitored the geometry of the deformed vessels during the compression process by processing the ultrasound images and found that the ratio of the degree of flattening of the artery and vein was an important indicator of the correctness of the execution. By analysing a larger population of healthy and sick individuals, we could determine the characteristic range of vascular pressure response for both groups.

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Synthesis and catalytic efficiency of organocatalysts based on (1R,2R)-(piperidin-1-yl)cyclohexane-1-amine scaffold

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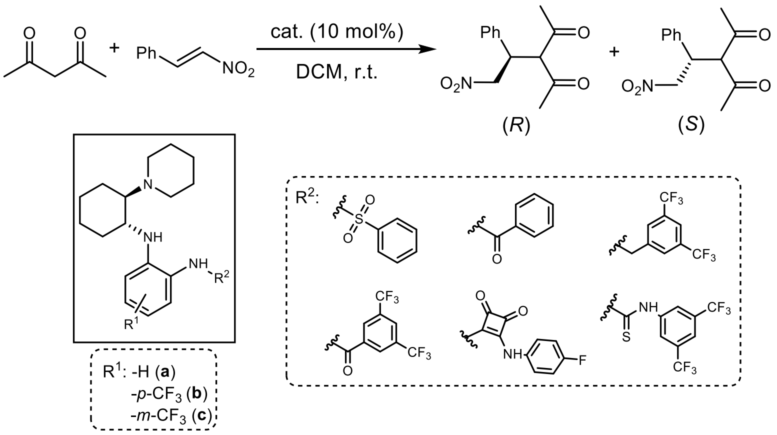
Over the past decade, the application of small chiral organic molecules as catalysts in enantioselective reactions has brought a significant breakthrough in the field of asymmetric catalysis.[1] The most intriguing catalysts to synthesize and observe are bifunctional H-bond noncovalent organocatalysts, due to their unique activation of substrates. While significant research efforts have focused on organocatalysts featuring thiourea and (thio)squaramide as double hydrogen bond donors, the exploration of diverse and novel hydrogen bond donors in organocatalysis remains relatively limited.[2] We therefore prepared new chiral H-bond donor bifunctional organocatalysts based on (1*R*,2*R*)-(piperidin-1-yl)cyclohexane-1-amine scaffold. Subsequently, these organocatalysts were employed in a model Michael addition of acetyacetone to *trans*-β-nitrosyrene (Scheme 1).[3] The catalytic activity of these newly prepared organocatalysts exhibited moderate enantioselectivity (18 examples, *ee* up to 58%).



Scheme 1: *Organocatalyzed Michael addition with the novel 1,2-benzenediamine organocatalysts.*

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Molecular cloning and preparation of the paraspeckle protein HNRNPK in Escherichia coli

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Paraspeckles are nuclear membraneless organelles (Fig. 1). They consist of long non-coding RNA (lncRNA) and various RNA-binding proteins such as splicing factor proline and glutamine rich (SFPQ) and Non-POU domain containing octamer binding protein (NONO). They form around the lncRNA NEAT1 (nuclear paraspeckle assembly transcript 1). Heterogeneous nuclear ribonucleoprotein K (HNRNPK) is an RNA-binding protein located in the nucleus. It enables alternative 3'-end processing of NEAT1, leading to the formation of the NEAT1_2 isoform, which is essential for paraspeckle formation.[1] The role of cellular paraspeckles is to regulate gene expression during differentiation, viral infections, and stress responses. Increased abundance of these nuclear organelles in neurons is characteristic of amyotrophic lateral sclerosis.[2] Our research focuses on the study of paraspeckle formation *in vitro*. To this end, we incorporated the HNRNPK and HNRNPK-NeonGreen sequences into a bacterial expression vector using Gibson assembly. We successfully expressed both HNRNPK constructs in *E. coli* and determined the optimal conditions for expression that can be used for larger-scale production of HNRNPK.

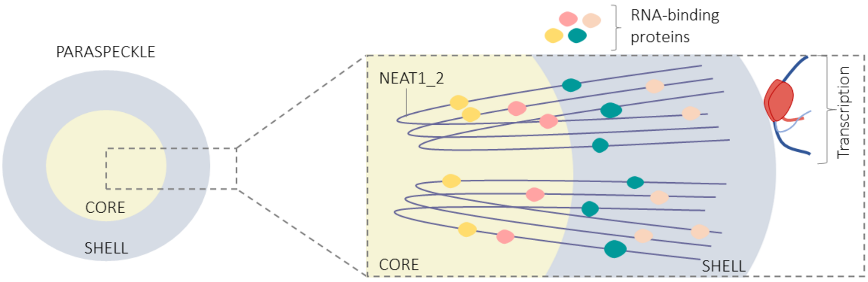

Figure 2: *Representation of the internal structure of the paraspeckle.*

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Photoredox Arylations of Bicyclic Heteroaryl Diazonium Tetrafluoroborates

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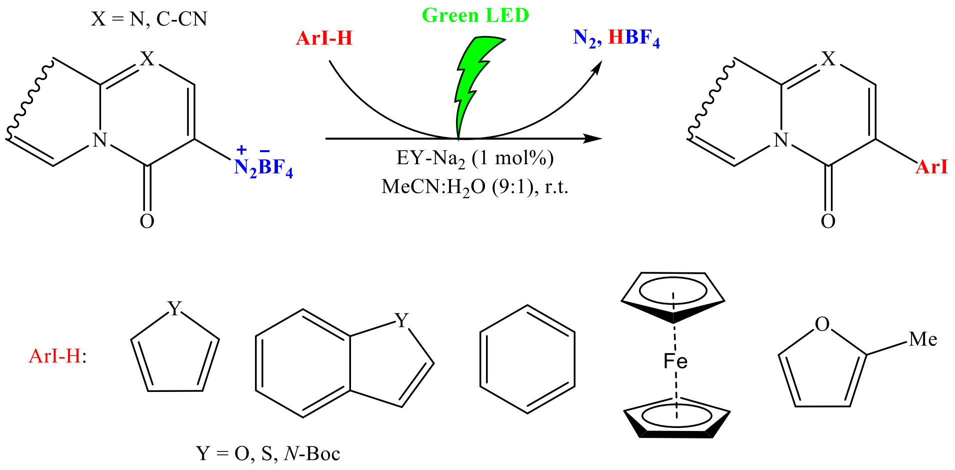
Following the procedures from the literature,[1,2] three title diazonium tetrafluoroborates containing bridgehead nitrogen atom were prepared. Inspired by previous work by König,[3] 4-oxo-4*H*-quinolizine-3-, 4-oxo-4*H*-pyrido[1,2-*a*]pyrimidine-3- and 5-oxo-5*H*-thiazolo[3,2-*a*]pyrimidine-6-diazonium salts were coupled with various (hetero)arenes under photoredox conditions. Reactions were performed at room temperature under green LED irradiation in the mixture of acetonitrile and water in the presence of photocatalyst eosin Y disodium salt (Scheme 1). Solvent mixture of acetonitrile and water enabled easy isolation of target compounds by column chromatography in moderate yields up to 63 %. Arylations also led to the first examples of ferrocenyl-substituted quinolizinone and azaquinolizinone-derivatives. Therefore, this method has broad substrate scope, furnishing 3- and 6-(hetero)aryl-substituted products with facile workup and represents metal-free alternative for the synthesis of target compounds.



Scheme 1: *Photoredox C-H arylations of title diazonium tetrafluoroborates.*

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Assessing the application of open-source data in determining environmental health risks

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Environmental pollution is responsible for approximately 9 million deaths per year, making it the world's largest environmental risk factor for disease and premature death1. In the frame of the Integrative Data Analysis for Healthy Society (IDA4Health) project, we searched for open-source urban environment and human health datasets to obtain data for analysing complex relationships between environmental factors and human health. We reviewed national and international databases (e.g. NIJZ, SURS, EUROSTAT, WHO) as well as crowdsourced databases such as Sensor.Community. Furthermore, we implemented a computational framework2 that collects and stores selected data using the Nomenclature of Territorial Units for Statistics (NUTS)3 classification system for regions. While some data was already available in the NUTS data format, others had to be preprocessed or approximated to align with a specific region. However, the architecture of the system is not reliant on the NUTS data format itself and can be used with various other data formats. Moreover, the framework integrates data within a machine learning and inference pipeline. This is achieved through a combination of statistical analysis techniques, such as linear regression analysis, correlation matrix analysis and calculation of correlation coefficients (Fig. 1). The framework can be further applied to an arbitrary location with available datasets. Finally, a pilot app was developed as a user interface to showcase our solution.

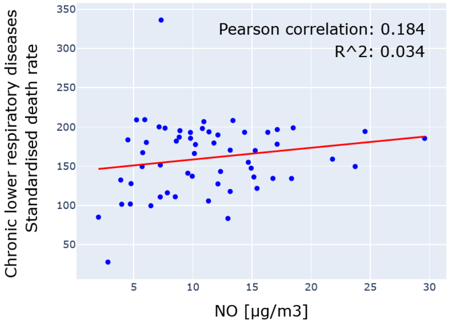

***Figure 1**: Example of a plot from the inference framework: correlation of nitric oxide (NO) with a standardised mortality rate of chronic lower respiratory disease. R^2 = coefficient of determination.*

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[3]Eurostat, Nomenclature of territorial units for statistics. *Eurostat*; Luxembourg, 1995.

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LCA Environmental impact assessment of a hamburger and soda

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As we become more aware of the impact of our food choices on the environment, it is important to understand how certain foods affect our planet. In this research, we analysed and compared the environmental impacts of beef and vegetarian hamburgers. We also carried out a comparison of a carbonated beverage and water using the method of Life Cycle Assessment (LCA), which was made possible by the OpenLCA computer program.

LCA is defined as the compilation and evaluation of the inputs, outputs and potential environmental impacts of a product system throughout its life cycle. The analysis covers processes from raw material extraction through material processing, production, distribution, use, repair and maintenance, to eventual disposal or recovery.[1] To start our assessment we collected all the needed data for the analysis, which was then put into the OpenLCA computer program, an open-source software, designed to make life cycle assessment calculations faster, simpler and more accurate.[2] After the calculations, the software presented us with graphs and tables, which were used to draw our conclusions of the study.

We have found that the most environmentally friendly product is a vegetarian burger, which is produced from local raw materials. The task has met our expectations and contributes to efforts to reduce negative environmental impacts.

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Risk evaluation and the ergonomic aspect of the restorer profession

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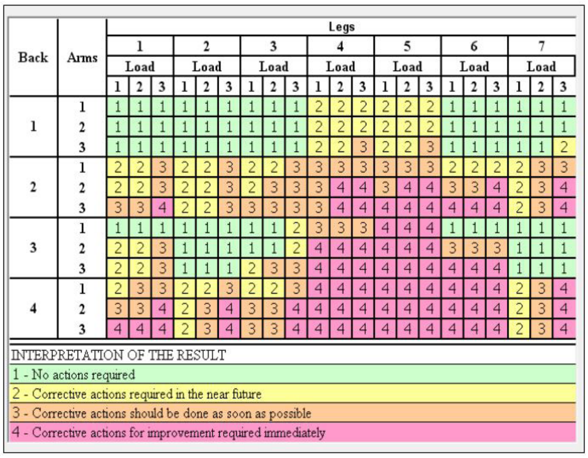
Providing a suitable working environment is considered one of the most important obligations of an employer. Workers may be exposed to a variety of factors in the course of their work that may affect their health in different ways.[1] We tend to focus on occupations that are dynamic in nature and, as a result, often neglect occupations that can be just as physically and mentally demanding but less dynamic. An example of such a profession is that of a restorer. I set myself the task of assessing the restoration profession in terms of exposure to various risks resulting from adverse factors in the workplace.[2] Differences in the risk evaluation can be caused due to the materials being the object of restauration and thus the work equipment that in being used.[3] In addition, I evaluated the profession from an ergonomic point of view by using the OWAS method and thus determined the strain caused by non-physiological posture. For an easier evaluation of the results, I helped myself with the use of the OWAS table shown in Table 1.

***Table 1**: Interpretation of OWAS method results.*



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4	1	2	3	3	2	2	3	2	2	3	4	4	4	4	4	4	4	4	4	2	3	4
	2	3	3	4	2	3	4	3	3	4	4	4	4	4	4	4	4	4	4	2	3	4
	3	4	4	4	2	3	4	3	3	4	4	4	4	4	4	4	4	4	4	2	3	4

INTERPRETATION OF THE RESULT
1 - No actions required
2 - Corrective actions required in the near future
3 - Corrective actions should be done as soon as possible
4 - Corrective actions for improvement required immediately

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Effect of monocarboxylic acids on properties of metal-organic frameworks

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Metal-organic frameworks (MOFs) are hybrid materials that can be used in a variety of ways because of their appealing properties.[1] We explored the influence of different monocarboxylic acid additives on the synthesis of one specific bioMOF.[2] We discovered that using different acid additives leads to efficient manipulation of the crystal size of these materials in alignment with Regime II.[3] Our conclusions demonstrate that the researched materials have a potential use in the biomedical field, especially because of their permanent microporosity and role as surface capping agents and modulators. In the end, we also confirmed that NO sorption is possible when it comes to these materials (Figure 3).

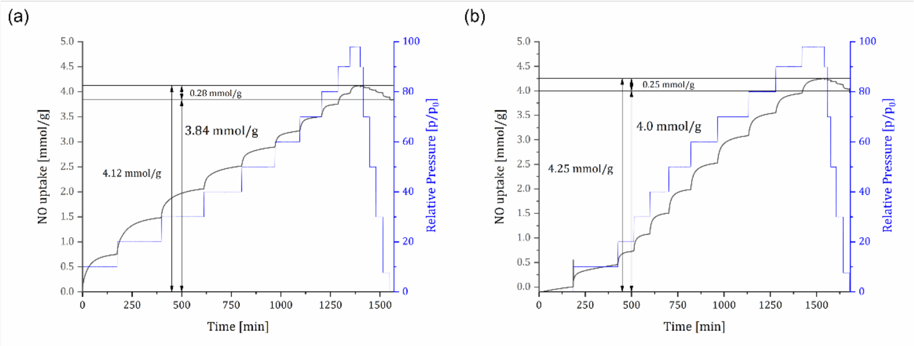

Figure 3: *NO sorption kinetics profile of analysed materials ((A) bioNICS1-MW-2h and (B) bioNICS1-PA-6-2h). The figure shows physiosorbed and chemisorbed NO and the NO that remained.*

[1] Horcajada, P.; Gref, R.; Baati, T.; Allan, P. K.; Maurin, G.; Couvreur, P.; Férey, G.; Morris, R. E.; Serre, C. Metal-Organic Frameworks in Biomedicine. *Chem. Rev.* **2012**, 112 (2), 1232–1268.
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Modulating gene expression via fusion of Rpd3 with dCas9

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Transcriptional regulation in eukaryotes is strongly influenced by post-translational modifications of histones, specifically by acetylation and deacetylation. Hyperacetylation leads to increased expression of specific genes, while hypoacetylation, achieved through deacetylation by histone deacetylases such as Rpd3, causes the expression of the corresponding genes to decrease.[1]

Acetyl-CoA is one of the key intermediates in cellular metabolism. Therefore, the genes involved in acetyl-CoA biosynthesis and transport are expected to be highly expressed under most growth conditions.[2] Our goal was to demonstrate that by fusing Rpd3 histone deacetylase to dCas9 protein, we can target specific genes involved in acetyl-CoA-associated pathways, and down-regulate their expression by binding dCas9-Rpd3 to a sequence around 100bp upstream of their transcription start sites. The effects of the presence of Rpd3 deacetylase in the vicinity of the corresponding histones on the expression of the target genes and associated phenotypic effects will be presented.

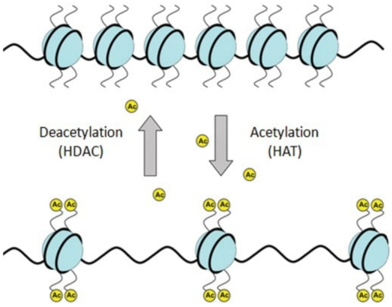

Figure 1: *Histone acetylation and deacetylation. HDAC, histone deacetylase; HAT, histone acetylase.*[3]

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Asymmetric phase transfer bifunctional catalysts based on camphor

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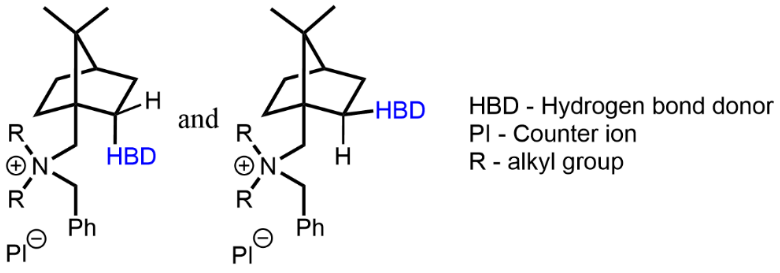
Various chiral bases are used in the synthesis of asymmetric bifunctional organocatalysts. Among them, cinchona alkaloid derivatives are commonly used, while camphor amine derivatives are a promising alternative to these established bases.[1] Camphor, which has a naturally occurring chiral and rigid structure, is available in both enantiomeric forms. In the field of asymmetric bifunctional catalysis, camphor-squaramide type catalysts have already shown favorable results in the 1,4-addition of 1,3-dicarbonyl compounds to *trans*-β-nitrostyrene.[2] Camphor type catalysts have not yet been used as asymmetric phase transfer bifunctional catalysts. Asymmetric phase transfer catalysis serves as an alternative activation model for reactions in heterogeneous reaction mixtures.[3]

In this study, a new class of bifunctional catalysts was developed from camphor. These catalysts were synthesized in eight steps, resulting in a modest overall yield. The synthetic route allows the preparation of structurally distinct catalysts with the potential to tune electron steric effects. In addition, both pseudo-enantiomeric catalysts are readily accessible. Our bifunctional camphor-based organocatalysts were tested in various asymmetric reactions and gave promising results.



Scheme 1: *Camphor-based phase transfer catalysts.*

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[2] Ričko S.; Svete, J.; Štefane B.; Perdih, A.; Golobič, A.; Meden, A.; Grošelj U. 1,3-Diamine-Derived Bifunctional Organocatalyst Prepared from Camphor. *Adv. Synth. Catal.* **2016** 358, 3786–3798.

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Immobilised and Recyclable Catalysts for Sustainable Deuterium Labelling of Organic Compounds

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Deuterium (D)-labelled organic compounds can be used in a wide range of applications. These include, for example: therapeutic treatment, drug discovery, mechanistic studies, and organic electronic materials.[1] Catalysts consisting of precious metals such as Ir, Pd and Pt are commonly used for their ability to facilitate selective and mild synthesis.[2] However, reliance on costly precious metal catalysts presents sustainability challenges, while recovering homogeneous small-molecule catalysts containing these metals from reactions is difficult and costly. Immobilisation of homogeneous catalysts is one approach to overcoming these obstacles. For example, the immobilisation of catalysts offers increased stability (partially through restrained aggregation), reduced metal contamination, more facile catalyst recovery, and reusability.[3] This aligns with Circular Chemistry principles, emphasising catalyst cyclic reuse and reducing the environmental impact of organic compound synthesis.[4]

Therefore, our ongoing research aims to investigate various approaches for the development of immobilised recoverable and recyclable catalysts for the synthesis of D-labelled organic compounds based on existing catalyst frameworks (Figure 1). Our presentation will offer an overview of preliminary findings, highlighting their potential implications and advancements.

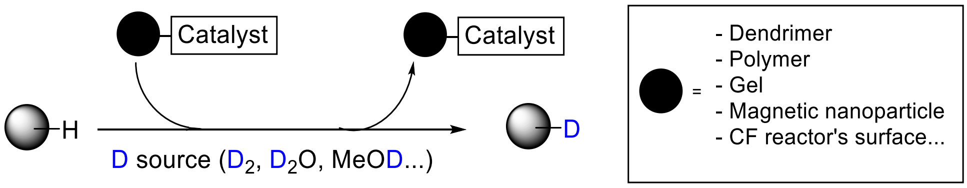

Figure 4: *General scheme for H/D exchange with immobilised catalysts.*

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[4]Keijer, T.; Bakker, V.; Slootweg, J.C. Circular chemistry to enable a circular economy. *Nat. Chem.* **2019**, 11 (3), 190–195.

Advantages and disadvantages of Food Supplements

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Dietary supplements have become an important topic in today's times, encountered almost everywhere. You can find more than 4.000 different food supplements on Slovene market.[1] They are not only promoted on television but are also written about in newspapers, and advertisements showcasing their effectiveness can be found online. Are dietary supplements truly as useful and harmless as advertisers claim, or are they just useless products that can even harm one's health in extreme cases?

In my assignment, I investigated what dietary supplements are, their significance, the legislation in this field, the categorization of dietary supplements, and the justification for their use. I posed the question of whether dietary supplements are necessary and when they are desirable, whether they are entirely unnecessary, and when they can be potentially dangerous. I gathered a significant amount of evidence supporting the use of dietary supplements, as well as examples demonstrating their potential harm associated with improper use, the use of counterfeit dietary supplements, and allergies to individual ingredients. After researching the use of dietary supplements worldwide and in Slovenia, I was also interested in the use of dietary supplements among high school students. I conducted a survey that I distributed to high school students. In the survey, I asked students about their personal experiences and awareness of dietary supplements, their opinions on dietary supplements, and their knowledge of them. I found that students could be more informed about dietary supplements, which would ensure their correct and safe use to a greater extent. Around the world, the consumption of dietary supplements has become almost a part of everyday life, and according to the expectations and forecasts of the American institute Future Market Insights, their sales are expected to double in the next 10 years. Already, every other person has consumed dietary supplements in the last month. The growth of the global dietary supplements market is increasing, primarily due to the growing health awareness among users. Usage varies from 39% to 71%, with older individuals consuming significantly more dietary supplements than younger ones. Approximately 39% of adults aged 19 to 30 consume dietary supplements, 49% of adults in the age group of 31 to 50, 65% among those aged 51 to 70, and a whopping 71% among those older than 70.[2] I found that dietary supplements themselves are generally not dangerous, but there are instances where complications can arise, which can be prevented with proper awareness, accurate information, and dietary supplements from reliable sources.

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Sustainable approach to wastewater management at KIMI company

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For many years, KIMI has embraced sustainable development and actively contributed to building a greener future. KIMI's core values have been also demonstrated through the Ecolabel product line for many years, as we aim to encourage environmental responsibility and economic viability within the company's operations and the broader community.

In accordance with the current trends and best practices in the field of industrial wastewater treatment,[1] we report the KIMI's path towards the optimization of the quantity and quality of wastewater, that also considers enhancing the economic efficiency of the process. We analysed the past data, which needs to be statistically organized in order to compare past data with improvements provided by new system, with a specific emphasis on the volume of water dedicated to circular economy practices.

One of the key improvements in the wastewater management system is the implementation of a novel electronically controlled CIP (Cleaning In Place) system for reactors cleaning, which enables us to optimize cleaning times and flows, resulting in potential reductions in water consumption and significant improvements in cleaning efficiency. Our aim is to propose an optimal solution that strikes the right balance between wastewater quantity and pollution levels.

Another aspect of our study involves evaluating the feasibility of investing in an additional treatment facility to reduce the pollutant load (COD and surfactants) of wastewater.[2,3] Furthermore, we explore the potential application of rainwater in the cleaning process, considering its environmental benefits.

Throughout the research, we considered all stakeholders involved in the comprehensive wastewater treatment process. This includes KIMI company, and its technology cleaning processes as well as the public water supply system with a focus on the price and volume of process water. Additionally, we considered the requirements and costs associated with the central wastewater treatment plant Domžale-Kamnik and environmental requirements of the Ministry of Natural Resources and Spatial Planning (Slovenia).

[1]Dutta, D.; Arya, S.; Kumar, S., Industrial wastewater treatment: Current trends, bottlenecks, and best practices. *Chemosphere* **2021**, *285*, 131245.
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[3]Mao, G.; Han, Y.; Liu, X., Technology status and trends of industrial wastewater treatment. *Chemosphere* **2022**, *288*, 132483.

From Controlling Selectivity in Iodination of Phenols to Transition-Metal-Free Coupling Reaction

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Iodophenols are versatile compounds with diverse applications ranging from drugs, radioactive markers, and intermediates in synthetic organic chemistry. A selective, robust, and operationally simple introduction of iodine atom(s) to phenols is desirable, while modern methods rely on the oxidative iodination strategy.[1] Herein, we present a study on the selectivity of mono- and diiodination of phenols utilizing $I_2/H_2O_2/H_2SO_4$ iodination system. We extended our method to selective synthesis of biologically interesting mono- and diiodophenols, i.e., tyrosine derivatives. Formation of formal ortho-phenolic homocoupling side-product was observed during iodination of model substrates. Gratifyingly, employing basic conditions with autocatalytic I_2 allowed us to exploit this side-reaction and convert iodophenols to the respective $C(sp^2)–C(sp^2)$ homocoupling products in the absence of metals. The formed biaryl axis scaffold is present in numerous natural products and chiral organic ligands.[2] Mechanistic investigations support a radical mechanism via a formal homolytic cleavage of the $C(sp^2)–I$ bond in the key step of the mechanism.

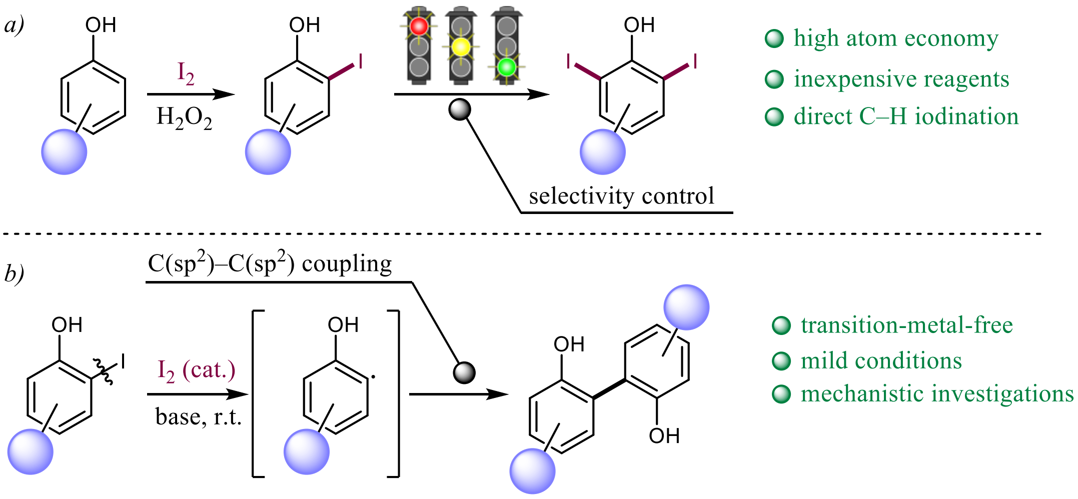

Figure 1: *a) Selective iodination of phenols. b) Radical C(sp2)–C(sp2) coupling of iodophenols.*

[1] Podgoršek, A.; Eissen, M.; Fleckenstein, J.; Stavber, S.; Zupan, M.; Iskra, J. Selective Aerobic Oxidative Dibromination of Alkenes with Aqueous HBr and Sodium Nitrite as a Catalyst. *Green Chem.* **2009**, 11 (1), 120–12.

[2] Yuan, S.; Chang, J.; Yu, B. Construction of Biologically Important Biaryl Scaffolds through Direct C–H Bond Activation: Advances and Prospects. *Top. Curr. Chem.* **2020**, 378 (2), 23.

Designed sensors of viral activity based on re-engineered innate immunity components

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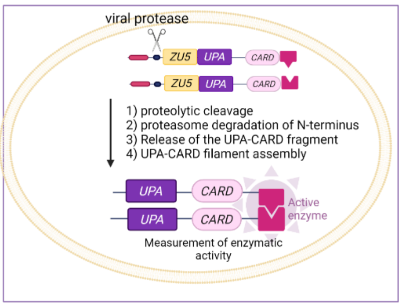
The COVID-19 pandemic demonstrated that innovative ways of virus detection are needed such as the development of novel biosensors. The traditional methods for detecting viruses require time and can fail to detect mutated viruses, biosensors present a way to create robust alternatives. One of the natural viral detection systems is the caspase recruitment domain family member 8 (CARD8) inflammasome.[1] Our study aimed to develop a viral detection sensor by rewiring the CARD8 receptor using synthetic biology approaches. Using molecular cloning, confocal microscopy, and cell culture techniques, we designed and tested a biosensor comprised of the sensor component (modified CARD8) and the enzymatic component (split-protein system). The sensor was transfected into the HEK293T cells and following the proteolytic cleavage, the CARD8 oligomerized and lead to the reconstruction of the split protein, allowing us to measure its activity. For the first sensor, CARD8 was fused to split beta-lactamase (CARD8-TEV-splitBetaLac) and in the second case, CARD8 was fused to split luciferase (CARD8-TEV-splitLuc). While the CARD8-TEV-splitBetaLac did not detect viral protease activity, the CARD8-TEV-splitLuc sensor successfully detected HIV protease and TEV protease. The main advantages of this sensor are that it does not detect a specific viral sequence and is thus independent of mutations and its adaptability since it can be modified to detect any viral proteases. Developed sensors could be used for diagnostics and also for the development of antiviral drugs targeting viral proteases.



Scheme 1: *Schematic of biosensor design. Created with Biorender.*

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[1] Wang, Q.; Gao, H.; Clark, K. M.; Mugisha, C. S.; Davis, K.; Tang, J. P.; Harlan, G. H.; DeSelm, C. J.; Presti, R. M.; Kutluay, S. B.; Shan, L., CARD8 is an inflammasome sensor for HIV-1 protease activity. *Science* **2021,** *371*, 1707.

Use of recycled PET plastic particles in mortars for plastic waste reduction

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Increasing plastic production results in huge amounts of plastic waste and consequently in global plastic pollution.[1] Waste plastic can be managed in many ways, based on energy or material recovery, depending upon composition and purity of the materials. The biggest demand for plastic especially for polyethylene terephthalate (PET) comes from the packaging industry which presents one of the biggest sources of plastic waste leading to formation of environmental problematic microplastics and nanoplastics. Although PET plastic has a high collective and recycling rate it causes environmental issues all over the world due to its large use.[2] Several studies confirmed using PET plastic waste in building materials could contribute to waste reduction in terms of recycling and reuse.[3]

The aim of this study was to determine the properties of mortars containing recycled PET plastic particles of different shapes and quantities as partial natural aggregate replacement. Results showed the more the plastic particle resembles the natural aggregate in mortar, the more similar were properties to plain mortar.

Figure 1. *Natural aggregate and most appropriate shape of PET plastic particles as replacement.*

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Development of a biosensor based on potato peelings and curcumin

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A biosensor[1] sensitive to changes in the concentration of ammonia (NH_3) in an aqueous medium is present in the research paper It is made from starch obtained from potato peels. The sensor contains curcumin,[2] a plant pigment that changes colour in response to a known concentration of ammonia.[3] We checked the operation of the sensor in the temperature range from 17°C - 25°C. The lower limit of detection is 50 ppm, response within 1 min. Responsiveness is inversely proportional to ammonia concentration. The sensor does not need any source of electricity for its operation, it is very affordable and completely biodegradable.[1]

***Scheme 1**: Color change of the sensor at elevated ammonia concentration.*

[1] Peternelj, A., Vključevanje vsebin o bioplastiki v pouk kemije v osnovni šoli. Magistrsko delo, Pedagoška fakuletata v Ljubljani, Univerza v Ljubljani, **2018**.

[2] Priyadarshi, R.; Ezati, P.; Rhim, J.- W., Recent Advances in Intelligent Food Packaging Applications Using Natural Food Colorants. *ACS Food Sci. Technol.* **2021**, 124–138.

[3] Sutton, M., A.; Samantha, S., R.; Baker, M.,H., Detecting emission changes and environmental impacts. Results of an Expert Workshop under the Convention on Long-range Transboundary Air Pollution. *Centre for Ecology & Hydrology. UK* **2009**.

Synthesis and characterization of photocatalytic mesoporous TiO_2-CeO_2 composites

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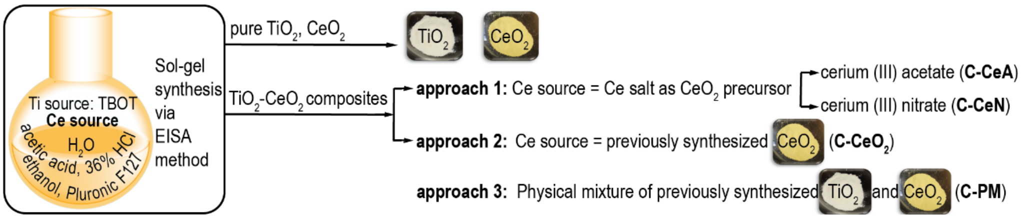
Photocatalysts possess the capacity to use solar energy to catalyse reactions for valuable chemical production or pollutant degradation[1]. Mesoporous TiO_2, CeO_2, and TiO_2-CeO_2 materials were prepared by sol-gel synthesis via the evaporation-induced self-assembly (EISA) method[2] in controlled conditions (40 °C and 33 % relative humidity), followed by calcination. The TiO_2-CeO_2 composites were synthesized using different approaches (Scheme 1) and different amounts of cerium sources by varying the Ce:Ti ratio (0, 0.2, 1, 5, 20 %). The obtained materials featured narrow pore size distribution (5-7 nm) and high specific surface area (80-180 m^2/g). The photocatalytic activity (ppm/h) was determined as the rate of oxidation of isopropanol into acetone in a gas-solid reactor system (Table 1). The highest activity was achieved using the synthesis approach 3 (physical mixtures, C-PM).



Scheme 3: *Synthesis of TiO_2-CeO_2 composites using different approaches.*

Table 2: *Photocatalytic activity (ppm/h) of TiO_2-CeO_2 composites prepared by different approaches.*

Ce:Ti ratio (%)	***0***	***0.2***	***1***	***5***	***20***
C-CeA	*932*	*1032*	*458*	*125*	*30*
C-CeN	*932*	*792*	*407*	*87*	*22*
C-CeO_2	*932*	*1167*	*865*	*1102*	*806*
C-PM	*1014*	*1245*	*1503*	*1773*	*1556*

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Extraction of active substance cordycepin from Cordyceps militaris and its determination using HPLC

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Cordyceps militaris is a medicinal fungus highly valued in traditional Asian medicine, with cordycepin as its main bioactive compound.[1] The aim of research was to optimize the extraction of cordycepin from dried and powdered *C. militaris*. For monitoring the efficiency of the extraction, an HPLC analytical method for determination of cordycepin in extracts, was partially validated. Optimization was carried out through single-factor experiments, evaluating the extraction efficiency based on the optimal cordycepin extraction ratio and the percentage of impurities found in the dry extract. The research comprised of five major groups of experiments, evaluating the influence of: (i) ethanol concentration in the solvent on the extraction efficiency, (ii) different ratios of solvent volume to dry sample mass on the extraction efficiency, (iii) leaching of cordycepin from a sample from which the extract was sequentially removed and fresh solvent added, (iv) pH of the sample-solvent mixture on the extraction efficiency, and (v) percolation performed at different temperatures. The optimal extraction parameters were determined as follows: a solvent-to-sample ratio of 20 mL/g, a temperature of 60°C, and a solvent composition of 76.8% (V/V) ethanol, as shown in Figure 1. It was found that the pH of the solvent-sample mixture had no significant effect on the extraction efficiency.

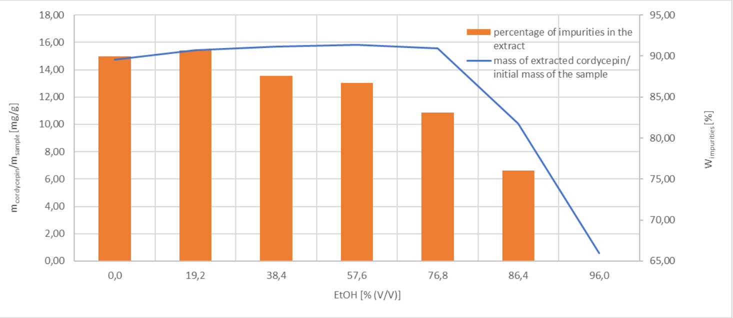

Figure 1: *Comparison of the dependency of extracted cordycepin on the sample mass and the dependency of impurity content on the ethanol proportion in the solvent.*

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Delaying water droplet freezing with superhydrophobic laser-engineered surfaces

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Corrosion and ice accumulation represent an enormous challenge in industrial systems, where it can cause equipment damage and failure, leading to financial losses or health hazards.[1] Passive methods, such as ice-phobic surface modifications, are being focused on as an alternative to replace the traditional active ice and frost management approaches.[2]

In this study, we present a facile approach for fabricating functionalized aluminum surfaces with enhanced anti-icing and anti-corrosion properties. Aluminum surfaces (1050A, H24 temper) were first laser textured with a nanosecond marking laser to produce micro- and nanostructures [Figure 1(a)], which was followed by application of a superhydrophobic coating (a self-assembled monolayer) of fluorinated alkyl phosphonic acid (3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-fluorododecylphosphonic acid - FDPA).

Experimental evaluation of the corrosion properties of the developed surfaces showed significantly enhanced corrosion protection during immersion in a corrosion medium. Furthermore, delayed freezing of 4 µL sessile water droplets compared with an untreated reference surface over a wide range of temperatures was observed [Figure 1(b,c)].

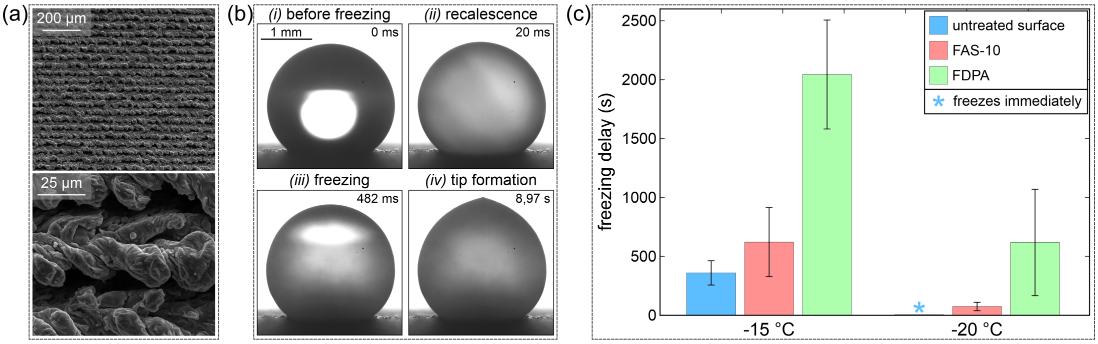

Figure 1: *SEM images of the laser-textured surface (a), water droplet freezing process (b) and comparison of freezing delay on untreated and functionalized surfaces at different temperatures (c).*

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Advances in Alzheimer Disease Detection: Synthesis of Fluorescent Probes and Their Photophysical Evaluation

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The absence of minimally invasive diagnostic method for Alzheimer's disease (AD) motivated us to prepare molecular fluorescent sensors capable of identifying AD biomarker amyloid β (Aβ) plaques, preferably *ex vivo* in blood samples[1]. To achieve this, we combined conventional chemical approaches with palladium-catalyzed cross-coupling reactions to synthesize molecular probes containing an electron-donating moiety, a delocalized π-system scaffold, and an electron-accepting group[2]. The diverse structural motifs of these compounds allowed for a methodical exploration of their optical characteristics in different solvents.

To evaluate the suitability of the newly developed fluorophores for biological optical imaging, we recorded spectra for absorption, emission, and excitation in solvents with varying polarities, namely *n*-hexane, dichloromethane, acetonitrile, methanol, and HEPES buffer. By employing time-dependent density functional theory and implicit solvation models, we conducted theoretical examination of the photophysical properties of the synthesized compounds. This comprehensive investigation provided valuable insight into the fundamental mechanisms governing the processes of (de)excitation, which supported meaningfully experimental structure–optical properties relationship.

Our efforts have yielded a series of molecular sensors that exhibit exceptional properties, including enhanced Stokes shift, increased quantum yield in dichloromethane, and, importantly, also strong affinity towards Aβ_{1-42} fibrils. These properties show significant potential for further development of AD diagnostic tools and highlight the promising clinical applications associated with such fluorescent dyes.

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A new candidate type I toxin-antitoxin system in the cyanobacterium Microcystis aeruginosa PCC 7806

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Toxin antitoxin (TA) systems are bacterial genetic elements that encode a relatively stable toxin and a labile antitoxin. The notorious bloom-forming cyanobacterium *Microcystis aeruginosa* is especially interesting in terms of TA systems as it contains the highest number of type II TA loci of any bacteria. Despite this, only one locus has been experimentally studied up to now[1] while type I TA systems were not found in this species so far. In type I systems, the toxin is a short membrane or cytosolic protein while the antitoxin is a short non-coding RNA[2].

Our bioinformatic analysis revealed fifteen candidate type I TA loci in the *M. aeruginosa* PCC 7806 genome and we experimentally characterized six of them. Based on our results, the expression of BH695_0320 and BH695_4017 (which we later renamed to MsoT1) has a negative effect on *Escherichia coli* cell growth while the expression of BH695_0311, BH695_3336, BH695_4989, and BH695_5020 has no effect (Fig. 1). Additionally, we found the expression of MsoT1 to have a delayed toxic effect when the cognate candidate antitoxin MsoA1 is also present on the plasmid. Using a synthetic-biology approach, we were also able to confirm the biologic activity of two predicted MsoA1 antitoxin promoters.

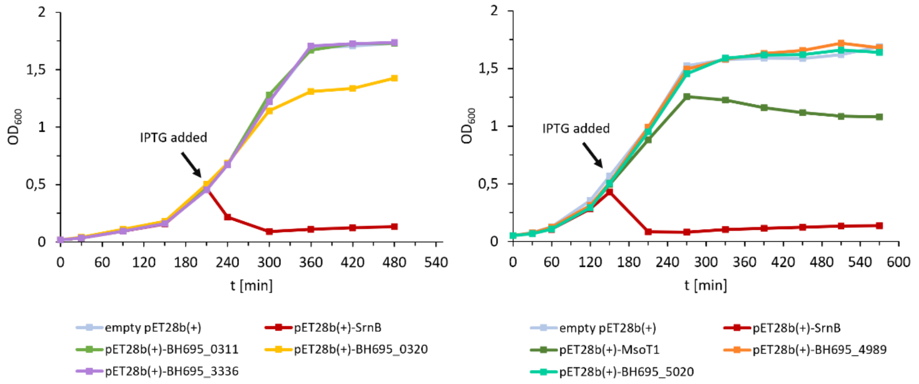

Figure 1: *Growth curves of E. coli BL21(DE3) pLysS expressing different candidate type I toxins.*

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Effect of single nucleotide polymorphism rs4129009 in TLR10 on immune response in A549 cell line

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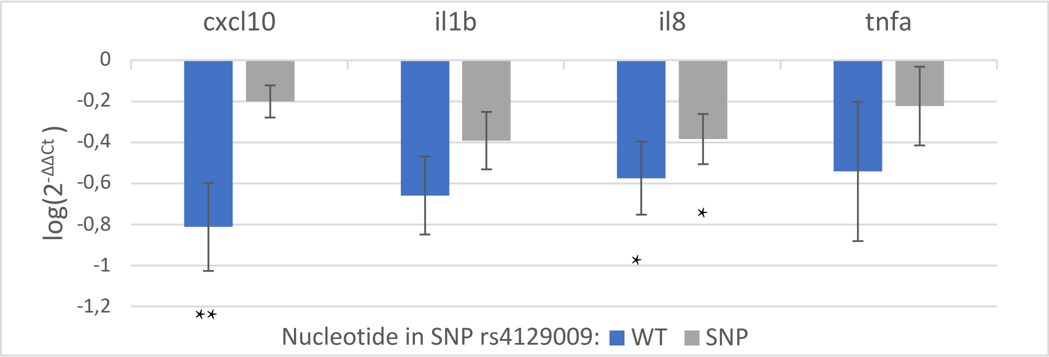
Even though TLR10 is the only TLR receptor of which ligands and mechanism of action have not yet been explicitly determines, previous researches have shown that TLR10 has immunomodulatory role. It was determined that overexpression of TLR10 has inhibiting effect on expression of pro-inflammatory cytokines. TLR10 is so the only inhibitory TLR receptor[1]. Variant of TLR10 gene rs4129009 (A>G) was shown in to be an advantage in lung related diseases in children.[2,3]

In this research we show that rs4129009 variant of TLR gene causes lower inhibition of transcription of genes for cytokines CXCL-10, IL-1β, IL-8, TNF-α then wild type TLR10 and so shows lower immune suppressor activity (Graph 1).



Graph 1: *expression of immune system related genes in cells of A549 cell line with wild type variant of TLR10 gene (WT) and rs4129009 variant (SNP).*

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CO_2 conversion to formic acid with indirect hydrogen source over different ZrO_2 catalysts

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Industrialization, overuse of fossil fuels and population growth are among the many culprits that have increased atmospheric CO_2 concentrations so much in recent decades that humanity is already facing serious environmental problems. By capturing, using and converting CO_2, we would not only reduce the amount of this greenhouse gas, but also gain valuable chemicals. One of the ways to reduce the concentration of CO_2 in the atmosphere is to convert CO_2 into HCOOH, which is not only an important liquid material for hydrogen storage but also a C1 building block for the chemical industry.[1,2]

The aim of this work was to propose a sustainable method for hydrogenation of CO_2 to formic acid using hydrazine hydrate as an indirect hydrogen source and to synthesize and select a catalyst that is highly active and selective (Fig. 1). Manganese-modified ZrO_2 supports with variable calcination temperature were synthesized and evaluated for the CO_2 hydrogenation to formic acid. The catalyst supported on monoclinic zirconia, Mn+ZrO_2-m, proved to be the most active among the studied catalysts.

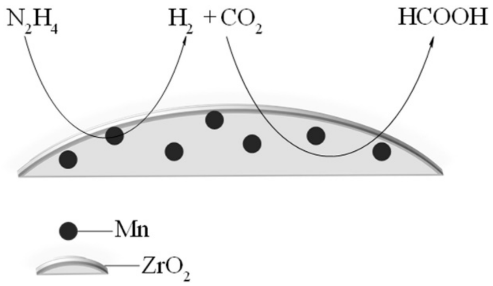

Figure 1: *Scheme of hydrogenation of CO_2 to HCOOH on Mn-modified ZrO_2 catalyst.*

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Monitoring of biodegradation of tire wear microplastics in the aquatic environment

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Tire Wear Particles (TWPs) are microplastics generated through friction between tires and road surface while driving. TWPs enter the environment either through runoff or air. Due to increased traffic and daily use of motor vehicles, TWPs are one of the main sources of microplastics in the environment nowadays.[1,2] When TWPs are released into the environment, they undergo various environmental processes and interactions with microorganisms that can lead to biofilm formation which is the first step prior their biodegradation.[3]

The aim of the research work was to study the biodegradation of TWPs over a period of 12 weeks in natural freshwater under controlled laboratory conditions. The TWPs used in the experiment were obtained from used tires and had a mean particle size of 47.39 ± 22.2 µm. Biodegradation was monitored by measuring oxygen consumption using a closed respirometer. In addition, scanning electron microscopy (SEM) was used to investigate the changes of TWPs surface, and Fourier transform infrared spectroscopy (FTIR) was used to observe possible changes in the chemical composition of TWPs due to the biodegradation.

The results showed that TWPs are not easily biodegradable, in fact, the biodegradation did not exceed 3.8 ± 2.2 % during the experiment. In addition, FTIR analysis showed the presence of newly formed functional groups, that can be attributed to the formation of a biofilm on the TWPs but not to biodegradation. SEM images confirmed the presence of microorganisms on the TWMs surface but their presence was scarce. No other changes in TWMs morphology were observed. The low biodegradability suggests that TWMs may persist and accumulate in the freshwater environment.

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Enhanced corrosion protection of aluminium using superhydrophobic coating

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Superhydrophobicity is the phenomenon where water assumes a spherical shape on a substrate's surface due to surface tension, Figure 1. The effectiveness of this property relies on the surface structure and the presence of hydrophobic compounds or molecules.[1,2] The objective of the research was to explore the creation of a superhydrophobic aluminum surface with excellent corrosion resistance and self-cleaning capabilities.

We investigated the impact of surface roughness achieved through etching with $CuCl_2$, as well as the influence of the perfluorosilane molecule on superhydrophobicity. We assessed changes in sample mass, surface morphology, and wettability. The surface was examined using a scanning electron microscope, and corrosion protection was evaluated through standard laboratory tests. Additionally, we tested the self-cleaning properties.

The results confirmed that the superhydrophobic surface, created through an optimal etching process with $CuCl_2$ and modified with perfluorosilane, exhibited superior resistance to corrosion compared to polished aluminum. Furthermore, the surface demonstrated self-cleaning properties.

Consequently, we successfully achieved superhydrophobic properties on aluminum in a straightforward, cost-effective, and industrially feasible manner. This surface modification technique holds practical value for applications requiring the maintenance of a clean surface.

Figure 1: *A drop of water on superhydrophobic aluminium surface.*

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Optimization of solid-phase extraction for selected phthalates, PAHs, and bisphenols on microplastics in aqueous environment

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In today's world, we face numerous environmental and health challenges. The category of pollutants that pose a risk to the environment and health also includes the pollutants discussed in my work: phthalates, polycyclic aromatic hydrocarbons (PAHs), and bisphenols. Phthalates affect the reproductive system of humans and induce decreased number of erythrocytes and anaemia.[1] PAHs cause various toxic effects in living organisms, including carcinogenicity.[2] Bisphenols can be classified as endocrine-disrupting substances, and they play a role in the genesis of cancer, brain function disorders, obesity, immunodeficiency, etc.[3] In my work, I focused on optimization of solid-phase extraction (SPE) of the dimethyl phthalate, diethyl phthalate, dibutyl phthalate, naphthalene, acenaphthene, phenanthrene, fluoranthene, bisphenol A, and bisphenol S. The studied parameters were: different types of SPE cartridges, the salt concentration and pH of the sample, the influence of the washing step, various elution solvents, and their volumes. After the conditioning step and equilibration step, the sample containing analytes with the addition of salt was applied onto the HLB cartridge. A mixture of methanol, acetonitrile, and ethyl acetate in an appropriate ratio was used as elution solvent. For the quantification of the analytes, a pre-optimized HPLC/DAD method was applied.

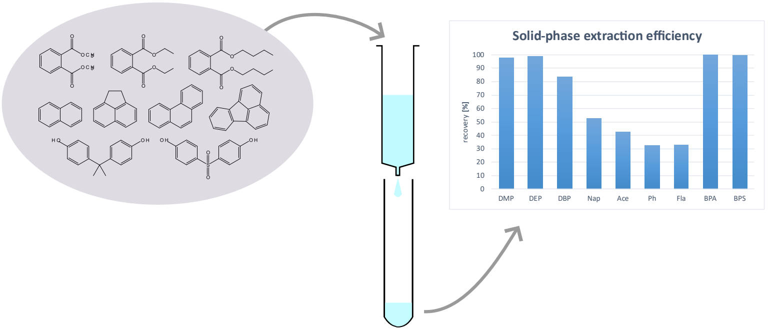

Figure 1*: Schematic representation of the present study.*

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Fate and transport of microplastics in constructed wetland

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Microplastics (MPs) are plastic particles smaller than 1 mm.[1] Due to their widespread presence in the environment, many studies have focused on investigating technologies to reduce MPs in the environment, such as constructed wetlands (CWs).[2] In this context, the aim of our study was to investigate the fate and transport of MPs in two different types of CWs. Two comparable experiments were performed; in the first one, the CW contained five different aquatic plants, while the second experiment was performed in the absence of plants. At the beginning of each experiment, synthetic wastewater with known quantities of MPs (synthetic microfibers, polyethylene fragments and tyre wear particles) was introduced, and in the following 12 days, the distribution of MPs in the CW was monitored, by counting the number of MPs attached in the effluent. At the end of the first experiment, the number of MPs attached to the vegetation, MPs in the water body, and in the sediment was determined, while in the second experiment, only the number of MPs in the water body and in the sediment was determined. Based on the results, it can be concluded that vegetation has a great influence on the horizontal and vertical transport of MPs in CWs, as more MPs were found in the sediment and in the effluent when plants were not present in the CW.

Figure 5: *Vegetated constructed wetland with the continuous surface flow.*

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The need for improved fire safety guidelines for rooftop PV systems

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Reducing carbon-based energy is essential for a sustainable future. Among sustainable energy sources, photovoltaics (PV) is a well-recognized option, endorsed by various national and supranational entities. The European Commission outlined an ambitious plan (REPowerEU)[1] to introduce over 600 GW of PVs by 2030, thus decreasing reliance on carbon-based sources. This initiative will increase the already rising rate of new PV installations. However, putting a PV system on the roof has been shown to increase the extent of damage in case of a fire,[2] both because it can be the source of a fire (including the DC and AC parts of the installation) and because the consequences of a roof fire increase. Current estimates show that the annual expected number of fires related to PV systems is 29 fires/GW of the installed power.[3] Many causes (in cases where the PV systems were the source of fire) were related to the processes of installation and maintenance of the PV installation.

Numerous PV installation guidelines were reviewed to assess how they address the fire safety aspects. Topics ranging from certification of maintenance and instalment personnel, requirements about the panels, requirements about the roofing materials, and rules for the array design (size, separation distances) were assessed and compared between the documents. The analysis showed that there is a clear lack of referencing regarding the proposed safety measures, thus making it difficult to find scientifically sound sources for the suggested arrangements. In particular, the pass/fail selection of roofing membranes through test standards was found not to provide sufficient safety. To enhance the scientific approach on the topic, carefully designed experiments were conducted to determine the effectiveness of the proposed safety measures through a parametric study. Some of the parameters investigated were the separation distance between multiple PV arrays on the roof and the type of roofing membrane. The results from the experiments clearly indicate that a scientific approach is needed in assessing the safety of various PV system solutions on roofs, thus confirming that the current prescriptive selection through roofing test standards fails to capture risk nuances between installed systems.

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[3] Mohd Nizam Ong, N. A. F.; Sadiq, M. A.; Md Said, M. S.; Jomaas, G.; Mohd Tohir, M. Z.; Kristensen, J. S. Fault Tree Analysis of Fires on Rooftops with Photovoltaic Systems. *Journal of Building Engineering* **2022**, 46, 103752.

Molecular cloning and preliminary expression and purification of fluorescently labeled components of the beta-catenin destruction complex

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Colorectal cancers (CRCs) stem from colon or rectum epithelial cells. Most sporadic CRC cases (over 80%) exhibit changes in the APC gene, an early event in disease development. These changes result from mutations in the Wnt signaling pathway, crucial for embryonic neural patterning and organ formation.[1] Mutations disrupt the β-catenin destruction complex, responsible for regulating β-catenin levels. Phosphorylation by GSK3β and CK1 primes β-catenin for ubiquitination and degradation. The complex involving Axin, APC, and Dvl acts as a scaffold during active Wnt signaling. If the destruction complex falters, β-catenin accumulates and enters the nucleus (Fig. 1). There, it interacts with TCF transcription factors, leading to the transcription of Wnt target genes that govern cellular processes.[2] The purpose of our work was to prepare fluorescently labeled proteins in order to study protein-protein interactions. We prepared five different protein constructs for the proteins Axin, Dvl, CK1a, beta-catenin, and GSK3β, which contained the coding sequence for a hexahistidine tag, GFP fluorescent tag, and a cleavage site for the TEV protease. We successfully cloned and expressed them in the bacterial strain *E. coli* BL21 with and without the pRARE plasmid. Subsequently, we performed an analysis of protein expression and purified them using nickel affinity chromatography.

Our constructs enable detailed research on component roles and interactions, illuminating β-catenin destruction complex behavior in physiology and the impact of cancer mutations on Wnt signaling.

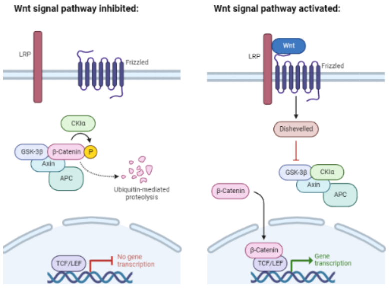

Figure 1: *Canonical Wnt or Wnt/β-catenin signaling pathway. Left: inhibited pathway by phosphorylation of β-catenin and subsequent degradation. Right: activated pathway by binding of Wnt to the receptor complex consisting of frizzled and LRP.*

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[2] Komiya, Y. & Habas, R., Wnt signal transduction pathways. *Organogenesis 4* **2008**, 68-75.

Corrosion protection of aluminium using a superhydrophobic coating

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Laser treatment was explored for facile and environmentally acceptable surface roughening. The aim was to achieve a hierarchical surface topography and chemical bonding (grafting) of silane molecule on an aluminium surface through immersion in an ethanol solution containing 1H,1H,2H,2H-perfluorodecyltriethoxysilane (FAS-10)[1,2], Figure 1.

The selected laser-treated aluminium surfaces (before and after grafting) were characterised using a contact profilometer, optical tensiometer, scanning electron microscope coupled with an energy-dispersive spectroscope and X-ray photoelectron spectroscope to evaluate surface roughness, wettability, surface morphology and composition. The corrosion properties were evaluated using potentiodynamic measurements in dilute Harrison's solution (DHS, 0.35 wt.% $(NH_4)_2SO_4$ + 0.05 wt.% NaCl). The dynamic properties were also assessed to determine the bouncing and self-cleaning effects.

The laser-treated aluminium surface with micro/nano-structures and a grafted perfluoroalkyl silane film demonstrated excellent superhydrophobicity, enhanced corrosion protection and bounce dynamics in water droplet tests. Prepared superhydrophobic aluminium surface achieved efficient self-cleaning ability against solid pollutants.

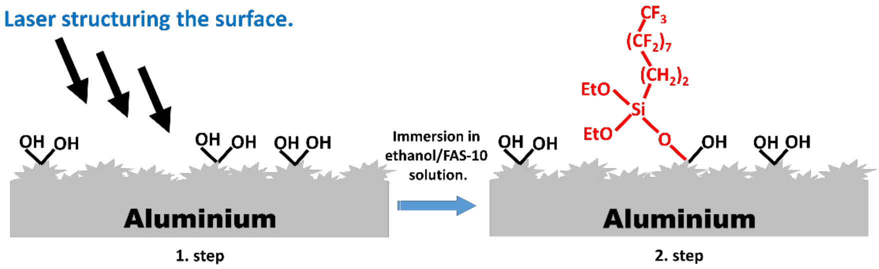

Figure 1: *Schematic illustration of forming a (super)hydrophobic aluminium surface prepared by the laser structuring the surface followed by grafting with perfluoroalkyl silane, FAS-10.*

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[1] Rodič, P., Kapun, B., Milošev, I., Easy and Fast Fabrication of Self-Cleaning and Anti-Icing Perfluoroalkyl Silane Film on Aluminium, *Coatings* **2020**, 10, 234.

[2] Rodič, P., Kapun, B., Milošev, I., Superhydrophobic Aluminium Surface to Enhance Corrosion Resistance and Obtain Self-Cleaning and Anti-Icing Ability. *Molecules* **2022**, 27, 1099.

The impact of ozonation of polypropylene and polyethylene terephthalate microplastics on leaching

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Microplastics (MPs) are becoming emerging micropollutants in environment. MPs have been found in marine and terrestrial ecosystems, including ground and surface waters, soil and even in animals. It has strong ability to adsorb toxic compounds that could impact on organisms and cause unknown effects.[1]

Total organic carbon (TOC) is an essential parameter in various scientific disciplines and provides valuable information about the organic content of sample and can be used to evaluate the overall quality and contamination of water.[1,2] We investigated the effect of ozonation on leaching of adsorbed compounds of MP by TOC measurement. Ozonation is used for treatment of drinking and surface waters, wastewaters and waste sludge which often contain MPs. During ozonation various compounds could be leached or formed affecting quality of the treated waters and performance of the post-ozonation processes.[3] We used PP and PET particles, smaller than 1 mm (0,5 g was of each type was added). Different ozone dosages (3.54 g h^{-1}, 3.99 g h^{-1} and 4.47 g h^{-1}) for three different time (0, 60 and 120 min) were used. Samples were stored in vials and total organic carbon (TOC) was measured. As shown in Figure 1, it seems, that ozonation of both types of MPs had some impact but there is no correlation between dose of ozone and time of oxidation on TOC. It can also be seen, that ozonation of PP had more impact on TOC and it can be assumed, that more adsorbed compounds started leaching from PP.

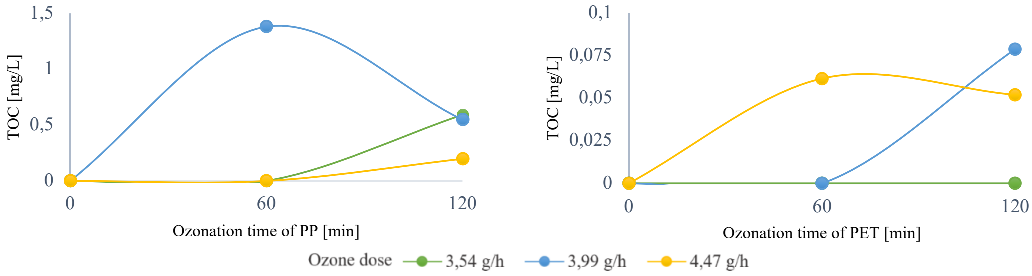

Figure 1: *TOC in relation to ozonation time based on ozone dose (PP left, PET right).*

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Development of dispersive micro solid-phase extraction for determination of emerging pollutants in water

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Anthropogenic activities and chemicalization of modern societies have led to gradual omnipresence of emerging pollutants (EPs) in surface waters. Therefore, it is necessary to develop ultrasensitive multi-residue analytical methods for their determination in complex matrices to monitor and study their behaviour. In water analysis, solid-phase extraction (SPE) sample treatment step using SPE cartridges, followed by LC-MS/MS instrumental analysis has been shown effective to reach environmentally relevant sub-10 ng/L sensitivity range.[1] But in recent years, dispersive micro solid-phase extraction (DMSPE) has become a promising sample preparation method due to its versatility, fast analysis, and low consumption of organic solvents. Moreover, its significant advantage is the possibility of using mixtures of various sorbents, which increases multiplexing capacity.[2] The aim of our study was to develop DMSPE method coupled to UHPLC-MS/MS for a single-run analysis of 20 diverse EPs that could potentially be present in Slovenian surface waters; only two of them have been screened so far.[3] By testing different sorbent types and optimizing the extraction and desorption conditions (Fig. 1) using UHPLC-DAD and UHPLC-MS/MS, we achieved preconcentration factors of 5–29 for the determination of a large number of compounds with diverse physicochemical properties, using a mixture of C18 and strong-anion exchange (SAX) sorbents. As such, this study shows a methodology useful for developments of DMSPE and may contribute to the popularization of this fast, wide-scope, green, and sensitive sample preparation technique for water samples.

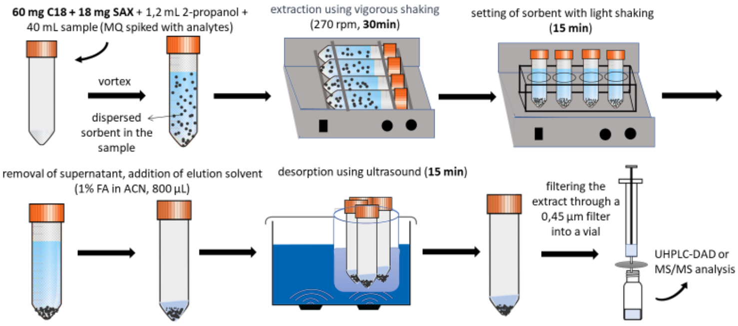

Figure 1: *Optimized DMSPE method.*

[1] Kumar, R., Qureshi, M., Kumar Vishwakarma, D., Al-Ansari, N., Kuriqi, A., Elbeltagi, A., Saraswat, A., A review on emerging water contaminants and the application of sustainable removal technologies. *Case Stud. Therm. Eng.* **2022**, 6, 1–14.

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[3] Klančar, A., Trontelj, J, Roškar, R., Development of a Multi-Residue Method for Monitoring 44 Pharmaceuticals in Slovene Surface Water by SPE-LC-MS/MS. *Water Air Soil Pollut.* **2018**, 229, 192.

Degradation of Petroleum Substances in Ozonation Fluidized Bed Reactor

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This study focuses on the comprehensive analysis of an ozonation fluidized bed reactor system, combining hydraulics investigation, biodegradability assessment, and kinetic modeling. The aim was to optimize the reactor's performance for the treatment of petroleum substances, specifically motor oil.

Ozonation and catalytic ozonation processes were realized. A modified zeolite with iron was used as a catalyst.[1] Parameters such as ozone generator power and oxygen inflow rate were varied and ozone saturation concentration results were analyzed to assess reactor efficiency and operating conditions. Experimental investigation revealed that the highest ozone saturation concentration was achieved at 60% of ozone generator power and an oxygen flow rate of 0.4 L/min. The hydraulics of the fluidized bed reactor were analyzed to understand the fluid dynamics within the system.[2]

Respirometry measurements with activated sludge were employed as a measure of immediate biodegradability.[3] The results indicated a significant enhancement in the immediate biodegradability of the motor oil following the ozonation process. By comparing respiration rates after ozonation with and without zeolite, it was observed that the inclusion of zeolite enhanced the immediate degradation process, suggesting its potential for improved ozonation.

To further enhance the understanding of the biodegradation process, various kinetic equations were considered and analyzed to identify the most appropriate one that best represented the process of biodegradation. The most favorable model, according to our analysis, was the Aiba model.

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Wisteria – ornamental, poisonous or useful?

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Poisons and toxins have been used since ancient times, and their properties as poisons and medicines are still being researched today. We decided to focus on Wisteria, a popular ornamental flower with beautiful purple blossoms. Its branches can climb up to 20 meters in the air with the right support.[1]

Extracts were obtained from different parts of Wisteria (leaves, flowers, stems, fruit pericarp, and fruit seeds) by simple maceration. The solvent used for extraction was water or a 70 % ethanol solution. The extracts were used for experiments on seeds of cress and mungo bean plants and on brine shrimps. The experiments were based on allelopathy, which, simply said, is about a positive or negative influence between organisms depending on the chemicals the organism secretes.[2] The results show that most of the extracts stimulate germination and plant growth, and that most of them kill other organisms, as we have seen in experiments on brine shrimps. The choice of solvent and the concentration of the extract in the solution used, also impact their effect on plants and brine shrimp. These results pose a base for further research as the extracts could potentially be used as a fertilizer and insecticide. We would also like to do HPLC tests to determine the content of these extracts.

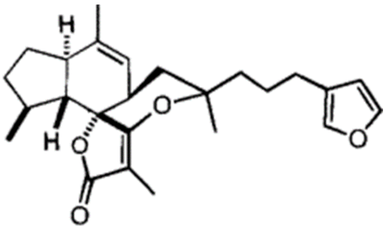

***Figure 6**: Skeletal formula of vistarin.*[3]

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Zooming into the relationship between neurotropic flaviviruses and autophagy in human astrocytes

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[2]Celica Biomedical, Tehnološki park 24, *SI*-1000 Ljubljana, Slovenia
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Accumulating evidence suggests that astrocytes, glial cells involved in maintaining brain homeostasis and supporting neuronal function, represent hotspots for viral replication and dissemination within the brain. Autophagy, a cellular pathway for degradation of damaged organelles and proteins, has emerged as a critical mechanism during viral infections, exhibiting both protective and detrimental effects. The interplay between autophagy and the life cycle of viruses is context-dependent, as it varies between different viruses, cell types and host species.[1] Using fluorescence microscopy (Fig. 1) we investigated whether neurotropic flaviviruses, known for causing severe neurological symptoms in humans, affect autophagy in human astrocytes. In addition, the involvement of astrocytic autophagy in regulation of flavivirus replication was assessed.[2] We showed autophagy is stimulated upon flavivirus infection of human astrocytes. Interestingly, flavivirus replication in these cells is autophagy-independent.

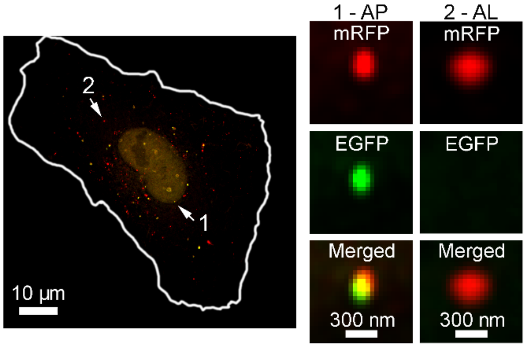

***Figure 1:** Human astrocyte, expressing fluorescent protein mRFP-EGFP-LC3, imaged by super-resolution fluorescence microscopy. Determining the number of autophagosomes (1) and autolysosomes (2) can be used to evaluate alterations in autophagic activity.*

[1] Choi, Y.; Bowman, J. W.; Jung, J. U., Autophagy during Viral Infection — a Double-Edged Sword. *Nat. Rev. Microbiol.* **2018**, 16 (6), 341–354.

[2] Tavčar Verdev, P.; Potokar, M.; Korva, M.; Resman Rus, K.; Kolenc, M.; Avšič Županc, T.; Zorec, R.; Jorgačevski, J., In Human Astrocytes Neurotropic Flaviviruses Increase Autophagy, yet Their Replication Is Autophagy-Independent. *Cell. Mol. Life Sci.* **2022**, 79 (11), 566.

Molecular Dynamics Simulations for a System of Particles with a Multiple Characteristic Length Potential

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We used a pair potential with multiple characteristic lengths (Fig. 1) in order to describe a two-dimensional system with multiple critical points. The study was done with computer simulations in both NPT and NVT ensembles. We calculated the relationship between different thermodynamic variables and interpreted the results. We also determined the local structure of the system, by determining the radial distribution function and the translation order parameter.[1]

Since the potential has two regions with a steep decrease where it is positive, we expected two anomalous regions with two critical points. The results confirmed our hypothesis. The pair potential was first proposed by M. A. A. Barbosa, E. Salcedo and M. C. Barbosa. They managed to produce similar results for a one- and three-dimensional system: "… potential can be designed to exhibit three liquid phases (LDL, HDL and VHDL), two liquid-liquid critical points and two density anomalous regions.[2]"

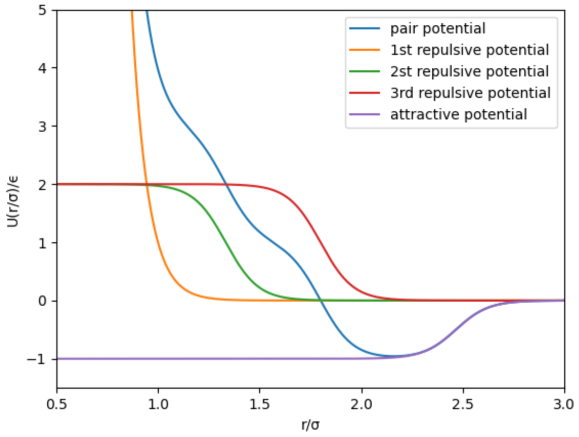

Figure 1: *Multiple Characteristic Length Potential.*

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Importance of cell casing choice in lithium metal battery electrochemistry

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Electrochemical impedance spectroscopy (EIS) is an important electrochemical tool that can give valuable insight into various phenomena occurring in batteries.[1,2] In order to perform reliable and reproducible measurements, some effort needs to be dedicated to the cell design intended for EIS measurements. Theoretically, the preferred type of cells are three electrode cells which give the most accurate and direct electrochemical information of the studied electrode.[3] However, many researchers prefer configurations that resemble the ones used for testing battery performance, e.g. two parallel electrodes separated with as thin as possible electrolyte-soaked separator.

It was shown experimentally that in some cases of practical interest, the impedance response of the same electrode in a coin cell or Swagelok cell configuration can be significantly different compared to a pouch cell design. The difference occurs when the electrolyte wets both the electrode under study as well as the metal case in stainless steel based casings. In our particular case – a passivated Li electrode – simultaneous wetting of the Li electrode and the stainless steel case caused the main impedance arc to split into two arcs. The phenomenon was explained by a simple equivalent circuit. Although the present study is limited to the metallic Li electrode, it must be emphasised that in most cases where both the electrode under study and another conductive surface (e.g. the cell casing) are in contact with the same electrolyte a significant alteration of impedance response may be expected. This effect is avoided by using a non-metallic casing (pouch cell casing) together with a limited surface area of contact strips, ideally placed in parallel and far apart. This design of cell casing avoids a large portion of the surface area of the metallic casing entering the direct electric field of the cell.

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Adsorption of a water-soluble polyacrylic acid-based polymer on activated sludge

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Synthetic polymers in the environment are still one of the most controversial and important environmental issues today. Water-soluble synthetic polymers (WSPs) have been widely used in vast quantities and their annual production in Europe alone is estimated to be several million tonnes,[1, 2] but the knowledge about their effects and fate in wastewater treatment plants is limited.[3] Therefore, the aim of our study was to evaluate the adsorption of a water-soluble polyacrylic acid-based polymer on activated sludge. WSP was rapidly adsorbed on activated sludge – during a period of six hours 95% of WSP was adsorbed. A change in pH had no effect on the adsorption. Potential biodegradation was also monitored but the measurement of oxygen consumption did not indicate any biodegradation. Therefore, it is evident that the WSP interacted with activated sludge and may, over time, affect the treatment efficiency of wastewater treatment plants.

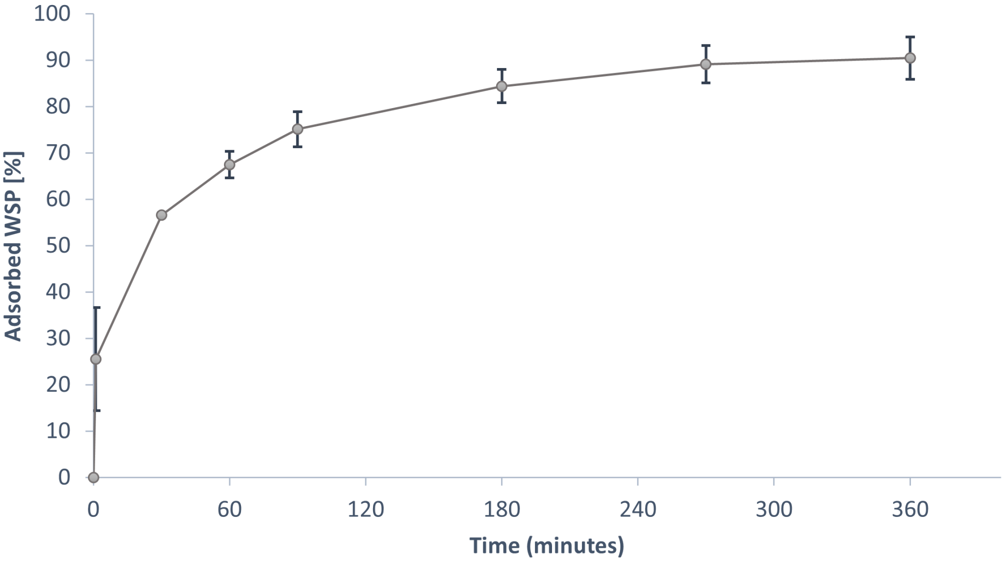

***Figure 1:** Adsorption of the water-soluble polymer (WSP) on the activated sludge.*

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[1]H. Arp, H. Knudsten, Could We Spare a Moment of the Spotlight for Persistent, Water¬Soluble Polymers?. *Environ. Sci. Technol.* **2020**, 54.

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Mutations of therapeutic targets of SARS-CoV-2 viral variants and the impact of mutations on the development drugs

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SARS-CoV-2 emerged in late 2019 from China, sparking global attention. The number of cases has exceeded 609 million with 6.5 million deaths. We chose SARS-CoV-2 as the topic of our research to understand the reasons for the pandemic, infections despite vaccination and prevention strategies.[1] To control the epidemic of SARS-CoV-2, the development of vaccines and drugs is crucial. Among the current 216 candidates, 92 vaccines are in human testing.[2] While both vaccines and medicines are important, the mechanism is completely different – vaccines trigger immune responses of the host with weakened virus particles, medicines act directly on the proteins of the virus.[3]

We studied the structure of SARS-CoV-2 therapeutic targets (S-protein, PLpro, 3CLpro/Mpro and RdRp), mapped the mutations of viral variants on them, used the molecular visualisation software PyMol, that we installed on our computers. We evaluated their interactions with experimental drugs (Tixagevimab, Nirmatrelvir, Remdesivir, and GRL0617) and found mutations significantly disturb the binding between the therapeutic target and the drug, causing the drug to lose effectiveness.

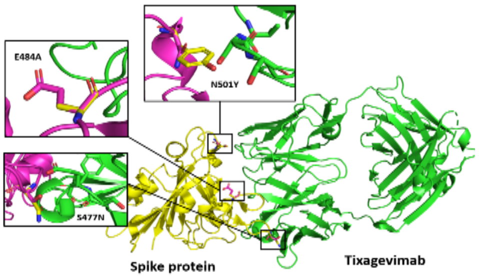

Figure 1: *Mutations on the S-protein.*

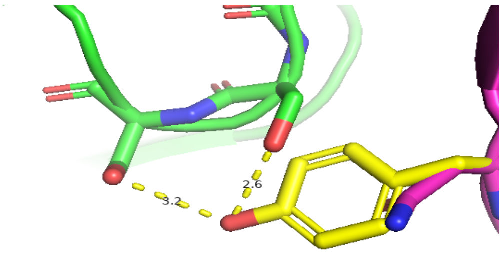

Figure 2: *Example of measurement of S-protein binding to Tixagevimab antibody.*

[1] World Health Organization. WHO Coronavirus (COVID-19) Dashboard. https://covid19.who.int/

[2] COVID-19 Vaccine & Therapeuti https://www.biorender.com/covid-vaccine-tracker

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Photocatalytic nitrogen reduction: a first-principles investigation

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Photocatalytic activation of an inert and stable nitrogen molecule is an environmentally friendly alternative to the established Haber-Bosch process of thermocatalytic ammonia synthesis [1,2]. In our study, we performed density functional theory (DFT) calculations to investigate the photocatalytic nitrogen reduction over Ru-doped TiO_2 clusters.

Calculations were performed in GPAW using the Perdew-Burke-Ernzerhof (PBE) functional, the local atomic orbitals (LCAO) basis set, and the projector-augmented-wave method (PAW) [3]. Based on the determined most promising active sites for the adsorption of nitrogen, ammonia, and hydrogen, the reaction mechanism was studied. We investigated the dissociative mechanism, the distal associative mechanism, the alternating associative mechanism, and the enzymatic associative mechanism. First-principles reaction mechanism was studied in the ground state and the lowest excited state. The excited state calculations were performed using the maximum overlap method (MOM) [4] and the parameters described above. The excited state calculations allow consideration of the photocatalytic properties, which is crucial for elucidating the photocatalytic reduction of nitrogen.

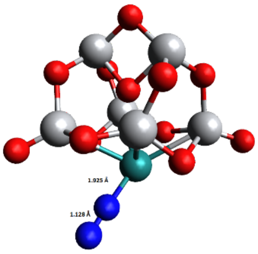

***Figure 1**: Adsorption of N_2 on Ru-$(TiO_2)_6$ cluster.*

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Ni/C-assisted lignin depolymerisation: effect of lignin structure on product distribution

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Fossil fuels are detrimental to the environment as they cause CO_2 emissions, pollute the air and environment, and lead to the extinction of animal species. A promising and important alternative is the biomass-derived polymer lignin, which is a renewable source of aromatics. The aim of our research was to optimise the isolation of organosolv lignin from biomass and to characterise the depolymerisation products.

Lignin was isolated from beech wood sawdust using the organosolv process to separate cellulose from hemicellulose and lignin. Lignin was then precipitated by three proportions of water to obtain three lignin fractions (Fig. 1). The non-fractionated lignin was also isolated for comparison. Lignin was depolymerised with and without Ni/C catalyst in a reductive environment. Isolated lignins and depolymerised products were characterised by different methods. GC-MS was used to analyse the monomeric compounds, while SEC, ^{31}P and 2D HSQC NMR were used to characterise the oligomers and the non-depolymerised lignin[1].

Lignin fractionation leads to more homogeneous lignin fractions. Catalytic depolymerisation results in a higher amount of monomeric compounds and reduces the formation of undesirable solid residue. GC-MS showed that the most abundant monomer was 2-methoxy-4-propylphenol, which is of interest to Fenolit, a company currently producing phenolic resins from the non-renewable phenolic-based material.[2]

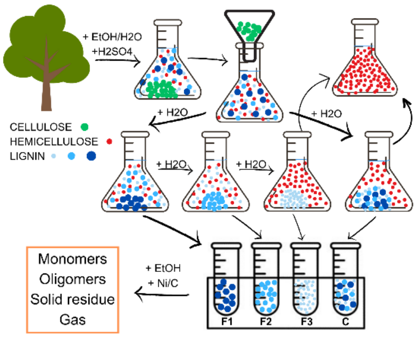

***Figure 7**: Lignin isolation with and without applied fractionation protocol, and depolymerisation.*

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Liquid-liquid phase separation of hen egg-white lysozyme

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Liquid-liquid phase separation (LLPS), a phenomenon initially demonstrated in cells a decade ago, has garnered significant attention due to its implications in cellular organization and function. This concept, derived from thermodynamics, describes the coexistence of insoluble liquids, analogous to oil in water, resulting in the formation of condensates. As our understanding of the thermodynamic and molecular forces driving condensate formation expands, numerous questions remain regarding their mechanisms of action, potential implications in aging and diseases, and their therapeutic potential for promoting human well-being.[1] In this study, we investigate the temperature dependence of phase separation in hen egg-white lysozyme solution, using a combined approach of theoretical modelling (Wertheim's perturbation theory) and experimental analysis.[2] The presented findings contribute to the growing body of literature on LLPS. By integrating theoretical modelling and experimental data, this research provides crucial insights into the underlying mechanisms of protein aggregation. By expanding our knowledge in this area, we aim to contribute to ongoing scientific efforts in unravelling the complexities of protein phase behaviour and its relevance to human health.

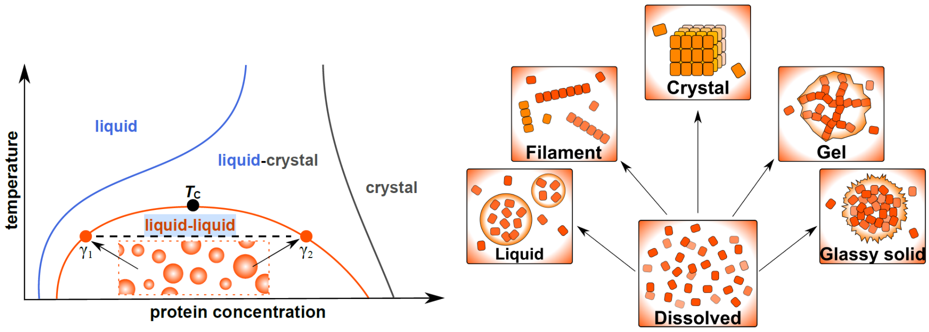

Figure 1: *Schematic representation of the thermodynamic phase diagram of aqueous globular protein solutions (left) and the most typical protein self-assembly structures formed during the "condensation" of proteins (right).*[3]

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From 1,2,3-Triazolium Salts to Mesoionic N-Heterocyclic Olefins

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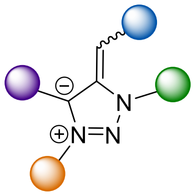
Following the success of N-heterocyclic carbenes (NHC) in the field of (organo)catalysis, N-heterocyclic olefins (NHO) emerged as a promising new class of carbon-based ligands[1]. Their structure is based on a NHC framework, to which a highly polarized alkylidene group is terminally appended. NHOs were first introduced by Kuhn in 1993[2], but a significant increase in research interest happened in the 2010s. Only recently a new type of NHOs, mesoionic N-heterocyclic olefins (mNHO) have been introduced[3]. This initial work included three rhodium complexes with different mNHOs and these remain the only examples of mNHO transition metal complexes currently published[3].

In this work we present the synthesis of novel mNHOs, which were designed to assess their coordinating ability. We were interested in exploring the effect of different substituents on stability, coordination and properties of potential mNHO transition metal complexes. You can achieve this not only through substitution on the triazole backbone but also at the olefinic carbon atom. We prepared a set of alkylated 1,2,3-triazolium salts, which upon deprotonation give access to mNHOs. Subsequently, we tested their reactivity with a selection of transition metal precursors.



Scheme 1: *Structure of a 1,2,3-Triazole-based mesoionic N-heterocyclic olefin.*

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Microscopic analysis of adhesive joint using beech wood

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Buildings are the single largest energy consumer in Europe, using 40% of our energy, and creating 36% of our greenhouse gas emissions. By the end of 2030 all new building are proposed to be zero-emission which could be achieved by using wood as a building material, including for multi-story buildings.[1] Softwood is the most commonly used building material, but the proportion of this type of wood in forests is decreasing due to climate change. Despite unfavorable characteristics such as dimensional instability and weight, the increasing proportion of hardwood could be used in timber construction.[2] However, the inclusion of this wood requires a thorough understanding of all relevant properties for use in demanding environments. In this study, we investigated the influence of compression time (60, 120 min), fiber orientation (radial - R, tangential - T), and the use of a primer on the penetration depth of polyurethane adhesive in beech wood. The specimens were prepared according to the standard EN 302, testing the shear strength and then making sections with a microtome for electron and optical microscope preparations.[3]

Based on the microscopic images, the thickness of the joint and the depth of penetration of the adhesive into each panel were determined using computer tools. The results showed that adhesive penetration was best when the panels were bonded with a radial-tangential grain orientation at a compression time of 120 minutes.

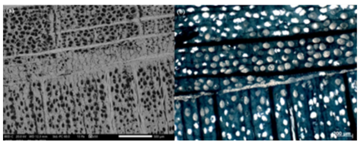

***Figure 1**: (a) SEM image of the adhesive joint between two plates with RT fiber orientation (sample thickness: 250 μm); (b) optical microscope image of the adhesive joint at 50x magnification: slide stained with 1% Astra blue FM solution (sample thickness: 200 μm).*

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Preparation of finish on cellulose fibres with nanoparticles of TiO_2, Ag and g-C_3N_4 with antimicrobial and photocatalytic performance

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Nanotechnology in textiles has already been well explored and nanomaterials show a great potential.[1] In this work, ternary nanocomposite for coating cellulose fibres, made of silver, titanium dioxide and graphitic carbon nitride, was successfully prepared. Its properties were compared to pristine cotton, fabric, coated with binary nanocomposites, and fabric, coated with single components only. Spectrophotometric analysis showed compatibility between components of coating which consequence in narrower band gap energy. That's why less energy is needed for electron excitation in case of ternary coating,[2,3] which was shown in coffee stains photodegradation experiment. Furthermore, it was shown that ternary coating made cotton fabric more protective against ultraviolet radiation and gives the best protection against bacteria (Figure 1) and viruses. Coated specimens were not cytotoxic. Experiments proved that thermic and mechanic properties of coated fabric haven't changed much. Cotton fabric, coated with this ternary nanocomposite was studied for the first time and has proven to be an effective sustainable solution for the textile functionalization.

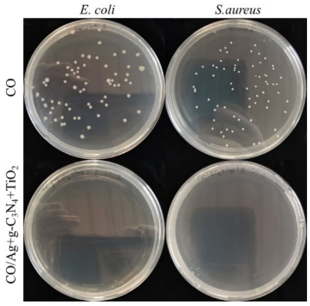

Figure 1: *Bacterial growth (E. coli and S. aureus) after incubation with samples of pristine cotton (CO) and cotton, coated with ternary nanocomposite (CO/Ag+g-C_3N_4+TiO_2).*

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Six G-quartet repeats as building blocks of tetrahelical DNA

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One of the most well-researched forms of noncanonical DNA are G-quadruplexes, which consist of at least two stacked G-quartets stabilised by monovalent cations. Each G-quartet is formed by four guanine bases in the same plane that are connected through Hoogsteen hydrogen bonds[1]. Recent bioinformatic analyses[2] of the reference human genome have discovered oligonucleotide sequences with the potential to form five and six stacked intramolecular G-quadruplexes. Such structures provide, due to the presence of an elongated stem, a prominent option for otherwise problematic specific targeting, which is why we decided to systematically study the influence of sequence and environmental factors on their formation.

We investigated the effects of gradual G-tract and loop elongation on oligonucleotide topology through means of magnetic resonance spectroscopy and polyacrylamide gel electrophoresis. We confirmed that titration with potassium cations promotes oligonucleotide folding, however, most samples displayed characteristics of a structural polymorphism. Thus we examined the influence of annealing, quenching and two-week-long incubation on folded structures, which allowed us to study thermodynamically and kinetically favoured topologies. We determined two parallel and one hybrid (3+1) topology with three G-quartets instead of the predicted five or six, which is a result of a limiting one-oligonucleotide loops being too short to span more G-quartets. We successfully demonstrated the formation of a six stacked intermolecular parallel G-quadruplex in absence of structural restraints in the loops.

Our deduction of conditions and structural restraints that influence folding of oligonucleotides with the potential to form five or six stacked G-quadruplexes is of great contribution to the assessment of novel approaches for specific G-quadruplex targeting and subsequent pharmaceutical applications.

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The influence of mix design and curing conditions to the mechanical properties of alkali-activated materials

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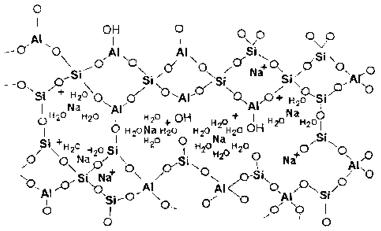
In the construction industry, it is becoming increasingly desirable to give more importance to the efficient and sustainable use of materials and the recycling of waste and by-products such as fly ash from thermal power plants, slag from the steel or construction industry, stone wool [1]. One such method is alkali activation, a chemical reaction between a solid aluminosilicate and an alkaline activator that forms a complex framework of tetrahedra. The resulting materials have similar properties to cement, concrete, and ceramics, but differ in composition [2]. The right balance must be found between the optimum conditions for sample preparation, curing, and the economics of the process.



***Scheme 1:** Model of aluminosilicate framework.*[3]

In the present work, electric arc furnace slag and stone wool were used as precursors for the preparation of alkali-activated materials (AAMs). Different mix designs with different particle size fractions, solid-liquid ratios, and two different alkali activators were prepared. The samples were characterized by studying the mechanical properties, chemical composition of the AAMs, the degree of reaction and leaching of potentially toxic elements from the final products to evaluate the potential use of the materials in different applications.

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In search of effective biological solutions against Xylella fastidiosa and its vector

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Xylella fastidiosa (XF) is a bacterial pathogen capable of infecting over 600 plant species, including olive, almond, figs, grapes. The bacterium is transmitted by a vector, *Philaenus spumarius* L., an insect feeding on xylem sap. One of the susceptible plants for the insect and the bacterium XF are olive trees, representing the historical heritage of the Mediterranean with agricultural importance for the local economy. Since the first detection of XF in 2013 in Italy, the bacterium has been alarmingly spreading mainly over parts of Italy, Spain, France, and Portugal, causing millions of trees to develop XF symptoms and eventually die. The severity of the disease means serious economic losses, and therefore combating strategies are needed. XF is regulated in the EU as a quarantine pest for which no effective treatment exists yet.[1] The BIOVEXO Project, funded by the HORIZON 2020 EU-BBI (now CBE) JU Framework, aims to develop environmentally sustainable and economically affordable biocontrol solutions for the prevention and treatment of XF infections to protect European agriculture and plants, particularly olive and almond. Two bacterial strains (BS), a microbial metabolite (MM), two plant extracts (PE), and an entomopathogenic fungus (EF) are being tested to combat XF and its vector, with our particular focus on one bacterial strain (Figure 1).[1,2]

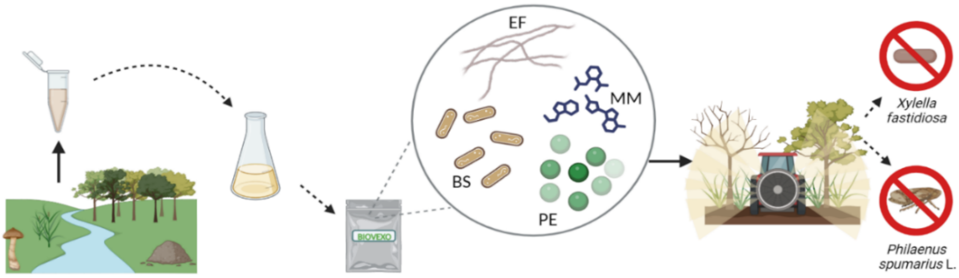

***Figure 1:** BIOVEXO biopesticides from natural sources, their production, and application in agriculture. BS, bacterial strain; EF, entomopathogenic fungus; MM, microbial metabolite; PE, plant extract. Created with BioRender.*

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The effect of methyl and butyl methacrylate in the hybrid sol-gel coating on corrosion protection of AA7075-T6

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The aerospace industry extensively uses aluminium alloy (AA) 7075-T6 due to its lightweight nature and passive response to atmospheric conditions. However, this alloy has low susceptibility to corrosion in chloride-containing solutions due to the presence of alloying elements like Zn, Cu, Mg, Si, etc.

Nowadays, numerous environmentally friendly surface treatments have been explored. Among these, the hybrid sol-gel coatings have been confirmed as an alternative to traditional corrosion protection methods reliant on chromate conversion treatments, which may include hazardous hexavalent chromium(VI). The sol-gel chemistry is based on the hydrolysis and condensation reactions of initial organically modified silica and silane reagents.[1] In addition, the coatings can be modified with different acrylate monomers to enhance the copolymerization.[1,2]

This study was focused on the hybrid sol-gel coatings with two different acrylate monomers applied on AA7075-T6. The coatings were prepared from organic precursors: 3-(methacryloyloxy)propyl trimethoxysilane and methyl or butyl methacrylate. The inorganic one was tetraethyl orthosilicate[1,2]. The solution and coating characterizations were cunducted by the Fourier-transform infrared spectroscope and a scanning electron microscope. The corrosion properties were evaluated by electrochemical measurements and by the Machu test during immersion in a corrosive medium.

The results indicated that synthesized hybrid sol-gel coatings form a continuous few micrometres thick film and o provide excellent barrier protection. The coating containing butyl methacrylate showed more durable corrosion performance in the studied medium than methyl methacrylate.

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Hydroxynaphthoic acid derivatives inhibit the growth of Gram-positive bacteria and interact with intracellular protein targets

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Bacterial resistance to conventional antibiotics is rapidly developing due to their overuse and misuse and poses a major threat to human health. Therefore, both the discovery and the development of novel antimicrobial agents against the most critical pathogens are urgently needed for the successful prevention and treatment of microbial infections[1].

It has been previously shown that two hydroxynaphthoic acid derivatives exhibit antimicrobial activity against different bacterial species[2]. The aim of our study was to test antimicrobial activity of selected hydroxynaphthoic acid derivatives, to find the most effective compound and to identify its protein target(s). Using various microbiology techniques, we identified 7-bromo-3-hydroxy-2-naphthoic acid and 1-hydroxy-2-naphthoic acid as the most potent compounds. Further characterization of antimicrobial activity by dilution antibiograms has shown that both compounds inhibit the growth of two Gram-positive bacterial strains, *Staphylococcus aureus* (Fig. 1), and *Bacillus thuringiensis*. We used 1-hydroxy-2-naphthoic acid as a starting compound for the synthesis of an affinity ligand. Furthermore, we were able to detect multiple cytosolic protein targets of 1-hydroxy-2-naphthoic acid in the soluble fraction of *S. aureus* lysate using affinity chromatography and found that a 25 kDa protein specifically binds to the ligand. On this basis, further research will focus on the identification of the detected protein targets in Gram-positive bacterial strains and the development of new compounds using hydroxynaphthoic acid derivatives as initial hits.

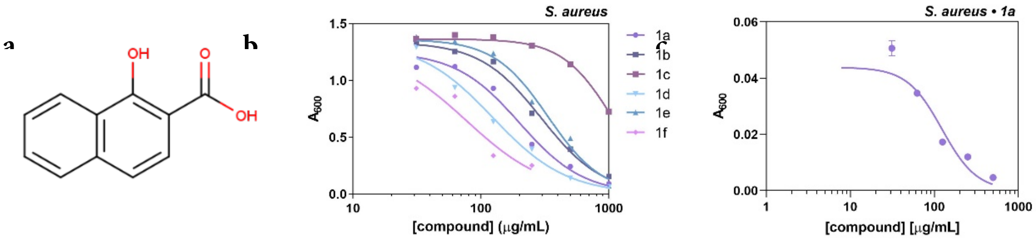

***Figure 1:** (a) Structure of 1-hydroxy-2-naphthoic acid and (b, c) dose-response growth inhibition curves of S. aureus with selected hydroxynaphthoic acid derivatives.*

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Creating a model system for production of nanobodies in yeast Saccharomyces cerevisiae

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Single-domain antibodies (nanobodies) have gained popularity in the last decade due to their stability and simple structure. Consisting of only one polypeptide chain, they can be synthesized by bacteria or yeasts as recombinant proteins, and still fold correctly[1,2]. This allows us to create production systems which are relatively cheap and accessible.

Upon transforming yeast cells with a plasmid containing a gene for a nanobody fused to alpha-factor signal sequence, the production is induced through an inducible promoter, then the nanobody is isolated. In this research, we show whether the suggested model system (Figure 8) is applicable for production of the chosen nanobody.

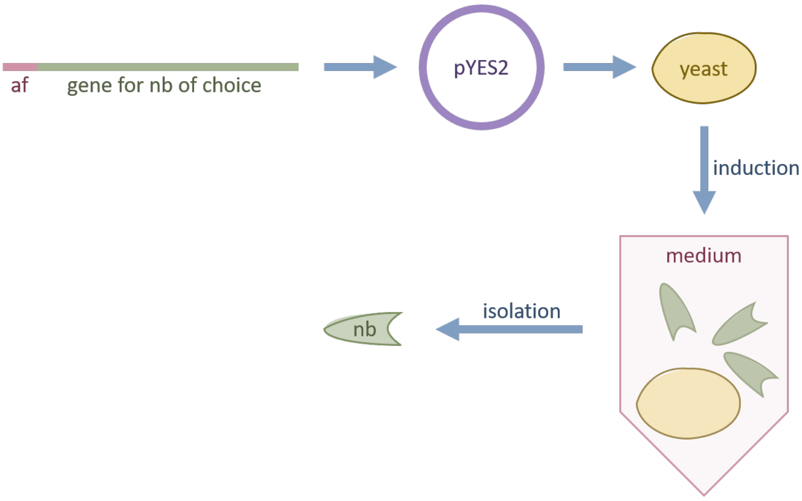

Figure 8: *Obtaining nanobodies from yeast cells. af: alpha-factor secretion signal; nb: nanobody; pYES2: plasmid with an inducible promoter; yeast: Saccharomyces cerevisiae.*

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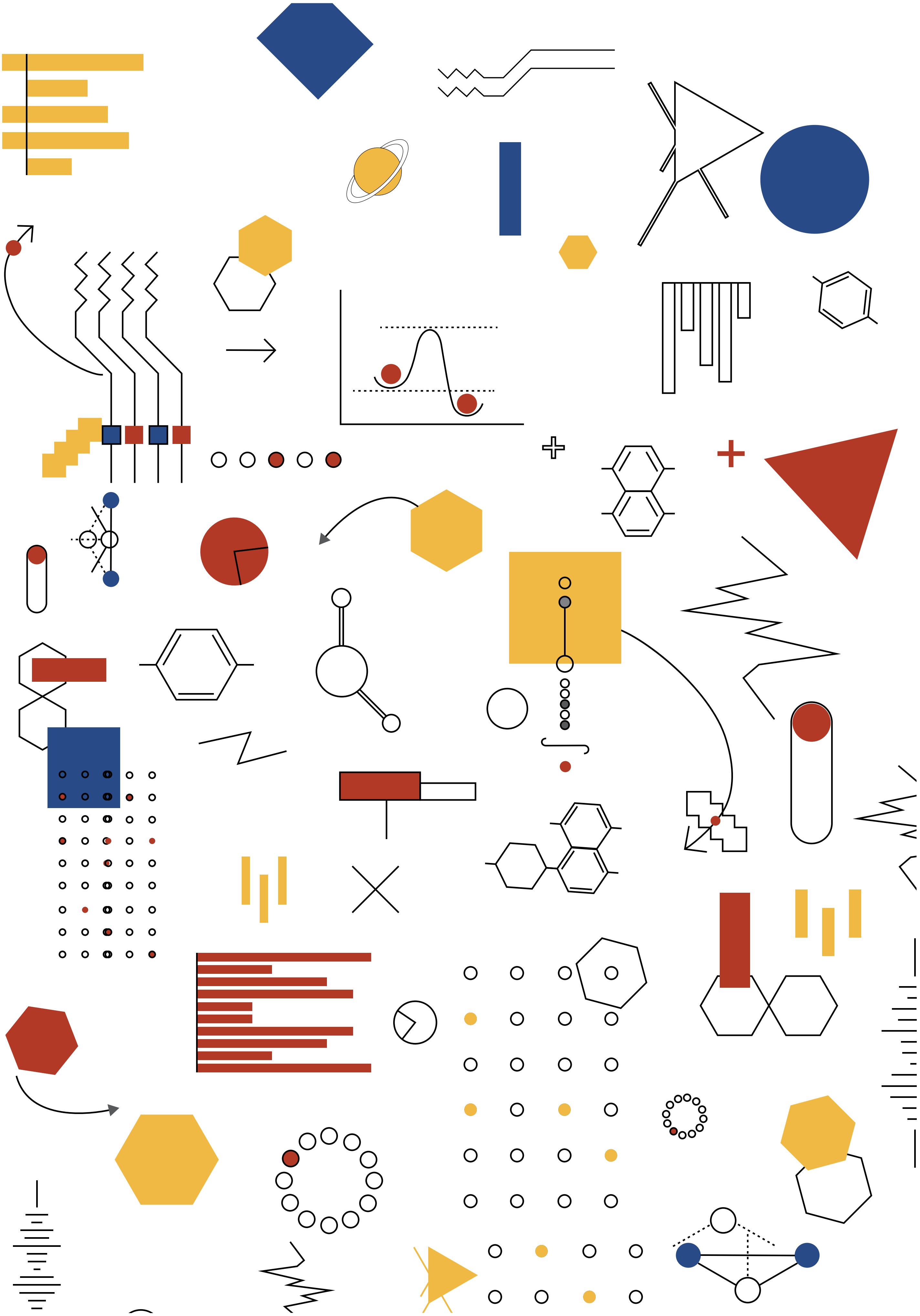
[1] Schoof, M. et al. An Ultrapotent Synthetic Nanobody Neutralizes SARS-CoV-2 by Stabilizing Inactive Spike. *Science* **2020**, 370 (6523), 1473–1479.

[2] de Marco, A. Recombinant Expression of Nanobodies and Nanobody-Derived Immunoreagents. *Protein Expr Purif* **2020**, 172, 105645.



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