NATURAL SCIENCE
BALTIC CONFERENCE

10-11.05.2025

BOOK OF ABSTRACT

nsbc.ug.edu.pl

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Information about The Natural Science Baltic Conference

The international "Natural Science Baltic Conference" (NSBC) took place, continuing the tradition of the popular Baltic Chemistry Conference. NSBC is a free international conference aimed at students and postgraduates, designed to enhance the scientific potential of young scientists. The event was completely free for both speakers and passive participants, attracting numerous attendees from various countries.

A total of 236 participants joined us, presenting 114 talks and posters, representing 37 different research institutions from 13 countries. This incredible outcome truly showcases the strength of our scientific community. We sincerely thank everyone for their participation and look forward to future gatherings that inspire further research.

Due to its interdisciplinary nature, the NSBC was divided into three thematic panels:

- CHEM PANEL: This panel featured research in the fields of chemical sciences, environmental sciences, ecology, and nanotechnology.
- BIO PANEL: This panel focused on biological sciences and biotechnology.
- PHYS PANEL: This panel covered topics in physical and mathematical sciences.

During the conference, young scientists, including students, doctoral candidates, and early-career researchers, had the opportunity to present their research findings and discuss popular science topics. Their presentations and posters were evaluated by members of the Scientific Committee, who selected the best ones.

NSBC was held exclusively online, enabling broad international participation without geographical limitations. The conference was a significant success, highlighting the growing importance of international collaboration and an interdisciplinary approach in the advancement of science.

We extend our heartfelt congratulations to all participants and award winners and thank everyone for their involvement in this year's edition of the Natural Science Baltic Conference.

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PhD Agnes Klar

University of Zurich

“A Next-Generation Dermo-Epidermal Skin Graft: Vascularized, Pigmented, and Fat-Enhanced”

Extensive skin loss due to trauma, burns, or disease presents a critical therapeutic challenge,particularlyin patients with limited donor sites for autologous grafting. To address this, we developed andcharacterized a novel bioengineered dermo-epidermal skin substitute (DESS) designed for clinical application 1,2. These skin constructs, composed of a stratified epidermis and a supportive dermal matrix, closely mimicthe structure and function of native human skin 3-5. Recently, DESS has successfully progressed to Phase 3clinical trials, underscoring its translational potential. To further enhance its clinical utility and physiologicalrelevance, we engineered an advanced skin construct incorporating a vascular component 6, 7for improved graft integration, melanocytes for pigmentation 8-10 (Fig. 1), and a third hypodermal fat layer 11to replicate full-thickness skin architecture. This next-generation, vascularized, pigmented, and fat-containing skin substitute offers a promising therapeutic option for patients with severe wounds, representing a significant advancement in regenerative medicine and skin reconstruction.

Special Guests

PhD Eng. Paweł Mazierski

University of Gdańsk

“Photocatalysis in 21st century: fundamentals and applications”

Photocatalysis has emerged as a very important technology in the 21st century,providing solutions to address urgent global issues in energy, environmental sustainabilityand chemical production. This presentation will provide a comprehensive overview of thefundamental principles of various photocatalytic processes, including light absorption,charge carrier dynamics, and surface redox reactions (Fig. 1) [1]. Special emphasis will beplaced on the advanced photocatalytic materials, such as heterojunctions, metal-organicframeworks, plasmonic nanostructures and hybrid systems, tailored for improving efficiency, selectivity and stability. Recent achievements in applications will be highlightedin view of hydrogen generation, CO2 reduction, air purification as well as organic synthesis. Case studies will illustrate the integration of photocatalysis in new technologies. Finally,the presentation will address current challenges and future directions to unlock the fullpotential of photocatalysis.

Presentations

A sustainable development perspective of marine recreational and sport fisheries in Kenya

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Abstract:

The marine recreational fishery also known as sport or game fishing in Kenya, has been practiced for several decades. Sport fishing is an important contributor to the socio-economic dynamics of coastal communities including provision of direct employment. This fishery was first introduced in Kenya in the 1950s and is mainly operated by private sport fishing clubs along the Kenya coast. We examined the status of marine recreational and sport fishery in Kenya using available information from published and grey literature sources. A total of 447 publications were initially retrieved and reduced to 15 after removing duplicates and those that did not meet the proper search criteria. We also assessed 17 grey literature records and historical data ranging from 1990 to 2006 from sport fishing clubs and boats.

Our findings indicate that sailfish belonging to family Istiophoridae dominated the fishery and that Malindi and Watamu were important sport fishing hotspots. Approximately, the fishery consisted of between 50 and 150 private and charter vessels with boat days declining from 1827 to 833 and 180 per fishing season in 1991, 2008 and 2021 respectively. Higher total numbers were recorded for the years 1991-1994, 2000 – 2001 and 2004 – 2005. Lowest numbers were recorded in 1996 and 2003. Within this 16-year period, the proportion of fish caught and released fluctuated due to various factors.

Our findings highlight that marine recreational and sport fishery in Kenya remain data deficient and are rapidly declining with the sub-sector conspicuously missing out from the annual national landings statistics and discourse on sustainable fisheries. Given the historical significance of these fisheries in Kenya, strengthening the various communities involved in the fishery will be crucial for revitalizing the opportunities that the fishery presents for livelihoods and ocean stewardship.

The authors acknowledge the Erasmus mobility fellowship, University of Szczecin Doctoral school and EFN Trudy fellowship for their support

First Principles and Machine Learning Investigations into Cement Hydrates' Atomic and Mechanical Properties

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Abstract:

Concrete is the second-most-used substance in the world after water, with more than 20 billion tons produced yearly. Yet, understanding the atomic and mechanical properties of the main component of the concrete, calcium-silicate-hydrate (C-H-S) cement hydrates – the complex binder phase of concrete –still poses a challenge [1].

In this work, we aim to investigate the atomic and mechanical properties of cement hydrates leveraging density-functional theory (DFT) and machine learning (ML) tools. We start by using DFT to study the electronic structure, bonding and mechanical responses of C-S-H at the atomic level [2]. Afterwards, we use ab inito molecular dynamics (AIMD) with ML to create a force filed on the fly for C-S-H, which will allow us to accurately simulate and capture the complex atomic interactions of cement hydrates while reducing the computation time. By integrating DFT, AIMD and ML, we seek to provide deeper insights into the fundamental properties of C-S-H and to develop a predictive model that could inform the design of new cementitious materials.

The author is sincerely grateful to Professor Henry Pinto for his valuable guidance and mentorship.

Literature:

[1] Qomi, M. J. A., Bauchy, M., Pellenq, R. J.-M. 2020. In Handbook of Materials Modeling: Applications: Current and Emerging Materials; Andreoni, W., Yip, S., Eds., Springer International Publishing: Cham, pp 1761–1792.

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Tracking cholesterol's role in colon cancer via Raman imaging, fluorescence, AFM, and chemometrics.

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Abstract:

Colorectal cancer (CRC) ranks as the third most frequently diagnosed cancer globally. Surgery remains the primary treatment approach for CRC. However, despite progress in surgical procedures, chemotherapy, and radiotherapy, CRC continues to be the second leading cause of cancer-related deaths worldwide. The significance of this public health issue drives ongoing research to develop new methods for rapid CRC detection and a deeper understanding of its risk factors.

In our study, we applied Raman spectroscopy and imaging to examine cholesterol levels in human colon tissues and cells, demonstrating an elevated cholesterol presence in colorectal cancer samples. Additionally, we used Raman techniques to investigate how mevastatin influences cholesterol biosynthesis. Our findings revealed that Raman spectroscopy and imaging are effective in assessing cholesterol levels in both normal and cancerous human colon tissues and individual cells. These methods also confirmed mevastatin's role in modulating the mevalonate pathway and reducing cholesterol levels. Chemometric methods, including Principal Component Analysis (PCA) and Partial Least Squares Discriminant Analysis (PLSDA), validated these observations. Furthermore, Atomic Force Microscopy (AFM) supported the beneficial effect of statins on cholesterol content, showing a marked increase in Young's modulus—a mechanical biomarker—in Caco-2 colon cancer cells treated with mevastatin compared to normal CCD-18 Co colon cells.

This work was supported by the National Science Centre of Poland (Narodowe Centrum Nauki) UMO-2017/25/B/ST4/01788 and by internal Grant no. W3/6D/2022 under the "FU2NFund for Upgrading the Skills of Young Scientists" program.

Literature:

[1] Beton, K., Wysocki, P., Brozek-Pluska, B., Spectrochim. Acta A Mol. Biomol. Spectrosc., 2022, 270, 120726; **[2]** Beton, K., Brożek-Płuska, B., J. Phys. Chem. B, 2022, 126(37), pp. 7088–7103.; **[3]** Julia Gala de Pablo et al., J Raman Spectrosc. 2018;49:1323–1332. [4] Abdullah S. Mondol et al., Analyst, 2019, 144, 6098.

Do tailocins matter? Insights from soft rot *Pectobacteriaceae.*

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Abstract:

Tailocins are phage tail-like nanostructures encoded in bacterial genomes and repurposed as precision weapons targeting closely related strains. In soft rot *Pectobacteriaceae* (SRP), tailocin production appears to be widespread and plays a role in shaping intra- and inter-genus interactions [1,2]. In our previous work, we demonstrated that tailocin-mediated killing is not uniform across SRP genera, with *Dickeya* spp. displaying broader activity than *Pectobacterium* spp. Comparative analysis of tailocin gene clusters among SRP strains revealed both conserved elements and strain-specific variations, potentially linked to differences in ecological targeting [2].

Building upon these findings, we investigated whether SRP-derived tailocins can influence microbial dynamics beyond their own group. Using a well-characterized model tailocin from *Dickeya dadantii* 3937 [1], we examined its impact on a diverse set of plant-associated bacteria occupying overlapping ecological niches. The results reveal diverse interspecies interactions, suggesting that tailocin-mediated competition may extend beyond genus boundaries.

Together, our data point to tailocins as potential microbiome-shaping agents, with ecological relevance that goes well beyond kin-killing. Whether these phage-derived structures act as opportunistic relics or they are a deliberate strategy applied by bacteria in environmental competition remains an open question — one we aim to answer.

This research was financially supported by the University of Gdansk via a research grant UGrants-start (533-BGB0-GS04-25) to Marcin Borowicz and by the National Science Center, Poland (Narodowe Centrum Nauki, Polska) via a research grant SONATA BIS 10 (2020/38/E/NZ9/00007) to Robert Czajkowski.

Literature:

[1] **Borowicz, M., Krzyżanowska, D.M., Sobolewska, M., Narajczyk, M., Mruk, I., Czaplewska, P., Pédron, J., Barny, M.-A., Canto, P.Y., Dziadkowiec, J. and Czajkowski, R.** (2025), Tailocin-Mediated Interactions Among Soft Rot *Pectobacteriaceae*. Mol Ecol, 34: e17728. https://doi.org/10.1111/mec.17728

[2] **Borowicz, M., Krzyżanowska, D.M., Narajczyk, M., Sobolewska, M., Rajewska, M. Czaplewska, P., Węgrzyn, K. and Czajkowski, R.** (2023), Soft Rot Pathogen *Dickeya dadantii* 3937 Produces Tailocins Resembling the Tails of *Peduovirus* P2. Frontiers in Microbiology 14: 1307349. https://doi.org/10.3389/fmicb.2023.1307349.

The influence of the chemical composition of FAME biofuel on oxidative stability

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Abstract:

Methyl ester fatty acids (FAME), or biodiesel, are produced by transesterification of vegetable oils or animal fats with alcohol, resulting in esters and glycerin. Biodiesel primarily consists of fatty acids with 16 or 18 carbon atoms, but some feedstocks, such as coconut oil, contain shorter-chain fatty acids like lauric acid [1].

In addition to esters, biodiesel contains small amounts of mono- and diacylglycerols, residual triacylglycerols, glycerin, methanol, free fatty acids, and sterols. The chemical composition affects biodiesel's cetane number and performance. Polyunsaturated esters reduce oxidative stability, while saturated esters affect low-temperature properties.

FAME may contain unsaturated double bonds or polyunsaturated fatty acids with multiple bonds separated by methylene groups. The oxidation stability of FAME follows the trend: C18:3 > C18:2 > C18:1, with reactive sites facilitating autoxidation. Bis-allylic sites, where double bonds are separated by methylene groups, play a critical role in oxidation.

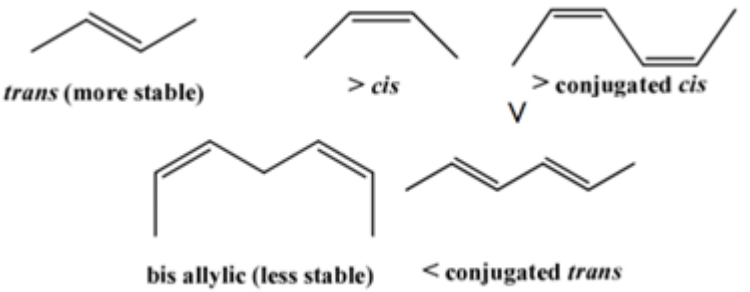

Fig. 1. The stability hierarchy of different alkene isomers

Polyunsaturated esters are more prone to oxidation than monounsaturated ones due to additional reactive sites, making FAME susceptible to oxidative instability [2].

Literature:

[1] Baczewski K., Kałdoński T. 2008. Paliwa do silników o zapłonie samoczynnym. Warszawa: Wydawnictwa Komunikacji i Łączności WKŁ. ISBN: 978-83-206-1705-4. 117-124.

[2] Ershov, M et al. 2022. Current challenge and innovative progress for producing HVO and FAME biodiesel fuels and their applications. Waste and Biomass Valorization, 14, 10.1007/s12649-022-01880-0.

Analysis of PolyP and DNA interactions with selected proteins

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Abstract:

Spatial separation within bacterial cells affects metabolic pathways by creating distinct local environments for proteins. One form of such compartmentalization may arise from condensates of polyphosphate (PolyP), resulting in the assembly of membrane-less organelles called 'PolyP granules'. PolyP is a linear polymer consisting of up to 1,000 phosphate (Pi) residues linked by ATP-like, high-energy phosphoanhydride bonds. Polyphosphate kinase (PPK) catalyzes the conversion of the terminal (γ) phosphate of ATP into PolyP, while exopolyphosphatase (PPX) hydrolyzes the terminal residues of PolyP to release inorganic phosphate (Pi). PolyP is conserved across all domains of life and is primarily synthesized in response to various environmental stresses, playing a key role in cellular survival. Moreover, it can substitute for ATP in kinase reactions, act as a reservoir of inorganic phosphate (Pi), and chelate metal ions such as Mg^{2+} and Ca^{2+}. Although some PolyP-binding proteins have been described in the literature, the structure, composition, and function of PolyP granules remain incompletely understood. Furthermore, the molecular mechanisms governing their assembly and disassembly have yet to be elucidated.

Our main hypothesis posits that PolyP may serve as an alternative scaffold for a number of proteins typically associated with DNA. Thus, it could alter the spatial distribution of protein activity, potentially leading to changes in their function.

To investigate this, I compared the interaction of selected proteins with PolyP versus DNA using Electrophoretic Mobility Shift Assay (EMSA) and Bio-Layer Interferometry (BLI). These comparative analyses address a key question: *How competitive is PolyP in binding DNA-associated proteins?* Additional experiments I performed provide insights into the PolyP–protein assemblies. Using Atomic Force Microscopy (AFM), I demonstrate which proteins influence the formation and maturation of PolyP condensates. By acting as a granule-forming scaffold for proteins, PolyP could play a pivotal role in shaping bacterial metabolism and coordinating responses to environmental challenges.

Investigating the therapeutic potential of morpholine-modified 1,3,5-triazines against colorectal cancer cell lines.

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Abstract:

Colorectal cancer (CRC) remains the second leading cause of cancer-related deaths worldwide. According to WHO data, in 2025 an estimated 2 million new cases and around 1 million deaths are expected. Alarmingly, an increasing number of cases are occurring in individuals under the age of 50. [1] Chemotherapy, primarily involving agents like 5-fluorouracil (5-FU), folinic acid, oxaliplatin, and capecitabine, remains the standard treatment for colorectal cancer (CRC). However, these cytostatic drugs often lead to severe side effects, and their overall efficacy has been questioned. Consequently, the focus is shifting towards personalized therapies with targeted drugs that promise enhanced safety and effectiveness. [2]

In 2020, Wróbel A. and colleagues reported that certain 1,3,5-aminotriazine derivatives exhibited cytotoxic activity against CRC cell lines, with the most potent compound demonstrating double the activity of 5-FU. [3] Building upon these findings, our research aimed to develop a new library of compounds with strong cytotoxic effects on CRC cell lines (SW480 and SW620) while sparing healthy cells (CCD841). We identified compounds with IC_{50} values below 10 μM, outperforming 5-FU. These compounds were synthesized using an innovative solvent-free, microwave-assisted method, allowing the generation of a diverse compound library in as little as 2.5 minutes.

The projectwas createdas part of the "DrugDesign" ScientificClub and the FutureLabPK (Project No. 68 A small molecule in a big battle – the search for a drug candidate for personalized therapy for colon cancer.)

Literature:

[1] Siegel, R. L.; Wagle, N. S.; Cercek, A.; Smith, R. A.; Jemal, A. 2023. Colorectal Cancer Statistics. CA Cancer J. Clin, 73 (3), 233–254.

[2] Krasteva, N., & Georgieva, M. 2022. Promising Therapeutic Strategies for Colorectal Cancer Treatment Based on Nanomaterials. Pharmaceutics, 14 (6), 1213.

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Fly Ash based Geopolymers: Bridging Waste Management and Sustainable Building Materials

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Abstract:
Fly ash, a byproduct of coal combustion in thermal power plants presents both environmental challenges and opportunities for sustainable construction. This study investigates the development of geopolymers using fly ash from the Gdansk Thermal Power Plant in Poland. Geopolymers are eco-friendly materials synthesized by reacting aluminosilicate source materials with alkaline solutions, offering durability and reduced environmental impact [1]. In this present study, geopolymer specimens were synthesized using fly ash and alkaline activators at different NaOH concentrations such as 6, 8, 10, 12, 14, 16, and 18 molars, respectively. The Na_2SiO_3 solutions were used along with the NaOH solution to initiate the reaction process. Mechanical testing (Compressive strength) indicated an optimal compressive strength value of 33 MPa was achieved with 14M NaOH solutions, attributed to enhanced geopolymerization. After 14 molar NaOH solutions, the strength shows the reverse trend. To correlate the mechanical properties, the fractured geopolymer specimen was characterized by FESEM, and FTIR, respectively. The lowest water absorption rate of 2.11% was achieved with the geopolymer specimen synthesized with 14 molar NaOH solutions.

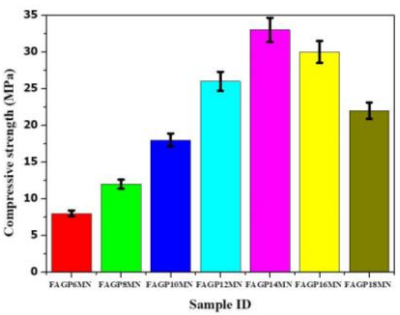

Fig. 1. Compressive strength of geopolymer specimen with different concentration of NaOH solution

Dipankar Das extends his heartfelt thanks to Fahrenheit Union of Universities in Gdańsk, Poland, for the Mayor of Gdańsk's Daniel Gabriel Fahrenheit Scholarship and the Department of Environmental Technology, University of Gdańsk, Poland.

Literature:

[1] Madirisha MM., Dada OR., Ikotun BD. 2024. Chemical fundamentals of geopolymers in sustainable construction. Materials Today Sustainability, 27:100842. https://doi.org/10.1016/j.mtsust.2024.100842

Investigation of catalytic activity, degradation and regeneration of platinum-doped perovskite for dry methane reforming

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Abstract:

Dry methane reforming (DRM) occurs when CH_4 and CO_2 (two greenhouse gases) react with each other in order to produce syngas, highly desired chemical resource. It is, however, highly catalyst driven and requires harsh temperature (over 600 degree Celsius) conditions. We propose to develop a catalyst based on ex-solved platinum nanoparticles on perovskite matrix. $(La_{0.3}Sr_{0.7})_{0.9}Ti_{1-x}Pt_xO_{3+\delta}$ perovskites with x = 0, 0.01, 0.02 and 0.05 were synthesized and characterized by x-ray diffraction (XRD), scanning electron microscopy (SEM) and Raman spectroscopy. Catalysts were tested in DRM experiments (employing gas chromatography for output determination).

Ex-solution process was successfully carried out for x = 0.01 and x = 0.02. Samples show promising dry reforming activity and regeneration ability, especially with more development in the future.

Chosen samples (in pristine, reduced, post-catalytic and regenerated forms) were additionally characterized by x-ray photoemission spectroscopy (XPS) at PHELIX beamline in SOLARIS. Acquired spectra show great differences in oxidation state structure between different samples, which provides insights for regeneration and degradation investigation.

Literature:

[1] Bhattar, S., Abedin, M.A., Kanitkar, S., & Spivey, J.J. (2021). A review on dry reforming of methane over perovskite derived catalysts. Catal. Today, 365, 2–23. https://doi.org/10.1016/j.cattod.2020.10.041

From biomass to beauty: Lignin valorization for sustainable hair conditioning solutions

Catarina Fernandes[1,2], Catarina Crespo[3], Ana Pocinho[3], Bruno Medronho[2], Luís Alves[1], Graça Rasteiro[1], Carla Varela[1]

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Abstract:

The use of cosmetic products is a highly popular practice. However, the increasing use of these products has raised concerns about their environmental impact. For example, some compounds commonly found in hair care formulations, such as cationic conditioning agents, are reported to be toxic to aquatic organisms [1]. The rinsing of hair care products results in their entry into wastewater systems, and, eventually, their discharge into rivers and oceans. These problems, and the increasing preference for natural products with low environmental impact, have motivated the research on renewable feedstocks for the development of cosmetic formulations [2]. Biopolymers, such as lignin, are excellent candidates to be used in bio-based formulations. Lignin is a natural polyphenol that can be seen as a multi-functional cosmetic ingredient for hair care, offering antibacterial, antioxidant, and sun-protective activities [2]. Lignin's hydrophobic nature can help to restore the hydrophobic barrier characteristic of healthy hair, and its functional groups allow chemical modifications, which can enhance the interactions with hair. In this work, lignin was extracted from acacia wood and then chemically modified to prepare cationic derivatives that could act as hair conditioning agents. The effect of the cationization conditions on the degree of substitution and surface charge of the prepared polymer were evaluated. The ability of these new lignin-based conditioning agents to efficiently repair damaged hair was assessed by evaluating their deposition into model surfaces of the hair. Lignin derivatives showed lower ecotoxicity to aquatic organisms of different trophic levels compared to a conventional commercial polymer (polyquaternium-11). These lignin-based conditioning agents were then incorporated into preliminary formulations and their stability and sensorial properties evaluated.

This work was financially supported by the Portuguese Foundation for Science and Technology (FCT) through the projects https://doi.org/10.54499/2022.06810.PTDC and https://doi.org/10.54499/UIDB/00102/2020. Catarina Fernandes acknowledges FCT for the PhD grant (https://doi.org/10.54499/2021.05991.BD).

Literature:

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Enhancing the antiproliferative activity of organoruthenium complexes using polydiacetylene nanocarrier

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Abstract:

Ruthenium complexes have been actively explored to overcome the limitations of platinum-based anticancer drugs clinically approved for treating different types of cancer. However, the clinical translation of Ru-based anticancer agents is significantly hampered by their poor stability, solubility issues, lack of specificity, and toxicity.[1] Several advantages can be exploited when the conventional metal complex is converted into metallodrug-nanoconjugate or by delivering metallodrugs using engineered nanocarriers.[2,3]

We prepared novel organoruthenium complexes bearing natural products/bio-active ligands, explored their structure-activity relationship, and investigated the molecular mechanism through which the complexes exert anticancer activity against different cancer cells. To further enhance the antiproliferative activity of complexes, two different strategies have been adopted using polydiacetylene-based nanosystems — physical encapsulation and chemical conjugation to achieve the sustained-release, enhanced cancer cell uptake, reduced In vivo toxicity, and real-time release monitoring of delivery.

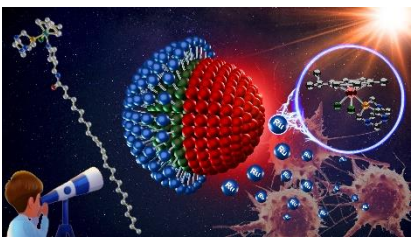

Fig. 1. Real-time release monitoring of metallodrug.

The author is sincerely grateful to the ANRF-SERB, India, for sanctioning the core research grant (CRG/2023/001155).

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Neuroprotective solution - potential role of tea in Alzheimer's disease

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Abstract:

Camellia sinensis is a plant from the Camelliaceae (Theaceae) family from which leaves tea is made. Tea infusion is the most popular version of this botanical product as well as one of the most consumed beverage globally. Green tea, in particular, is rich in polyphenols and has demonstrated various health benefits, including anti-inflammatory, anticancer, and neuroprotective effects, primarily attributed to its potent antioxidant capacity [1,2]. Alzheimer's disease (AD) is marked by progressive neurodegeneration and dementia. This neurodegenerative process is linked to the buildup of extracellular β-amyloid (Aβ) plaques and intracellular tau protein tangles within the brain.

A systematic review was conducted to consolidate and analyze data from published studies. Such approach provided a structured synthesis of methodologies and findings from existing research. The literature search was carried out using databases such as Google Scholar, PubMed, Scopus.

Green tea contains a range of polyphenolic compounds, including catechins like epigallocatechin gallate (EGCG), flavonoids as well as phenolic acids that possess potent antioxidant activity. These compounds deter production and activity of reactive oxygen species, mitigating mitochondrial damage and neuronal apoptosis associated with neurodegenerative processes [1,2]. EGCG was found particularly effective in decreasing β-amyloid accumulation and promoting tau protein clearance in neuronal cells. In Alzheimer's mouse models, EGCG significantly reduced Aβ levels in the hippocampus and frontal cortex. Another compound in green tea, L-Theanine, was found to improve hippocampal long-term potentiation in mice, thereby enhancing memory function [1,3].

The antioxidant compounds found in green tea may interfere with the molecular processes that drive neurodegeneration and the progression of AD. In addition to its protective effects on the brain, green tea has demonstrated anti-inflammatory and anticancer properties. However, more extensive research, especially involving human trials and additional in vivo models, is needed to validate these encouraging results.

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Unraveling the nature of SDSS J101353.45+492758.1: a weak emission line quasar with extreme X-ray weakness

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Abstract:

Most galaxies are believed to host a supermassive black hole (SMBH) at their center [1,2]. During their active phase, these SMBHs are fueled by accretion processes occurring in their surroundings [3,4], classifying them as active galactic nuclei (AGN). Weak emission line quasars (WLQs) form a peculiar subclass of quasars, the most luminous type of AGN. They exhibit extremely weak – sometimes undetectable – emission lines in the optical and UV bands, despite having a continuum similar to that of classical quasars. Since their discovery [5], WLQs remain a subject of debate, particularly regarding the estimation of the SMBH mass they host [6] and the nature of their environment [7].

The quasar SDSS J101353.45+492758.1 (hereafter J101353) is especially intriguing, as it shows almost no emission lines. Although weak, the Mg II line is visible. Additionally, this quasar is exceptionally faint in X-rays, raising questions about its environment and the mechanisms responsible for its emission lines. In this study, we analyze the broad-band spectral energy distribution (SED) of J101353 using a fitting approach to accurately determine its fundamental parameters. We also perform photoionization simulations to explore the optimal conditions for emission line production. By investigating different scenarios, we aim to explain both the extreme X-ray weakness and the absence of strong emission lines, particularly examining the role of a hot corona and a warm region, key components in the emission line formation process.

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Impact of the use of silver nanoparticles in potato cultivation

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Abstract:

One of the world's most numerous crops is the potato, which is exposed to unfavorable weather conditions affecting the development of bacterial and viral infections. In recent years, several plant protection products containing nanoparticles, especially silver nanoparticles, have appeared on the agricultural market. Silver nanoparticles are known for their broad antimicrobial properties. However, due to the nanoscale particle size, there is a risk of heavy metal accumulation in the edible parts of plants.

This study aimed to synthesize and verify the effect of foliar application of silver nanoparticles during potato vegetation. The applied silver nanoparticles were synthesized with sodium citrate and sodium dodecyl sulfate as stabilizing agents. The concentration of silver nanoparticles was 0.1, 1.0, and 10 mg/dm3.

The study showed that the accumulation of silver ions in potato tubers was observed for the AgNPs spray synthesized with SDS, however, the values were very low. The SDS synthesis method was more favorable in terms of the nutritional content of potato tubers. Using a lower concentration of AgNPs_SDS increased the content of phenolic compounds in the potato tuber. These correlations were confirmed by principal component analysis.

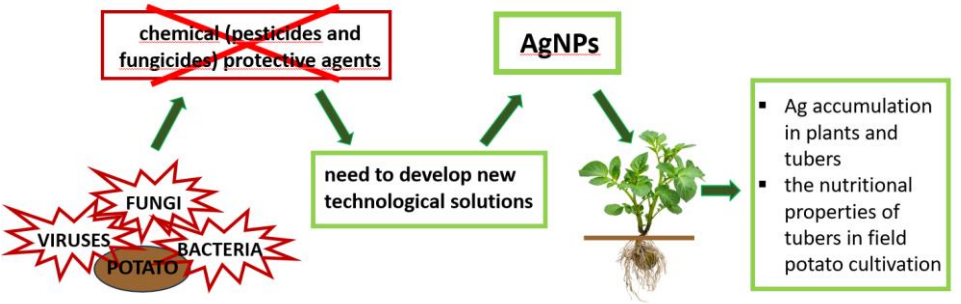

Fig. 1. The relationship between the methodology for obtaining AgNPs and Ag accumulation in plants and tubers and the nutritional properties of tubers in field potato cultivation.

Hybrid drug carriers: Combining SEDDS and polymer particles obtained by dewetting

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Abstract:

My research focuses on three types of drug carriers: self-emulsifying drug delivery systems (SEDDS), polymer particles deposited on a solid substrate, and a combination of both. Self-emulsifying drug delivery systems are three-component systems containing a lipid phase, surfactant, and co-surfactant. Mixing these ingredients yields a stable emulsion. Polymer (polylactide) particles deposited on a solid substrate are obtained by dewetting, a process where an unstable polymer layer disintegrates upon melting in contact with a high boiling point polar solvent. Upon cooling, the polymer forms solid particles attached to the substrate [1]. The third type of drug carriers includes structures prepared by fusion of emulsion droplets (SEEDS) onto polylactide particles supported on the substrate surface. The fusion results in polymer particles being covered with a thin layer of a liquid lipidic compound. The obtained systems have the potential to be used to incorporate guest species, e.g. doxorubicin (an anticancer drug).

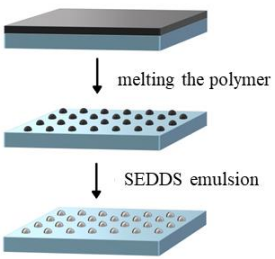

Fig. 1. Preparation of polymer particles with shells consisting of SEDDS.

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Enhanced Electrocatalytic Performance of NiB@NiCu(OH)$_2$/NF Electrode for Ammonia Oxidation Reaction

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Abstract:
The development of highly active and stable electrocatalysts The development of efficient, stable, and cost-effective electrocatalysts for the ammonia oxidation reaction (AOR) is crucial for advancing next-generation energy conversion systems and promoting sustainable fuel technologies. In this study, we report the design and fabrication of a novel nanostructured electrocatalyst, NiB@NiCu(OH)$_2$ supported on nickel foam (NF), synthesized through a facile hydrothermal approach followed by controlled dip-coating cycles.

Three variants were prepared with varying numbers of boron dip-coating cycles (5, 10, and 15) to systematically investigate the effect of boron content on catalytic performance. Comprehensive structural and morphological characterization using X-ray diffraction (XRD) and scanning electron microscopy (SEM) confirmed the successful formation of crystalline Ni(OH)$_2$ and the presence of Cu and NiB, which were homogeneously distributed on the surface of the NF substrate.

Electrochemical performance evaluation revealed a superior catalytic activity of NiB$_{10}$@NiCu(OH)$_2$/NF towards AOR, achieving a remarkable current density of 247.81 mA cm^{-2} at 1.55 V vs. RHE, along with the lowest charge transfer resistance (Rct) of 0.334 Ω, as determined by electrochemical impedance spectroscopy (EIS). The Tafel slope analysis indicated a Heyrovsky-like rate-determining step, implying rapid electron transfer and favorable reaction kinetics. The enhanced performance is attributed to the synergistic effects of boron incorporation, which facilitates strong intermediate adsorption and accelerates electron transfer, and copper modification, which contributes to improved electrical conductivity and structural stability.

This study not only demonstrates the effectiveness of compositional and morphological tuning in optimizing electrocatalytic activity but also positions NiB@NiCu(OH)$_2$/NF as a highly promising electrode for practical AOR applications. The findings provide valuable insights into the rational design of bimetallic and doped hydroxide-based electrocatalysts for energy and environmental technologies.

The author gratefully acknowledges Prof. Justyna Łuckzak for her valuable guidance. This work was funded by the National Science Centre, Poland (OPUS, UMO-2021/41/B/ST4/03255), and conducted at the Department of Process Engineering and Chemical Technology, Gdańsk University of Technology.

Tailored Interactions of Silica Nanoparticles with Intestinal Cells: Connecting Shape and Surface Chemistry with Barrier Function

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An in-depth understanding of the adaptive potential of the intestinal compartment to physical cues, including those derived from interactions with drug carriers, is essential for oral delivery applications. Taking advantage of the technological versatility of mesoporous silica nanoparticles (MSNs), spherical, rod-shaped, and virus-like materials were synthesized to evaluate morphology-dependent interactions with Caco-2/HT29-MTX-E12 cells. The novel quantification protocol developed for this aim combined live cell imaging and immunofluorescence data in correlation with cell viability and membrane integrity assays and mechanical measurements using atomic force microscopy [1]. Contributions of shape, aspect ratio, surface roughness, and size of the MSNs were explored, considering the influence of the mucus layer and intracellular uptake pathways. Several post-grafting strategies were additionally implemented for the functionalization of spherical particles and further examination of the influence of surface chemistry, charge, and colloidal stability [2]. Small particle size and surface roughness favored the highest penetration through the mucus but limited interaction with the cell monolayer and efficient internalization. However, the larger aspect ratio of the MSNs seemed to privilege paracellular permeation and increased cell-cell distances without hampering barrier integrity. Similar effects were observed for medium-sized spheres, modified with hydrophilic and negatively charged functionalities, which enhanced both mucus penetration and particle-cell interactions. The redistribution of tight junctions, privileged by phosphonated MSNs, seemed to be essential in membrane function, altering its adaptation and biomechanical compliance. Furthermore, the inhibition of clathrin-mediated endocytosis and modulation of the membrane architecture, organization, and fluidity effectively tuned these responses, confirming both morphology and chemically dependent interactions elicited by silica particles.

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Sustainable esterification of chlorogenic acid using lipase immobilized on spent coffee grounds: Characterization of a potential food additive

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Abstract:

Phenolic compounds in plants and fungi are gaining attention for their antioxidant, anti-inflammatory, and antimicrobial effects. Despite their promising bioactivity, their poor solubility in lipids limits their incorporation into fat-based food products. To overcome this, a technique known as *lipophilization* is used, which involves attaching hydrophobic groups—such as fatty acids or fatty alcohol residues—to enhance lipid solubility, typically through ester formation. In alignment with Green Chemistry principles, lipase enzymes can catalyse these biotransformations [1,2,3].

This study focused on the enzymatic modification of chlorogenic acid using a four-carbon alcohol catalyzed by microbial lipases immobilized on food waste material. Specifically, the biocatalysts were prepared by adsorbing lipases onto spent coffee grounds. These immobilized enzymes were then used in esterification reactions, followed by purification and analysis of the resulting ester to assess solubility and antioxidant activity.

The results demonstrated that this sustainable, waste-derived biocatalyst effectively catalyzed the targeted esterification reaction, yielding a specific chlorogenic acid ester, as confirmed by NMR analysis. The resulting compound maintained strong antioxidant activity—attributed to chlorogenic acid—while displaying increased lipophilicity. This dual hydrophilic-lipophilic nature broadens the potential applications of the ester, particularly as a functional additive in lipid-rich food systems.

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The effect of Mumio Shilajit combined with UVA and UVC radiation on MDA-MB-231 breast cancer cells and healthy VH10 human fibroblasts

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Abstract:

Mumio Shilajit is a substance used in unconventional treatment in Ayurvedic medicine. It occurs in the Himalayas, the Tibetan Plateau and the Altai. It is formed as a result of the death of organic plant matter. It is used in the treatment of diseases of the skeletal, cardiovascular and nervous systems, as well as in the treatment of skin diseases and diabetes. [1]

UV radiation is light invisible to humans, with a wavelength shorter than visible light. Due to the effects of ultraviolet radiation on living organisms, three types of this radiation are distinguished: UVA, UVB and UVC. UVA and UVC radiation were used in the research due to their use in medicine for photoradiotherapy (UVA) and anticancer radiotherapy (UVC). [2][3]

The aim of the study was to analyze the effect of UVA and UVC radiation in combination with Mumio Shilajit in MDA-MB-231 breast cancer cells and healthy VH10 human fibroblasts.

The tests used for examining cytotoxicity of mumio Shilajit alone and in combination with UV radiation is: cell cycle analysis, Annexin V apoptosis assay, clonogenic assay and MTS assay, for genotoxicity a gamma - H2AX assay.

The authors are sincerely grateful to dr A. Węgierek-Ciuk for valuable guidance and comments.

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Characterization of gelatin-alginate-inulin hydrogels for potential biomedical applications

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Abstract:

Wound healing is a complex process that requires a moist and supportive environment. Traditional dressings, such as cotton gauze, can be dry and stick to the wound, impeding healing. Hydrogel dressings offer a promising alternative due to their ability to keep the wound bed moist and promote healing. Additionally, hydrogel dressings can be created using 3D printing techniques, making them more personalized to the patient's needs. Gelatin-alginate gels are the subject of intensive research in the context of application in both dressing materials and 3D printing. An innovation of our research is the addition of inulin, which is a prebiotic, biocompatible polysaccharide. Although it is mainly used in the food industry, studies show that it can find applications in medicine and drug delivery systems.

The aim of this study was to investigate the specific properties of hydrogels based on gelatine, alginate, and inulin that could serve as dressing material. The hydrogels with different inulin contents were c subjected to mechanical properties analysis by compression tests to assess their hardness and elasticity, and thermogravimetric (TG) tests investigated thermal stability. Based on the results, it can be concluded that an increase in inulin content leads to higher hardness of the obtained hydrogels. However, thermogravimetric measurements indicate that these materials are less thermally stable.

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Does the length of the aliphatic chain affect the photophysical properties? - studies on the phenothiazine-triazole system

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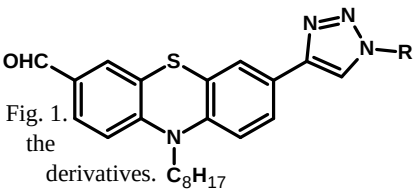
Abstract:

Heterocyclic compounds are a vital class of organic compounds due to their diverse photophysical and biological properties, making them applicable in various fields, including pharmaceuticals, medicine, and optoelectronics [1]. Due to the possibility of modifying their structure, they can play a key role in donor-acceptor systems, which enable fine-tuning of physicochemical properties through the appropriate selection of electron-donor and electron-acceptor fragments. This, in turn, facilitates the design of new materials with specific parameters.

In the present work, six triazole-based phenothiazine derivatives, differing in the length of the aliphatic chains at the triazole substituents, were designed and synthesized (Fig. 1). Additionally, the influence of aliphatic chain length on photophysical properties, such as absorption, emission, quantum yield in solvents of different polarities, and cellular bioimaging capabilities of the tested derivatives were investigated. The obtained results were interpreted based on quantum chemical calculations performed using the DFT method.



C6 R=C_6H_{13}
C8 R=C_8H_{17}
C10 R=$C_{10}H_{21}$
C12 R=$C_{12}H_{25}$
C14 R=$C_{14}H_{29}$
C16 R=$C_{16}H_{33}$

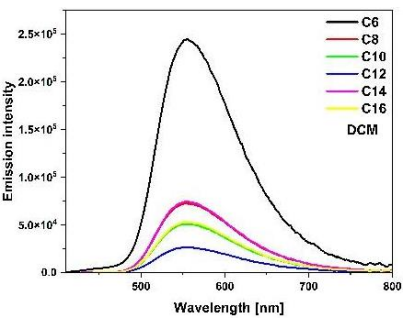


Fig. 1. Structures of obtained the derivatives.

Literature:

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EXPOSURE TO POLYSTYRENE NANOPARTICLES LEADS TO DYSFUNCTION IN DNA REAPIR MECHANISMS IN CACO-2 CELLS

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Nanoplastic (NP) occurs ubiquitously in aquatic and terrestrial environments, and its harmful biological effects have been observed in a variety of organisms, i.e. bacteria, plants, and animals [1]. Studies on human cells provide fundamental information on key mechanisms of toxicity that will provide answers to the question of whether and how NP poses a health risk. Mechanisms of toxicity mainly include membrane disruption, and production of reactive oxygen species, and may induce DNA damage including oxidative DNA damage (single-strand breaks, SSBs) and DNA double-strand breaks (DSBs) [2]. The emerging concern over environmental nanoparticles, particularly polystyrene (PS) nanoparticles, involves that there is some evidence suggesting that PS particles may be genotoxic in mammalian cells, however, the molecular basis is unclear [3].

This study investigates the interactions between NPs and an immortalized cell line of human colorectal adenocarcinoma cells (Caco-2) by exposing them to various NPs concentrations 50, 100, 400, 800, and 1200 μg/ml). The Caco-2 human epithelial cell line is a prevalent model for studying the intestinal epithelial barrier [4]. Derived from colon cancer, a noteworthy feature of this cell line is its spontaneous differentiation into a monolayer that closely resembles absorptive enterocytes functionally and morphologically, reflecting those found in the intestine.

We assessed potential cytotoxicity using viability tests (trypan blue and clonogenic assay) and explored NP genotoxicity *via* flow cytometry assays (PARP1-dependent apoptosis, cell cycle changes, and DSBs). Our findings indicate a moderate level of cytotoxicity due to PS, seen in both trypan blue and clonogenic assay. Moreover, our preliminary results demonstrated no changes in cell cycle distribution, no significant increase in the level of DSBs, and a minimal increase in the level of apoptotic cells. As we did not observe direct effects, we expect indirect effects mediated by other molecules (*e.g.*, induction of reactive oxygen species (ROS), inhibition of DNA repair mechanisms), therefore our future studies will determine ROS levels, oxidative DNA damage and expression of genes encoding proteins belonging to oxidative DNA damage repair pathways (base excision repair pathway, BER) [5].

Further investigations are still needed to understand the implications of environmental pollution on human health, particularly concerning the cytotoxicity and genotoxicity of NPs to evaluate the carcinogenic risk of NP [3].

This work was supported by National Science Center (NCN) Poland no. 2024/53/B/NZ3/01635 and System of Financial Support for Scientists and Research Teams – SGGW (Warsaw University of Life Sciences) No. S23007 to P.B.

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Investigation of the structural and electrical properties of nanocomposite $SiO_x(Si)\&Fe_yO_z(Fe)$ films depending on the annealing temperature

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Abstract:

Nanocomposite films with the metal and silicon nanoinclusions in an oxide matrix can be used for a variety of applications due to their unique and useful properties [1]. The purpose of this work is to investigate the influence of the annealing temperature in the range of T = 400-1000 °C on the structural and electrical characteristics of nanocomposite $SiO_x(Si)\&Fe_yO_z(Fe)$ films.

Fig. 1 shows the *I-U* characteristic of the initial sample measured in the temperature range from 95 K to 340 K, where the dielectric-metal transition can be distinguished. This transition shifts to the lower voltages as the annealing temperature increases, which is related to the structural transformations investigated using X-ray diffraction, IR spectroscopy, and Raman spectroscopy methods.

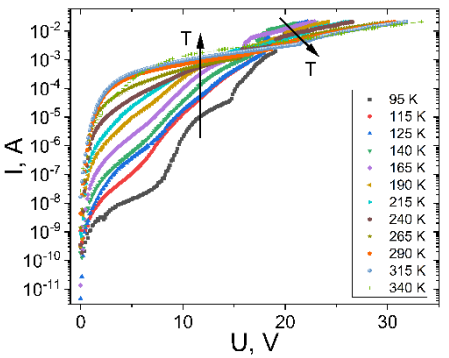

Fig. 1. *I-U* characteristics of the initial sample in semilogarithmic coordinates. The direction of the temperature increase is indicated by arrows.

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Single-Click Approach to Molecular Docking-Based Virtual Screening via SwiftDock

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Abstract:

Molecular docking-based virtual screening (MDVS) is a computational approach used to dock libraries of small molecules against a target macromolecule to identify potential lead compounds exhibiting favorable bioactivity [1]. Various VS tools, including PyRx, InstaDock, and MultiDock Screening Tool, perform this task employing docking software such as AutoDock4 (AD4) and AutoDock Vina (ADV) [1,2,3,4,5]. Although several automation scripts and software solutions are available to facilitate VS using AD4, none offer a fully automated single-click workflow encompassing file preparation, docking execution, and optimal pose extraction. To address this gap, we introduce SwiftDock (https://github.com/notacoder-dz/SwiftDock), an open-source virtual screening tool for Windows users that performs a fully automated AD4-based MDVS with a single click, thereby eliminating the need for prior expertise or usage knowledge of the necessary software. SwiftDock should be deployed in a working directory containing protein and ligand files, then executed to carry out all required pre-docking, docking, and post-docking steps automatically. Despite certain limitations, SwiftDock aims to enhance the accessibility of MD and VS for non-bioinformaticians, facilitating experimental and therapeutic research.

The authors extend their deepest gratitude to everyone who has played a part in shaping this work and contributing to its fruition.

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Pyrochlore thermoelectric materials, based on oxide/oxide and oxide/metal alloy composition.

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Abstract:

Pyrochlore oxides are dielectric materials used in various industries, such as the atomic industry, electronics, and catalysts [1]. Thermoelectric properties are closely related to carrier concentration and band gap size. As a result, pyrochlore oxides typically exhibit low thermal and electrical conductivity, along with a high Seebeck coefficient off mV/K order [2]. However, the figure of merit (ZT) for standalone pyrochlore oxides is low, making them unsuitable for thermoelectric applications.

A multicomponent system was used to improve thermoelectric properties. In recent years, multicomponent compounds have been under intense investigation across various materials for their ability to modify and enhance material properties. One of the changes is the reduction of lattice thermal conductivity in materials, mostly thanks to increased phonon scattering [3].

In this work, two pyrochlore oxides were synthesized, $SrBi_2Ti_2O_7$ (SBTO) and multicomponent pyrochlore oxide $(Zr_{0.2}Sn_{0.2}Ti_{0.2}Hf_{0.2}Fe_{0.2})(Sr_{0.25}La_{0.75})O_7$ as (MEPO). Each one was combined with different compounds to enhance its thermoelectric properties. The first composite is based on SBTO with $La_{0.7}Sr_{0.3}CoO_3$ (LSTO), and the second is based on multicomponent pyrochlore oxide (MEPO) and metal alloy (Fe-Cu).

X-ray Diffractometry (XRD) and Scanning Electron Microscopy (SEM) were used to study the structure and microstructure of the materials. The temperature dependence of the total Seebeck coefficient was measured and analyzed. For electrical conductivity measurements, dependent on temperature, a DC four-wire technique was used. During the experiment, measurements of the Seebeck coefficient and electrical conductivity were held in two different atmospheric conditions, with high and low concentration of water vapour.

Financial support of these studies from Gdańsk University of Technology by the DEC-2/1/2023/IDUB/III.1a/Ra grant under the RADIUM - 'Excellence Initiative - Research University' program is gratefully acknowledged.

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The effect of TiO_2 nanotubes reduction for wastewater treatment by photocatalysis

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Abstract:

Different water contaminants, such as pharmaceuticals and personal care products, are being detected in water resources worldwide, due to the inefficacy of municipal wastewater treatment plants (WWTPs) in removing them [1].

The use of advanced oxidation processes, namely photocatalysis, can be a possible solution to implement in WWTPs and decrease this problem. These processes use the •OH radicals to efficiently destroy the organic contaminants into CO_2 and H_2O [2].

The use of powders and artificial radiation can be a barrier to implement this technology at real-scale. Thus, anodized TiO_2 nanotubes can be a suitable solution since it can be easily separated from water and reused several times [3]. Moreover, the introduction of oxygen vacancies by a simple thermal treatment in reducing atmospheres (as H_2/Ar) can suppress the recombination of electron-hole pairs and enable visible light activity leading to improved photocatalytic activity [4].

Therefore, in this work it was studied the reduction of anodized TiO_2 nanotubes by evaluating their photocatalytic activity towards the remediation of water contaminated with phenol or parabens.

The authors gratefully acknowledge to the Foundation of Science and Technology – FCT (Portugal) for the PhD grant (2021.06221.BD) and the financial support (CEECIND/01207/2018, UIDB/00102/2020 and UIDB/05183/2020).

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Design, synthesis and antimicrobial activities of fluconazole-based conjugates containing antimicrobial or cell penetrating peptide

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Abstract:

The increasing challenge of antimicrobial resistance necessitates the exploration of alternative therapeutic strategies. One promising approach involves the development of conjugates composed of antimicrobial drug and peptide, such as antimicrobial peptide (AMP) or/and cell-penetrating peptide (CPP). These conjugates are chemical compounds formed by a covalent bond between two molecules, typically of different chemical natures, which may exhibit new or improved biological properties compared to the original components. The design and synthesis of such conjugates with azole drugs may lead to molecules with synergistic activity and enhanced selectivity [1].

We report here chemical synthesis and biological activity of conjugates of antifungal drug fluconazole (FLC) with peptides named as P5 and P9 –fragments of a helical domain of type I interferon from *Aristicluthys nobilia*, which show significant activity against methicillin-resistant *Staphylococcus aureus* (MRSA) strains [2]; and Pep39 – a cationic marine-derived peptide with cell-penetrating properties and the ability to deliver biological cargo [3]. In all studied conjugates, glutaric acid served as a linker, forming covalent bonds between hydroxyl group of FLC and *N*-terminal amino group of the peptide (ester and amide moieties, respectively).

The resulting conjugates were subjected to antimicrobial profiling against selected strains of yeast as well as Gram-positive and Gram-negative bacteria. Broth microdilution method for MIC determination was used as a measure of antimicrobial activity**.** Our research showed that the P5 peptide and its conjugate have promising activity against selected fungi (*C. glabrata*, *C. krusei*, *C. albicans*) and bacteria (*B. subtilis*, *P. aeruginosa*). However, cytotoxicity assays on cancer and non-cancer cell lines indicate that the tested conjugates induce a relatively high cytotoxic effect (especially on the latter) compared to antibiotics widely used in the clinic. Therefore, they cannot be considered good candidates for drug development and need some modification and further research.

The research was funded by BMN (No. 539-T060-B137-24) and *BMN (No. 539-T060-B184-25)*

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Multifunctional Laser-Induced Graphene Sensors Enabled by Neutral-pH Aniline Electropolymerization

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Abstract:

Laser-Induced Graphene (LIG) electrodes represent a promising class of carbon-based materials for electrochemical sensing owing to their low production cost, reproducibility, high surface area, and facile functionalization.

In this study, we explore the LIG electrodes as versatile platform for sensing through tailored surface modifications to extend their sensing capabilities. First, electropolyemrization of aniline on LIG surface was performed at neutral pH conditions (pH 7.4), using polystyrene sulfonate (PSS) as a dopant. This approach allows the formation of a stable, fiber-like morphology for polyaniline (PANI) under mild conditions, overcoming the challenge associated with polymerization at acidic pH. The resulting PANI-LIG electrodes enabled the sensitive detection of β-blockers - metoprolol and propranolol - showing increasing current with concentration and significantly reduced limits of detection compared to unmodified LIG. Additionally, the electrode showed a strong pH detection capability, highlighting its potential application as multiplexed sensing platform.

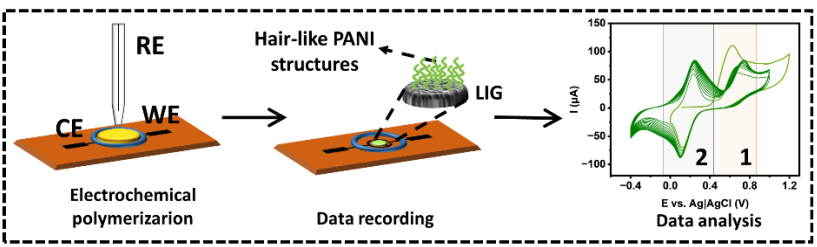

Fig. 1. Scheme of LIG modification.

This work was supported by the National Research Centre, Poland, grant no. 2023/51/I/ST7/01948.

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The role of Elongator as a translation regulator during plant photomorphogenesis

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Abstract:

Elongator is a protein complex composed of six subunits that occurs among all eukaryotes [1, 2]. In plants the complex is involved in seedlings development in light, called photomorphogenesis [3]. However, it is not entirely clear how Elongator regulates this process, because the complex is multifunctional and active in both nucleus and cytoplasm. In plants, the nuclear pool of Elongator is involved in the regulation of transcription by histone acetylation [4], while in cytoplasm it regulates the efficiency of translation by carrying out the modification of the 34th uridine of certain tRNAs [5]. What remains to be explored is how plant Elongator combines its two activities in both transcription and translation regulation and which one is dominant. To date, research has mainly focused on the role of the complex in regulating gene expression at the transcriptional level.

In order to fully assess both activities, a proteomic analysis has been carried out. For this purpose, global proteins were isolated from the plant sample and fractionated on SDS-PAGE, followed by quantification of the proteome using Shotgun-type label-free comparative analysis. On the basis of the data obtained, an ontological analysis was carried out using Dicots Plaza 5.0 software. Through subsequent comparison of the proteomes with the transcriptomes of the wild-type and *elo3-6* mutants, it will be possible to determine the interplay between the transcriptional and translational activities of the plant Elongator.

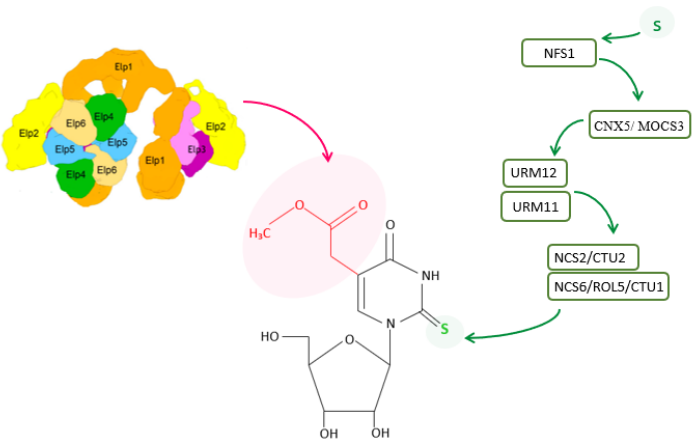

Fig. 1. Scheme of the modification of 34th tRNA uridine [5, 6, 7]

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Post-Synthetic Metalation of Al-PMOF for Enhanced Visible-Light CO_2 Photoconversion

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Abstract:

Porphyrin-based metal–organic frameworks (MOFs) have emerged as highly tunable platforms for photocatalytic CO_2 reduction. In this study, the visible-light-driven CO_2 photoconversion efficiency of an aluminum-based porphyrin MOF (Al-PMOF) was systematically tuned through post-synthetic incorporation of transition metals (Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}). The effects of metal identity and cobalt loading on the structural integrity, charge separation dynamics, CO_2 adsorption, and formic acid generation were investigated using a combination of spectroscopic, microscopic, and photochemical analyses. Among the modified materials, Al-PMOF(Co) with 8 wt.% loading exhibited superior activity (90 $\mu mol \cdot g^{-1}$ HCOOH in 4 h), attributed to improved charge separation and maintained crystallinity. In situ DRIFTS and GC-MS revealed mechanistic insights into reaction intermediates. This work highlights the potential of rational metalation strategies in porphyrin MOFs to engineer efficient and reusable photocatalysts for sustainable CO_2 utilization [1].

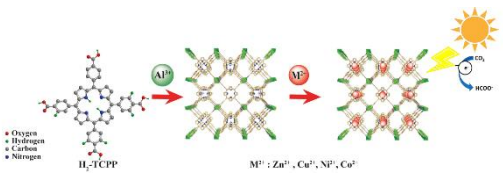

Fig. 1. Schematic illustration of the post-synthetic incorporation of transition metals (M = Co, Ni, Cu, Zn) into the Al-TCPP framework to yield M-Al-PMOF hybrids with enhanced photocatalytic CO_2 reduction performance. The structural integrity of the MOF is retained while the metalation of the porphyrin core introduces new active sites, improving charge separation and promoting visible-light-driven formic acid production

This research was supported by the Polish National Science Center under the grant 2021/41/B/ST4/00849.

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The Overview of Side effects from epidural analgesia

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Abstract:

Epidural anaesthesia involves injecting local anaesthetics and adjunct drugs into the epidural space (Fig.1) to block nerve signal transmission [1-3]. Amide-type anaesthetics like bupivacaine, lidocaine, and ropivacaine act by inhibiting voltage-gated sodium channels, preventing pain signal propagation [4-8]. Their effectiveness depends on properties such as lipid solubility, protein binding, and pKa. Opioids like fentanyl or sufentanil are often added to enhance analgesia via μ-opioid receptor activation, allowing for lower anaesthetic doses and reduced motor block [4]. Vasoconstrictors such as epinephrine may also be included to prolong action and limit systemic absorption [5-6]. While effective, epidural anaesthesia carries risks, including neuro- and cardiotoxicity—especially with bupivacaine due to its strong cardiac sodium channel affinity [1,3]. This study compares the mechanisms of these substances and their associated side effects.

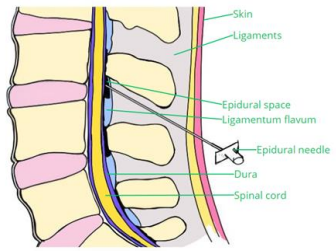

Fig. 1. Epidural needle insertion

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Selective functionalization of borylsilylalkenes *via* coupling reactions

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Abstract:

Borylsilylalkenes, due to the presence of boryl and silicon groups with different reactivities, represent an interesting group of building blocks in organic chemistry. These compounds can be modified using demetallation and cross-coupling reactions, leading to various possible products, such as tri- and tetrasubstituted olefins, which are highly valuable as they are present in anti-cancer drugs [1] or fluorescence materials. Developing procedures of regio- and stereoselective functionalization of borylsilylalkenes is essential for their implementation as building blocks. Borylsilylalkenes can be obtained using various reactions types, but *E* isomers are more difficult to obtain [2].

During the study [3], the functionalization of (*E*)-1,2-diboryl-1-silylethenes *via* Suzuki-Miyaura coupling reactions was optimized. The processes were carried out in a stepwise manner, allowing selective substitution of one or both boryl groups in a single step, as well as modification with two different aryl groups. This approach allowed for the precise optimization of each reaction step. The type of reactants used, catalyst concentration, type of solvent, reaction time, and temperature were optimized to obtain products with the highest possible yield and selectivity.

As a result of study, functionalization protocols of borylsilylalkenes *via* Suzuki-Miyaura coupling were developed. As part of the research, 21 functional alkenes were synthesized, 17 of which were obtained for the first time. The products were fully characterized by ^{1}H, ^{13}C, ^{29}Si, ^{11}B NMR spectroscopy, as well as GC MS. Additionally, the structures of 3 products were successfully confirmed by crystallographic analysis. The successful synthesis of these compounds demonstrates the compatibility of various functional groups with this protocol, leading to the formation of a wide range of substituted olefins.

Financial support from National Centre for Research and Development: Lider 9 programme (LIDER/6/0017/L-9/17/NCBR/2018) and Adam Mickiewicz University: ADVANCEDBestStudentGrant II (075/39/ID-UB/0011)

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Artificial Intelligence in Environmental Health: Modeling micro- and nanoplastics cytotoxicity

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Abstract

This study explores how machine learning techniques can enhance our understanding of the cytotoxic effects of micro- and nanoplastics on mammalian cell lines. By developing predictive computational models, we aim to assess potential health risks posed by these particles without relying solely on time-consuming and costly laboratory experiments. This data-driven approach contributes to environmental toxicology by offering faster, scalable tools for risk assessment and supporting the development of evidence-based strategies to protect both ecosystems and human health. In this context, machine learning has already proven useful in environmental sciences, helping to identify patterns and predict toxicological effects with increasing accuracy [1,2].

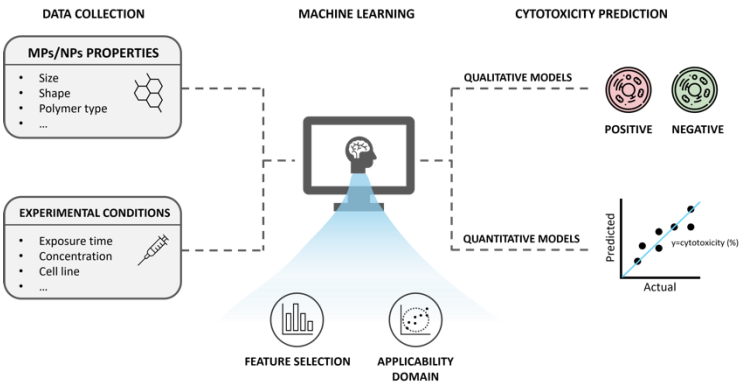

Fig. 1. Machine learning for micro- and nanoplastics cytotoxicity predition.

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Computational studies of the metal-organic framework MIP 202(Zr): stability, electronic structure, and defects.

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Abstract:

Metal-organic frameworks (MOFs) exhibit high porosity, large surface area, and numerous active sites, making them promising candidates for photocatalysis. Unlike conventional photocatalysts, MOFs can self-adjust their electronic and optical properties without additional species, enhancing their photocatalytic efficiency [1]. MIP-202(Zr) [2], based on L-aspartic acid, is particularly notable for its sustainability, scalability, and biocompatibility. This study aims to computationally analyze MIP-202(Zr) based structures through density-functional theory (DFT), exploring structural modifications such as metal exchange (e.g., Ti^{4+}), metal doping, and structural defects. These modifications tune the charge separation, band gap, and overall photocatalytic performance. However, DFT is computationally expensive for large systems such as MOFs. To tackle this limitation, machine learning (ML) techniques are employed to predict the stability and properties of modified MOFs more efficiently by capturing structure-property relationships. Specifically, the ML force fields (MLFF) feature in VASP enables the automatic generation and refinement of force fields through on-the-fly training based on MD simulations, significantly accelerating the prediction of forces, energies, and other dynamic properties [3].

This approach facilitates the selection of modified MOFs with enhanced photocatalytic performance, contributing to renewable energy solutions in response to global energy and environmental challenges.

The authors acknowledge Yachay Tech University's support and fruitful collaboration with the University of Gdańsk and QSAR Lab in Poland.

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First principles investigation into the electronic structure of disordered $Ba_{0.5}La_{0.5}CoO_3$ perovskite

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Abstract:
In this work we present the results of a theoretical study of the electronic structure of a perfect $Ba_{0.5}La_{0.5}CoO_3$ using the density functional theory (DFT) approach [1]. $Ba_{0.5}La_{0.5}CoO_{3-\delta}$ is known to exhibit high catalytic activity and mixed ionic-electronic properties that make it a suitable candidate for cathode materials used in protonic fuel cells [2]. The pseudopotentials used for DFT were obtained using a novel multi-objective evolutionary algorithm based on decomposition approach (MOEA/D). [3] The hard pseudopotentials generated using MOEA/D give more accurate total energies, lattice parameters, bond lengths, band dispersions and band gaps than soft pseudopotentials. [1,3,4] Hard pseudopotentials are better suited for calculations involving the defect chemistry and catalytic reactions in defective $Ba_{0.5}La_{0.5}CoO_{3-\delta}$.

(a) (b)

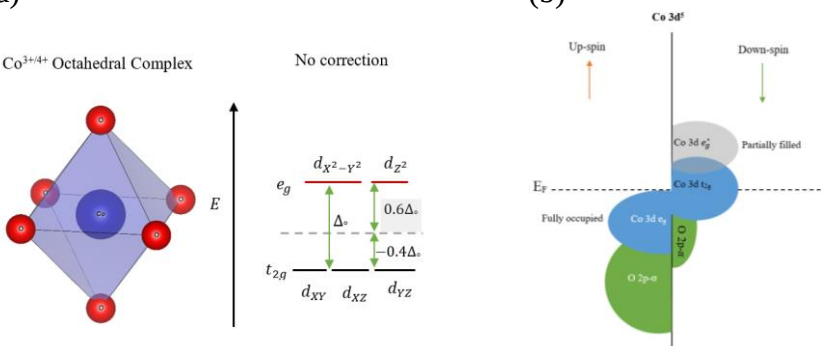

Fig. 1. Illustrative model of crystal field and exchange splitting at the $Co^{3+/4+}$ octahedral

The results to be presented include the Pareto fronts of Ba^{2+}, La^{3+}, $Co^{3/4+}$ and O^{2-} for eigenvalues, norms and energies**.** In addition, the bandstructure of $Ba_{0.5}La_{0.5}CoO_3$, total density of states and partial density of states of the Co3d will also be presented.

The author is grateful to the super-computing center at Gdansk University of Technology for providing computational resources for this work.

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Inhibition of PTP-1B as a chance to defeat cancer

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Abstract:

The purpose of the research is to synthesize selective inhibitors of the PTP-1B enzyme. I am going to achieve it by synthesizing peptides that are derived from APRs of the PTP-1B enzyme. These peptides should cause aggregation of PTB-1B molecules and decrease its activity.

PTP-1B is involved in the development of many types of cancer. PTP-1B is involved in carcinogenesis by activating the non-receptor tyrosine kinase Src. Increased Src kinase activity has been observed in many types of human cancer. Many studies have shown that PTP-1B can act as an activator of Src kinase, increase tumorigenesis, and promote tumor progression of cancer cells. The role of PTP-1B in the process of carcinogenesis has been particularly noted in the case of breast cancer. This enzyme probably plays a role as a promoter of this cancer development. PTP-1B increases the proliferation of breast cancer cells and simultaneously inhibits their apoptosis, which indicates that it greatly "helps" breast cancer to grow. The inhibition of this enzyme should help to stop the development of cancer.

The author is sincerely grateful to Dr Julia Witkowska for supervising the project.

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Advanced oxidation processes for azole degradation: a potential alternative or supplementary wastewater treatment

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Abstract:

Azole compounds demonstrate significant biological activity and are commonly used as antifungal agents in medicine, personal care products and agriculture for crop protection. Given their extensive application, the detection of azole compounds has been reported in surface water, groundwater, and wastewater in various countries [1]. Due to their high resistance to hydrolytic, photolytic and biological degradation, azoles are not effectively removed by conventional methods used in wastewater treatment plants, such as biodegradation using activated sludge [2]. To address this limitation, advanced oxidation processes (AOPs) may serve as an alternative or supplementary process in the removal of these contaminants. These include photochemical processes with the use of ultraviolet (UV) radiation and chemical processes involving strong oxidants such as Fenton's reagent, ozone, or persulfate ions, as well as integrated approaches that combine these techniques [3].

The purpose of this study was to perform the degradation of azole compounds by advanced oxidation processes and to optimize the process conditions. To better recreate the conditions at a wastewater treatment plant, treated wastewater from the facility was also used as the matrix in the favorable conditions. Samples were taken at specific time intervals and analyzed using high-performance liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS).

The results indicate that complete removal was obtained for most azoles tested in the photodegradation process. The action of UV radiation is also sufficient to remove azole compounds from the treated wastewater matrix, demonstrating the potential of this technique as a complementary wastewater treatment method in treatment plants.

This work was supported by the Polish Ministry of Education and Science (0911/SBAD/2506).

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Second life for used cigarette filters

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Abstract:

In the era of growing environmental awareness, increasing attention is being paid to the search for innovative solutions aimed at protecting the environment. One of the most serious ecological problems remains the leakage of petroleum into aquatic environments. It is estimated that every year, one hundred million gallons of oil are uncontrollably spilled into water bodies, which poses a significant threat to marine life and ecosystems. [1] In response to this challenge, scientists have proposed the use of spent cigarette filters as oil sorbents. Although the filter itself does not possess either hydrophobic or oleophilic properties, it gains the desired characteristics only after being coated with appropriate reagents. [2,3] These modifications allow the filter to effectively capture oil from the water's surface

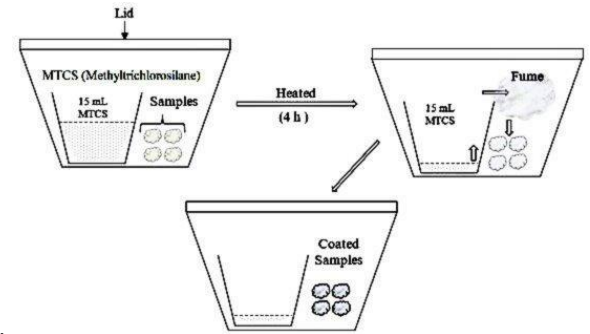

Figure 1. Schematic for the hydrophobic coating process.[2]

The goal of this presentation is to discuss the process of modifying cigarette filters and to present the potential of their use as an innovative sorption material supporting environmental protection.

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Triple-conducting $La_{0.5}Ba_{0.5}Co_{1-x}Fe_xO_{3-\delta}$ oxides as positrode for Proton Ceramic Electrochemical Cells

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Abstract:

Developing efficient and scalable hydrogen technology is a key component of the European Union's energy transition strategy. Protonic ceramic electrochemical cells (PCECs) are highly promising exhibit high efficiency[1], the ability to function at intermediate temperatures, and the capability to employ hydrogen directly as a fuel source[2]. Critical element of PCECs positrodes which assist in the oxygen reduction process and require high ionic and electronic conductivity. Triple-conducting oxides (TCOs), such as perovskite-type materials, are excellent candidates for these applications because they can conduct oxygen ions, electrons/electron holes, and protons. Leading materials are perovskite cobaltites[3]. To improve the key properties of those elements, studies of dopants in composition influence it[4]. This study focuses on the influence of the cobalt substitution with iron in lanthanum-barium cobaltite perovskites, $La_{0.5}Ba_{0.5}Co_{1-x}Fe_xO_{3-\delta}$ (LBCF) on critical factors like conductivity, thermal expansion, hydration, and mechanical stability[5]. This work gives insight into the possibility of controlling and tailoring the key properties of positrode material by controlling the composition.

Acknowledgements Project FunKeyCat is supported by the National Science Centre, Poland under the M-ERA.NET 2, which has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement no 685451.

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Biochemical properties of lipases of oil bodies of germinated jojoba seeds differ from lipases present in microsomal fractions

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Abstract:

Jojoba (Simmondsia chinensis) differs from other oilseed plants; as storage materials, it accumulates wax esters instead of triacylglycerols. This unique characteristic suggests that jojoba seed lipases may possess distinct properties. However, our previous studies did not show significant differences in biochemical properties of lipases of jojoba germinated seeds localized in microsomal fractions from biochemical properties of such lipases of germinated seeds of Crambe abyssinica and germinated seeds of Camelina sativa, two oilseed species that accumulate triacylglycerol as a storage material. However, the lipases localized in membranes of microsomal fractions could differ from those in oil body membranes. Thus, the presented studies aimed to characterize the biochemical properties of lipases of the oil body fraction of germinated jojoba seeds.

During preliminary research connected with this project, we established a successful protocol for isolating membrane fractions of oil bodies of germinated jojoba seeds with active lipases. Further, using this protocol, we isolated such membrane fractions from jojoba seeds at different stages of seed germination. Isolated membrane fractions were stored at -80 °C until further use for assays characterizing lipases present in these membranes.

For enzymatic assays characterizing tested lipases, lyophilized oil body membranes were used. In most assays tri-[14C]18:1-TAG served as the substrate for the tested enzymes. To freeze-dried membrane fractions it was added in benzene solution. The solvent was immediately evaporated, leaving the substrate integrated with the membranes. Reactions were started by the addition of incubation buffer and carried out in an incubator with regulated temperature and shaking. Lipase activity was assessed by quantifying the released [14C]-fatty acids from the added substrate. Quantification was performed by electronic autoradiography (Instant Imager) after separating the chloroform-extracted reaction mixture on a TLC plate.

The obtained results demonstrated that lipase activity in the tested membrane fractions, isolated from the oil bodies of germinated jojoba seeds, increased with the germination time. The optimal temperature for tested lipases was 30 °C. The enzymes were active over a broad pH value; however, the highest activity was recorded at pH 6. The addition of calcium or magnesium ions to the incubation buffer did not affect the tested lipase activity.

The presented properties of lipases of oil body membranes differ from the properties of lipases present in microsomal fractions of germinated jojoba seeds. Thus, it is likely that different lipase isoforms exist within these two cellular compartments. This finding also opens a gate from comparative studies of lipases of oil bodies from other than jojoba plant

species (accumulated TAG as a storage material), especially in substrate specificity of these lipases. Lack of significant differences in this aspect found by us earlier in assays with lipases of microsomal fractions from germinated seeds doesn't have to be true for lipases of oil body membranes.

Is adsorption a valuable method for water purification?

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Abstract:

Water pollution is one of the key problems related to environmental protection and the health of living organisms. In addition to the basic pollutants of natural origin, water also contains so-called emerging contaminants – substances that have been relatively recently recognized as harmful, and their removal from water is difficult. Although they are common in water and occur in very low concentrations, they have a negative impact on living organisms due to their ability to bioaccumulate. A significant part of ECs are pharmaceuticals, antibiotics, pesticides, hormones, agricultural waste [1,2].

A promising solution seems to be the adsorption of ECs on various solid adsorbents. This process is characterized by high efficiency and is economical. Natural adsorbents such as zeolites, clay, chitin are used to remove metals, dyes and organic compounds. Due to its properties, activated carbon shows effective removal of various types of pollutants on an industrial scale. It is a promising material for the removal of organic compounds containing aromatic groups, pharmaceuticals and large, complex molecules [2,3]. The adsorption capacity and surface character can be adjusted to obtain more favorable conditions for high effective adsorption [4].

The use of adsorbents for water treatment is a necessary step. The right selection of the adsorbent is crucial, which, thanks to its low selectivity, enables effective adsorption of various pollutants [5].

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Ecotoxicology of Cosmetics – The Impact of Cosmetic Ingredients on the Baltic Sea Ecosystem

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Abstract:

The widespread use of cosmetics and personal care products has raised concerns about their environmental impact, particularly on aquatic ecosystems. Many cosmetic ingredients, such as UV filters, parabens, silicones, and microplastics, enter water systems through wastewater and accumulate in marine environments. The Baltic Sea, with its unique brackish water ecosystem and limited water exchange, is particularly vulnerable to pollution from cosmetic residues.

This presentation explores the ecotoxicological effects of cosmetic ingredients on marine organisms, including fish, plankton, and benthic species. Scientific studies indicate that some UV filters disrupt endocrine functions in aquatic life, while microplastics contribute to bioaccumulation and trophic transfer. Additionally, certain preservatives and surfactants exhibit toxicity to marine microorganisms, affecting the food web and ecosystem stability. The discussion will also address the role of regulatory frameworks, such as EU cosmetics regulations and water protection policies, in mitigating cosmetic pollution. Furthermore, the potential of biodegradable and eco-friendly cosmetic formulations will be analyzed as a sustainable alternative. Raising awareness among consumers and industry stakeholders is crucial for reducing the environmental footprint of cosmetics and preserving the fragile Baltic Sea ecosystem.

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Data Mining in the Search for New Terahertz Generators

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Abstract:

Terahertz (THz) radiation lies between infrared and microwaves on the electromagnetic spectrum and can penetrate non-conductive materials, making it valuable for diagnostics, quality control, and 6G telecommunications. Its development is hindered by the so-called "terahertz gap"—the lack of efficient, low-cost THz sources with strong electric fields. One promising generation method is optical rectification, which requires single crystals with specific properties [1, 2].

Currently known materials reach an optical rectification efficiency of up to 3.8% ($LiNbO_3$). However, studies from 2022 suggest that many crystal structures in the CSD database may possess significantly better characteristics[3]. So far, data mining combined with DFT calculations has mainly been applied to organic compounds. In this project, the same approach will be used to identify coordination compounds with promising potential for THz generation.

The presentation will cover the current progress in the search for new materials capable of efficiently generating terahertz radiation.

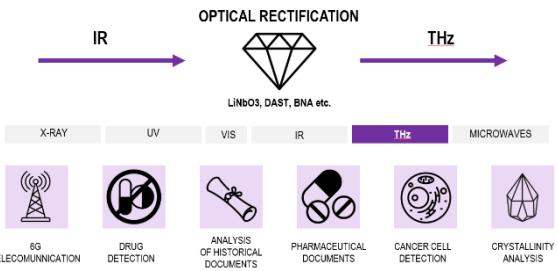

Fig. 1. Characteristics of terahertz radiation.

This work was supported by the 'The Excellence Initiative - Research University' program, under the 'Study@Research' initiative, agreement no. 155/34/UAM/0066.

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Electron Paramagnetic Resonance spectroscopy in the detection of reactive oxygen species generated by indocyanine green

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Abstract:

Electron Paramagnetic Resonance (EPR) spectroscopy analyzes materials with unpaired electrons by detecting changes in microwave energy absorption. This provides insights into the electronic structure, chemical environment, and molecular dynamics [1].

Reactive oxygen species (ROS) are a group of compounds formed as a result of incomplete oxygen reduction, including the superoxide radical (O_2^{-}•), hydroxyl radical (OH•), and non-radical oxidizing agents such as singlet oxygen ($1O_2$). Evaluation of singlet oxygen and free radicals using EPR is possible because they have unpaired electrons. However, their short lifetime necessitates the use of specialized, low-reactivity molecules known as spin traps, which facilitate detection and concentration monitoring over time [2].

The aim of this study was to evaluate free radical production by indocyanine green (ICG) under both irradiated and non-irradiated conditions and to analyze the reactions occurring during irradiation. The spin trap DMPO (5,5-Dimethyl-1-pyrroline N-oxide) was used for radical detection, with special attention given to the correlation between the volume ratio of the spin trap and the ICG solution.

The obtained EPR signal is a composite of signals from different reactive oxygen species. The changes in the intensity of the corresponding EPR signal fragments corresponding to individual radicals, which are proportional to their concentration in the tested samples, will be presented.

Quantitative ROS detection using spin traps is crucial for evaluating the effectiveness of photosensitizers used in innovative cancer treatment methods, such as photodynamic therapy (PDT). PDT relies on the generation of singlet oxygen and other ROS through the interaction of a photosensitizer with light and the oxygen present in tissues, leading to selective destruction of cancer cells. Indocyanine green, a fluorescent compound, has gained interest as a potential photosensitizer for PDT. While ICG is already an approved agent for fluorescence imaging, further research is needed to standardize its role in photodynamic applications.

Literature:

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Application of the "click chemistry" concept in the synthesis of structures containing a 1,2,3-triazole ring and a chiral aminoalcohol subunit

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Abstract:

Compounds containing the 1,2,3-triazole ring with unique structural features has enormous potential in drug design against variety diseases as a pharmacophore, a structural platform or a bioisoster [1]. Three-member ring-opening reactions are classified as part of the Nobel Prize-winning concept of "click chemistry," which is based on the principles of ideal chemical reactions, which should be specific, efficient and selective in terms of regioselectivity and stereoselectivity [2].

The aim of the project was to carry out a series of reactions of chiral oxiranes with chiral aziridines, followed by the opening of the obtained aziridinoalcohols using azide ions and the final synthesis of 1,2,3-triazoles (Fig.1). The application of aziridine as a nitrogen nucleophile in the reaction enabled the opening of oxiranes without the need for additional metal-based catalysts, classifying it as "green chemistry." Importantly, it was found that the regiochemistry of the resulting product depends on the stereochemistry of the substrates used. The aziridine ring-opening reactions were carried out in a similar manner, and the final step was the synthesis of the corresponding triazoles in a copper-catalyzed reaction. Particularly important was the incorporation of the 1,2,3-triazole ring due to its bioisostericity with many commonly used pharmacophore systems. Additionally, as an extension of the conducted research, a regio- and stereoselective synthesis of an atenolol analogue, a well-known drug from the β-blocker group used in the treatment of cardiovascular diseases, was also performed.

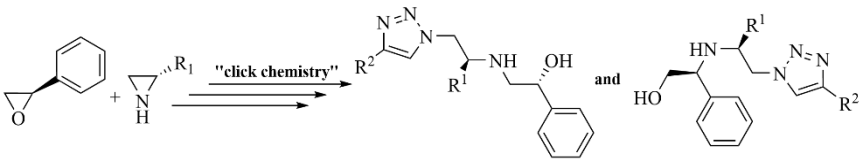

Fig. 1. Schematic representation of syntheses.

Literature:

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Synthesis and analysis of luminescent properties of coumarine chalcone derivatives

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Abstract:

The aim of the work is to synthesize luminescent coumarin derivatives using modern synthesis methods (mechanochemical and sonochemical) [1]. I strive to ensure that the obtained products exhibit luminescence in the solid state, specifically possessing Aggregation-Induced Emission (AIE) properties. This phenomenon allows solving the problem of emission quenching caused by aggregation (ACQ) and enables the use of materials, for example, in thin-film OLED displays, without the need for host-guest systems, which requires additional matching of the small molecule compound to the appropriate polymer matrix [2].

I began my research by preparing a series of aldehydes using Suzuki and Sonogashira coupling reactions, starting from diverse salicylaldehyde derivatives [3]. In the next step, I obtained acyl and ester derivatives of coumarin. In the final stage, I performed the appropriate chalcones through reactions with substituted aromatic aldehydes via classical heating [4]. To evaluate the luminescent properties in the solid state, as well as the film-forming properties, I prepared a series of thin solid layers using the drop casting method, which I then analyzed using a digital microscope. In the next stage, I examined the photophysical properties through absorption and emission studies in solutions and the solid state. To demonstrate the mechanochromism of the molecules, I also performed X-ray structural measurements for selected derivatives.

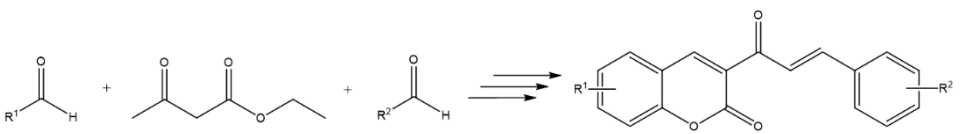

Fig. 1. General synthesis scheme.

Literature:

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Synthesis and photocatalytic applications of carbon dots/polymeric carbon nitride composites

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(TNR size 10, centered, bold, author presenting underlined)

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Abstract:

This study focuses on efficient synthetic approaches and the photocatalytic applications of non-metal carbon dots (CDs) incorporated into polymeric carbon nitride (pCN) semiconductors. Graphitic carbon nitride has been widely investigated in photocatalysis due to its unique electronic structure, moderate band gap (~2.7 eV), and excellent chemical and thermal stability [1]. However, it still faces challenges such as limited visible-light absorption, low specific surface area, and a high electron–hole recombination rate. Recently, carbon dots have attracted attention owing to their high photoluminescence, low toxicity, broad optical absorption, and excellent up-conversion properties. Incorporating carbon dots into g-C_3N_4 can enhance photocatalytic performance while maintaining the metal-free of the material. In this work, CDs/pCN composites were synthesized from lemon juice and urea, using four different methods: physical stirring, calcination, hydrothermal treatment, and exfoliation. These composites were applied to the degradation of the antibiotic ciprofloxacin (CIP) under visible light irradiation. Among the methods, the calcination route exhibited the highest photocatalytic activity in removing CIP. Furthermore, the degradation pathway of CIP was proposed based on the identification of intermediates using time-of-flight mass spectrometry (ToF-MS).

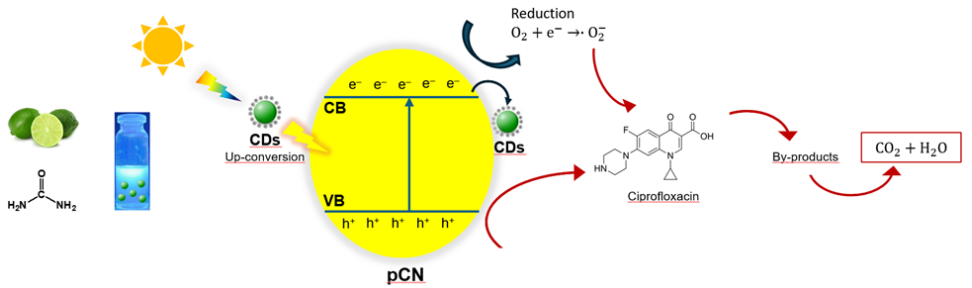

Fig. 1. Photocatalytic mechanism of carbon dots/polymeric carbon nitride for photodegradation of Ciprofloxacin under visible light irradiation.

Literature:

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Microbial lipids from *Yarrowia lipolytica*: a sustainable approach to vegan food innovation

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Abstract:

As the global population continues to rise, the resources necessary for food production are diminishing, highlighting the need for innovative strategies to ensure a sufficient and sustainable supply for both the current and future populations. Biotechnologies based on microorganisms have a long history in the food industry. Oleaginous yeasts are considered one of the tools for sustainably maximizing food production. Lipids are an essential component of microorganism cell membranes, but only about 25 yeast species can accumulate more than 20% of lipids in dry biomass as lipid bodies [1]. The main objective of the study was to develop a concept for the use of oleaginous *Y.lipolytica* biomass and single-cell oil (SCO) as a food components. SCOs were derived from the KKP 379 strain, cultured in media containing glucose, cold-pressed rapeseed oil, and low cost carbon sources such as molasses and post-frying rapeseed oil. Confocal microscopy analysis of the biomass and detailed analysis of the composition of fatty acids, sterols, and polycyclic aromatic hydrocarbons (PAHs) in the extracted lipids were conducted. The choice of substrates allowed to obtain SCO from post-frying rapeseed oil medium with the desired yield (3.27 g/L), composition (unsaturated fatty acids - 94%), and high oxidative stability. All SCOs from *Y. lipolytica* met the European Commission's requirements for marketed oils and fats for maximum levels of PAHs.

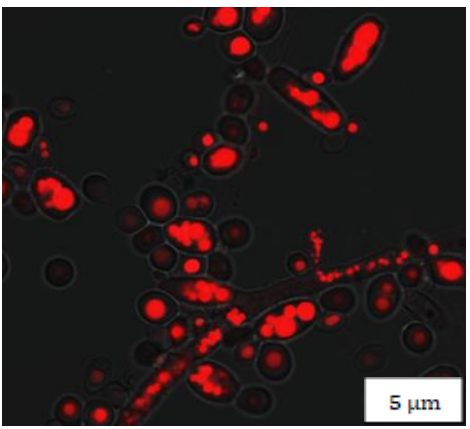

Fig. 1. Confocal microscopy of Nile red stained cellular lipids from *Y. lipolytica* cultures

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Chemical warfare agents in the Baltic Sea: acute & chronic toxicity in fish

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Abstract:

It is estimated that between 45,000 and 70,000 tons of chemical weapons were dumped into the Baltic Sea during the 20th century [1]. Due to corrosion, chemical warfare agents (CWAs) are being released from the marine-dumped munitions at an increasing rate [2]. This issue has been largely overlooked, resulting in a significant gap in ecotoxicological data. To comprehensively assess the risks associated with marine-dumped chemical weapons, it is essential to analyze the toxicity of CWAs to aquatic organisms, including fish.

The aim of this study was to assess the acute and chronic toxicity of several CWAs to fish. Standardized tests (OECD no. 215 and 236) were employed, using the model organism *Danio rerio*. A multi-biomarker approach was applied, encompassing the assessment of fundamental toxicity parameters (mortality, growth rate), toxicity thresholds (LC_{50}, $EC_{10,20,30}$), bioaccumulation of CWAs, as well as the expression levels and activity of molecular markers of oxidative stress.

The conducted study determined the acute toxicity profile of eight organoarsenic and six organic sulfur CWAs, as well as the chronic toxicity profile of two organoarsenic CWAs. The results provide valuable data on the potential ecological threats posed by CWAs and contribute to a better understanding of their short- and long-term environmental impacts.

The research was funded by grants no. 2020/37/N/NZ8/04099 and 2021/40/C/NZ8/00125 (National Science Centre, Poland), as well as grant no. #C056 BSR INTERREG, Marine Munition Remediation Roadmap (MUNIMAP).

Literature:

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Development of a Method for Detecting Concurrent Infectious Respiratory Diseases in a Selected Human Population Using Nanopore Sequencing

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Abstract:

The World Health Organisation (WHO) predicts a much more dangerous viral outbreak in the future than the COVID-19 pandemic, which will kill more than 50 million people worldwide [1]. The research problem presented in this work was addressed, because there is a need to develop a diagnostic method for the rapid, accurate and efficient detection of different viral variants co-occuring in the human population [2].

The aim of this work is to develop a diagnostic method based on nanopore sequencing to detect, in less than five hours, the co-occurence of viruses (SARS-CoV-2, influenza A and B, RSV, parainfluenza) responsible for causing infectious respiratory diseases in humans. The use of the latest generation sequencing method will enable the detection of specific viral variants present in the sample taken from the patient.

The above-mentioned method will provide an opportunity to develop personalized medicine. Futhermore, the method created will enable a better understanding of many viral pathogens, creating the possibility of developing new medical therapies, vaccines or drugs that will contribute to the alleviation, prevention or eradication of many of today's diseases.

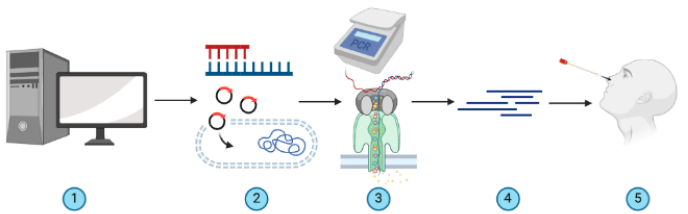

Fig. 1. The scheme of the work plan. The figure was created using BioRender software (https://www.biorender.com/)

Literature:

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Phytoremediation as a Method for Cleaning Soils Contaminated with Heavy Metals

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Abstract:

In recent years, the problem of environmental pollution has intensified significantly, mainly due to the dynamic development of industry, particularly mining, transportation, and agriculture. One of the most serious threats to environmental quality is heavy metals, which—unlike many organic compounds—do not undergo biodegradation but instead accumulate in the soil, leading to its degradation. One of the modern methods of soil decontamination is phytoremediation. This process involves the use of land plants to remove heavy metals and other toxins from the substrate. Depending on environmental conditions and the nature of a specific area, several types of phytoremediation can be distinguished, each selected individually to suit the needs of the specific site. The proper selection of plant species, which are capable of accumulating contaminants, also plays a important role in achieving the best possible remediation results. [1,2]

Literature:

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How bacteria can help us detect and monitor marine pollution: novel studies on bacterial communities in Baltic Sea sediments and the use of Vibrio sp. MM1 in heavy metals detection

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Abstract:

The Baltic Sea, though relatively small, ranks among the most polluted marine ecosystems in the world. Toxic and mutagenic substances accumulate in its sediments and coastal waters, posing serious environmental challenges. Recent research has shown that microbial methods provide high specificity and fast detection of various pollutants. These features make them ideal for assessing remediation efforts and tracking contamination.

A study near Kolberger Heide munitions dumpsite in the Baltic Sea demonstrated the effectiveness of microbial fingerprinting in detecting low levels of 2,4,6-trinitrotoluene (TNT). Using 16S rRNA gene sequencing and machine learning, researchers identified a TNT-specific microbial signature that allowed them to predict TNT presence with up to 81.5% accuracy. TNT was not a main driver of community shifts, demonstrating the high sensitivity of this approach. Additionally, microbial profiling was more sensitive than standard chemical testing methods used to assess pollutant concentrations [1].

In another study, a luminescent *Vibrio* strain MM1 isolated from the Caspian Sea exhibited high sensitivity to many heavy metals. Its EC50 values were significantly lower than those of commercial kits. These results suggest that MM1 could be used in bioluminescence-based assays for early pollution detection. This approach could be extended to the Baltic Sea by identifying native luminescent *Vibrio* species adapted to its unique conditions. Harnessing the biosensing potential of indigenous microbial strains may greatly enhance our ability to detect and respond to local pollution [2].

Preserving the Baltic's health requires innovative, nature-based solutions- and microbial biosensors may be one of them. Investing in such methods might be vital to preserving its delicate biodiversity.

The author is sincerely grateful to Professor Małgorzata Waleron for valuable guidance and comments.

Literature:

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A2 Milk: the buzz, the benefits, and a future

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Abstract:

Cow's milk can be categorized into three types based on the β-casein protein: A1A1, A1A2, and A2A2. Caseins are the main proteins in milk, and their composition depends on the animal's genotype. The A1A1 milk, often called "conventional" milk, is the most common due to its higher yield from cows. On the other hand, "old breeds" – which are less productive – mostly fall under the A2A2 genotype. Over the years, selective breeding for high milk production has led to the near elimination of these older breeds, making the A1A1 genotype dominant in industrial dairy farming.

The A1 and A2 variants of β-casein differ by a single amino acid. In A1 β-casein, histidine is present at the 67th position, whereas proline is found in the A2 version. This small difference makes a significant impact on how the protein is digested in the human body. Proline, in particular, forms a stronger bond with the preceding amino acid, influencing digestion. It also affects technological differences, which are important from an industrial perspective.

Consumer interest in health-promoting and functional products is growing, and A2 milk addresses many of their needs.

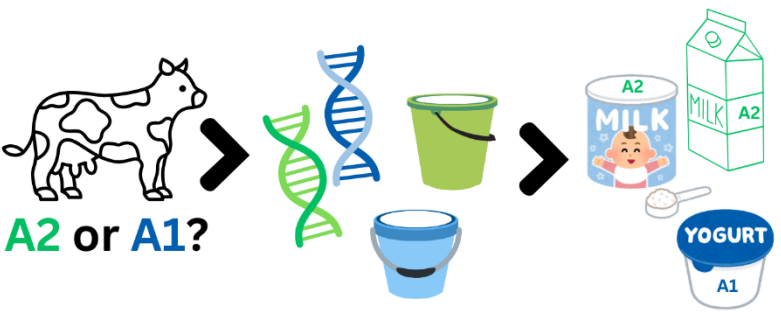

Fig. 1. A2 and A1 milk in the industry.

Literature:

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Posters

From Microarrays to Next-Generation Sequencing (NGS): Unveiling the Secrets of Transcriptomics

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Abstract:

This paper aims to present the available platforms for transcriptome analysis of studied organisms and the benefits of incorporating these techniques into one's research**.**

Microarrays dominated among platforms used for transcriptome analysis across a wide range of organisms, thus making a significant contribution to the development of pharmacology, molecular biology, and transcriptomics.

Scientific and technological advances have enabled NGS to become the successor to microarrays, allowing for the discovery and exploration of previously unknown aspects of the transcriptomic landscape. [1,2,3]

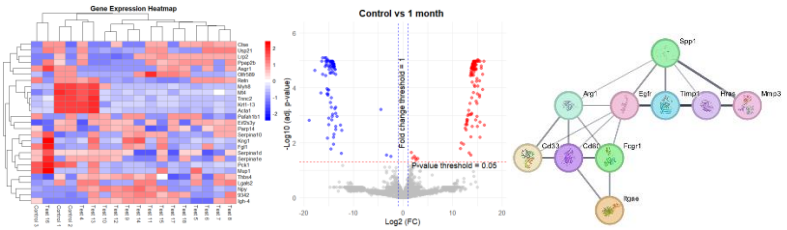

Fig. 1. Example results of transcriptome analysis

Literature:

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Characterization and significance of B lymphocytes in Non-small Cell Lung Cancer patients

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Abstract:

Advances in understanding immune system's role in cancer have driven major breakthroughs, particularly the development of immunotherapies utilizing T lymphocytes and Natural Killer (NK) cells (Ribas & Wolchok, 2018). While T and NK cells have been extensively studied, the contribution of B lymphocytes to anti-tumor immunity, though increasingly recognized, remains less characterized (Sharonov et al., 2020; Wouters & Nelson, 2018).

To better elucidate the role of B cells in Non-Small Cell Lung Cancer (NSCLC), we isolated immune cells from patient-matched tumor tissue, adjacent healthy tissue, and peripheral blood. These cells were stained using a multi-parameter antibody panel designed to identify distinct B lymphocyte subpopulations. Flow cytometry analysis was performed to compare B cell profiles across patient-derived samples and peripheral blood from healthy donors.

Our analysis revealed significant differences in the frequencies of key B cell subpopulations, including regulatory, memory, and naïve B cells, when comparing NSCLC patients to healthy controls. Furthermore, we observed altered expression patterns of critical surface markers on B cells from patients compared to healthy donors, as well as potential variations across different tissue compartments within patient.

In conclusion, these results demonstrate notable alterations within the B lymphocyte populations in NSCLC patients, highlighting the potentially significant, yet complex, role of B cells in the anti-tumor immune response. Our findings warrant further investigation into the specific functions of B cells within the NSCLC tumor microenvironment.

The authors are grateful to all the patients who provided samples that were used for this research.

Literature:

Ribas, A., & Wolchok, J. D. (2018). Cancer immunotherapy using checkpoint blockade. *Science*, *359*(6382), 1350–1355. https://doi.org/10.1126/SCIENCE.AAR4060

Sharonov, G. V., Serebrovskaya, E. O., Yuzhakova, D. V., Britanova, O. V., & Chudakov, D. M. (2020). B cells, plasma cells and antibody repertoires in the tumour microenvironment. *Nature Reviews. Immunology*, *20*(5), 294–307. https://doi.org/10.1038/S41577-019-0257-X

Wouters, M. C. A., & Nelson, B. H. (2018). Prognostic Significance of Tumor-Infiltrating B Cells and Plasma Cells in Human Cancer. *Clinical Cancer Research : An Official Journal of the American Association for Cancer Research*, *24*(24), 6125–6135. https://doi.org/10.1158/1078-0432.CCR-18-1481

MOFs - structures that absorb, catalyze and photocatalyze

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Abstract:

Metal-organic frameworks (MOFs) are a rapidly developing class of porous crystalline materials composed of metal ions or clusters coordinated to organic linkers. Their modular architecture, high surface area, tunable pore size, and chemical versatility make them exceptional candidates for a broad range of applications. This presentation will explore how MOFs function as multifunctional platforms capable of adsorption, catalysis, and photocatalysis.

First, we will examine their performance as advanced adsorbents in gas storage (e.g., hydrogen, methane, CO_2 capture), pollutant removal, and selective separation processes. Then, we will highlight the catalytic capabilities of MOFs in various organic transformations, emphasizing how their structure allows for precise control of active sites, enabling efficiency and selectivity not easily achieved with traditional catalysts. Finally, the presentation will focus on the emerging field of MOF-based photocatalysis — particularly their role in light-driven reactions such as water splitting, CO_2 reduction, and degradation of organic pollutants under mild conditions.

By analyzing case studies and recent advancements, we will demonstrate how the structural diversity of MOFs can be harnessed to tailor their properties for specific tasks. Special attention will be given to the design principles that govern their functionality, the challenges in their stability and scalability, and the potential they hold for sustainable chemistry and clean energy solutions in the near future.

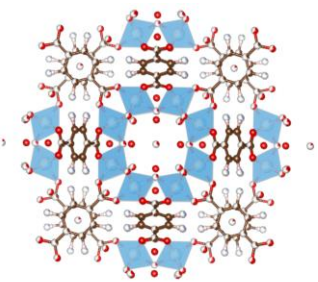

Fig. 1. Structure of NH_2-MIL-125 (Ti) (by Vesta Software)

TIGIT: A Rising Target in Cancer Immunotherapy

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Abstract:

T-cell immunoreceptor with immunoglobulin and ITIM domain (TIGIT) is an immune checkpoint receptor involved in tumor immune evasion. Expressed on T cells, natural killer (NK) cells, and tumor-infiltrating lymphocytes (TILs), it suppresses antitumor immunity by inhibiting T and NK cell activity, enhancing regulatory T cell (Treg) function, and interfering with CD226 co-stimulatory signaling. Due to its immunosuppressive role, TIGIT has become a promising target, particularly in combination with PD-(L)1 inhibitors, as these pathways are often co-expressed on exhausted CD8+ T cells [1].

Several monoclonal antibodies targeting TIGIT have been developed, with multiple agents undergoing clinical evaluation [2]. Tiragolumab has shown promising results in combination with atezolizumab, enhancing immune activation and improving clinical outcomes in non-small cell lung cancer (NSCLC) [3]. Domvanalimab, an Fc-silent antibody, has demonstrated potent immunostimulatory effects, particularly when combined with zimberelimab and chemotherapy [4]. Meanwhile, vibostolimab was tested alongside pembrolizumab in extensive-stage small cell lung cancer (ES-SCLC) but due to frequent adverse effects, treatment with vibostolimab/pembrolizumab was discontinued, highlighting the complexity of TIGIT blockade strategies [5].

While early clinical trials are encouraging, the therapeutic success of TIGIT inhibitors depends on their ability to enhance antitumor responses without excessive toxicity. Ongoing phase II and III studies will clarify their clinical potential. If proven effective, TIGIT blockade especially in combination with PD-(L)1 inhibitors could significantly expand immune checkpoint therapy options for cancer patients.

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Wsparcie żywieniowe w terapii chorego z zaawansowanym rakiem żołądka – opis przypadku

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Opis przypadku dotyczy 74-letniego pacjenta z postępującą utratą masy ciała (około 20% masy wyjściowej), kacheksją i objawami wysokiej niedrożności przewodu pokarmowego w przebiegu niskozróżnicowanego gruczolakoraka żołądka (G3). Pierwotne postępowanie terapeutyczne w szpitalu rejonowym obejmowało całkowite żywienie pozajelitowe przez dostęp obwodowy oraz leczenie objawowe, prowadząc do stabilizacji gospodarki wodno-elektrolitowej i częściowego odwrócenia katabolizmu. Dalsza diagnostyka i leczenie żywieniowe przez założoną mikrojejunostomię odżywczą w ośrodku wysokospecjalistycznym umożliwiły wczesne rozpoczęcie żywienia dojelitowego w warunkach domowych.

Pacjenta zakwalifikowano do chemioterapii okołooperacyjnej oraz leczenia operacyjnego. Dzięki wczesnej interwencji żywieniowej BMI wzrosło z 19,73 w momencie przyjęcia do 21,73 przed zabiegiem operacyjnym. Pooperacyjnie zastosowano żywienie pozajelitowe i dojelitowe, które pacjent dobrze tolerował, a stan odżywienia został utrzymany (BMI 22,4 po 6 miesiącach). Leczenie żywieniowe odegrało kluczową rolę w optymalizacji stanu klinicznego, zwiększeniu tolerancji leczenia onkologicznego i poprawie długoterminowego rokowania.

Przypadek ten podkreśla znaczenie wczesnego rozpoznania niedożywienia, indywidualizacji strategii żywieniowej oraz bliskiej współpracy wielodyscyplinarnej w leczeniu pacjentów onkologicznych [1,2].

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Effect of drought and gamma poly-γ-glutamic acid (γ-PGA)on cell wall structure in yellow lupine root

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Abstract:

Studies have shown that abiotic factors can reduce global crop productivity by up to 50%. Among these, soil water scarcity is the most influential, negatively affecting both the above-ground parts of plants and their roots, the first to respond to drought conditions [1]. For this reason, understanding how economically important species react to water stress is crucial. Yellow lupine (*Lupinus luteus* L.), in particular, is highly sensitive to drought, experiencing significant yield losses under reduced water availability [2, 3]. Drought-induced oxidative stress in plants alters cell wall structure, leading to changes in the levels and spatial distribution of specific components, such as pectins, including variations in their degree of methylation.

Certain rhizosphere bacteria, particularly from the *Bacillus* genus, produce poly-*γ*-glutamic acid (*γ*-PGA), a protective metabolite synthesized in response to environmental stress. This compound has been shown to enhance drought tolerance in oilseed rape by stimulating osmoprotective mechanisms [4, 5]. However, the mechanism of *γ*-PGA action under drought stress in other crops, such as legumes, remains poorly understood. In this study, we tested the hypothesis that *γ*-PGA can modify the root structure of yellow lupine under soil drought conditions. Drought induces both the accumulation of highly methylated homogalacturonans (HGs) and their subsequent demethylation, which may contribute to cell wall loosening. Dot blot analyses revealed that *γ*-PGA influences the pectin methylation status of HGs in lupine roots under drought stress, with the effect being dependent on the time of application and concentration of the metabolite. Treatment with *γ*-PGA on the 14th day of drought was particularly effective in reversing stress-induced changes in HG methylation.

Research work partly funded by the 2020-2024 science budget as a research project under the Diamond Grant IX program no. 0180/DIA/2020/49, and project IDUB NCU in Toruń, Grants 4NCU Students program no. 9001960020/2024/00591

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AI, Smart Sensors, and New Predictors for COPD Management

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Abstract:

Chronic Obstructive Pulmonary Disease (COPD) is a major cause of morbidity and mortality worldwide. Telemonitoring plays a significant role in the management of COPD since it enables healthcare providers to detect early signs of COPD exacerbations, allowing for prompt intervention, and potentially preventing hospitalizations. While existing telemonitoring approaches have shown promise in reducing hospitalization rates, further studies are needed to evaluate the impact of telemonitoring on quality of life.

Through the CICERONE project, we introduce a home telemonitoring system that gathers multimodal data. This study presents the first developments, including a mobile application, an environmental air quality monitoring system, and an electronic patient record that brings all heterogeneous data in one place. This app has been developed using a user-centered design methodology with a group of 31 participants and empowers patients through surveys, games, voice and cough sound recording, and integration with vital sensors (peak flow meter, smart wristband, and a scale). Collected data is transmitted to a centralized electronic record, enabling continuous patient monitoring.

Currently, the system is gathering data in an observational study with a group of COPD patients. Machine learning models will be trained and validated to enhance the early detection of imminent COPD exacerbations. We aim to contribute to the advancement of COPD management by developing tools that foster proactive and individualized care.

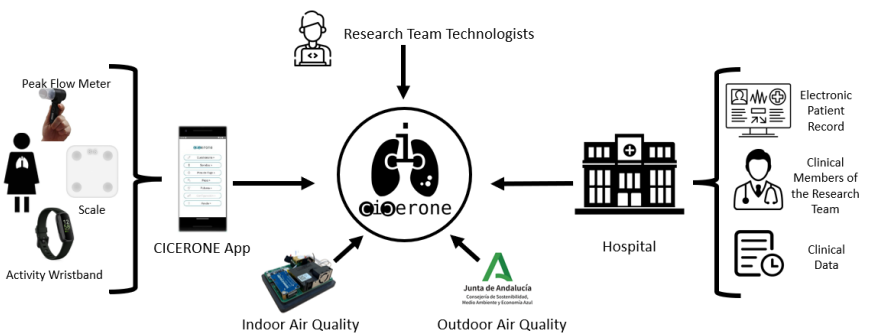

Fig. 1. System Architecture of CICERONE.

This study is part of the R&D&I project CICERONE, with reference PID2021-126810OB-I00, funded by MICIU/AEI/10.13039/501100011033 and by FEDER/EU.

Predictive Chemistry and Market Realities: Translational Challenges from Molecule to Market

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Abstract:

Predictive chemistry—using computational tools such as QSAR, molecular docking, and ADMET modeling—has become a cornerstone of modern molecular design. These techniques accelerate early-stage compound screening and enable rational design workflows. However, a persistent challenge lies in translating computational success into real-world applications.

This poster explores the growing disconnect between in silico–optimized molecules and their market viability. Factors such as synthetic complexity, scalability, cost, regulatory hurdles, and patentability often derail even the most promising compounds. Using examples from drug discovery and industrial chemistry, I highlight the "Valley of Death" where innovation fails due to non-scientific barriers.

There exists a need for an expanded role of predictive chemistry that incorporates not only biological and physicochemical parameters, but also economic and logistical feasibility. Emerging strategies—including AI-based tools that factor in synthesis cost and supply chain constraints—may offer a more realistic path from molecule to market.

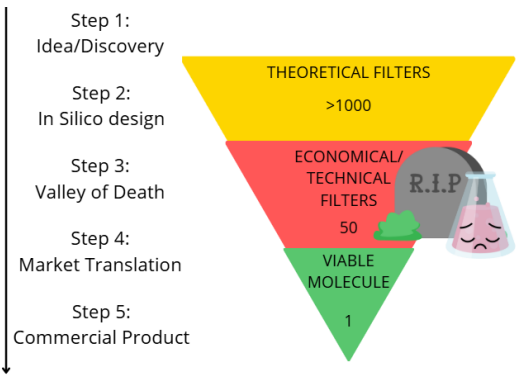

Fig. 1. From Predicted Commercial Reality.

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Assessment of calcium content of daily food rations offered by diet catering services.

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Abstract:

Calcium is a macronutrient that plays a key role in many biological and physiological processes. It is responsible for the mineralization of bones and teeth, the conduction of nerve impulses, and muscle contractions. Despite its crucial role, it is estimated that over half of the global population does not meet the recommended daily intake of calcium [1].

The aim of the study was to determine the calcium content in the daily food rations (DFR) offered by dietary catering services and compare it with reference values for calcium requirements in the diet.

The study involved analyzing meals offered by dietary catering services in the city of Białystok. A total of 30 DFR, each providing 2000±128.5 kcal per day and consisting of 5 meals, were examined. The DFR were provided by 10 different catering companies over 3 consecutive days. During the study, calcium content was determined using atomic absorption spectrometry (AAS) with a flame technique (Hitachi Z-5000, Japan). The calcium content in the DFR was calculated using the Dieta 6.0 software. The obtained results were compared with the nutrition standards estimated average requirement (1000 mg/day) [2].

The statistical analysis showed significant differences between the calcium content measured by the AAS analytical method and the computational method ($p<0.0045$). The calcium values in DFR measured by the AAS method ranged from 188.2 to 1130.5 mg/day, with an average of 474.7±199.0 mg, while the computational method ranged from 223.1 to 1613.9 mg/day, with an average of 673.0±289.7 mg.

The results obtained by the AAS method indicate that almost all DFR (96.7%) did not meet the recommended daily intake (RDA) for calcium. The full-day diets offered by dietary catering services are a poor source of calcium and, for the most part, do not cover the recommended daily intake for this element.

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Research methods to study the permeability of active drug substances through the blood-brain barrier

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Abstract:

The blood-brain barrier (BBB) is a highly selective physiological structure that plays a crucial role in protecting the central nervous system (CNS) by regulating the passage of substances from the bloodstream into the brain. Due to its semi-permeability, the BBB presents a major obstacle in the development of CNS drugs. [1]

This poster presents an overview of current methods used to evaluate the permeation capacity of active pharmaceutical ingredients (APIs) across the BBB. Both *in vivo* and *in vitro* models are discussed, including their advantages, limitations, and relevance to mimicking human BBB permeability. [2]

Special attention is given to the Parallel Artificial Membrane Permeability Assay for the Blood-Brain Barrier (PAMPA-BBB), an *in vitro* technique that models passive diffusion across the BBB using a lipid-infused artificial membrane.

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Modification of biopolymer blends with natural plant extracts to improve their mechanical and thermal properties

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Abstract:

Growing interest in biodegradable materials has intensified research into biopolymer modifications aimed at enhancing their functional properties. The objective of this work was the modification of gelatin-based biopolymer blends by using selected natural plant extracts. The study aimed to evaluate the impact of these extracts on the chemical structure, mechanical, and thermal properties of the obtained biodegradable films. The modification process was conducted under controlled conditions, including homogenization and drying of the mixtures.

According to available literature, the use of natural biopolymers in packaging production contributes to reducing negative environmental impacts by limiting the use of petrochemical-based plastics and ensuring biodegradability and non-toxicity [1, 2]. FTIR analysis revealed changes in the intensity of amide and carbonyl bands, indicating an increased degree of crosslinking in the blends. DSC studies confirmed an increase in glass transition (Tg) and melting temperatures (Tm), indicating improved thermal stability of the materials. The addition of plant extracts significantly increased tensile strength, elongation at break, and Shore hardness compared to control samples.

Biodegradation tests demonstrated enhanced resistance to biological degradation. The obtained results confirm the application potential of the modified blends as biodegradable packaging films with improved functional properties.

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Influence of Dietary Habits on the Concentrations of Zinc and Copper in the Serum of Patients with Age-Related Cataract

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Abstract:

Zinc (Zn) and copper (Cu) are trace elements that play an essential role in the human body. Disruptions in their homeostasis induce oxidative stress, which can be a risk factor for various diseases, since those biometals are vital cofactors of antioxidant enzyme pathways [1]. Age-related cataract (ARC) is an opacification of the lens and the leading cause of vision loss worldwide. While the etiology of this condition is not fully understood, oxidative stress, UV exposure, cigarette smoking as well as malnutrition are considered the most likely causes of cataracts [2]. That is why lifestyle modifications, especially dietary changes, may be particularly beneficial in preventing or delaying the progression of ARC.

The objective of the study was to assess the effect of dietary habits on serum Zn and Cu concentrations in ARC patients.

A total of 63 patients with ARC (aged 48–91 years) and 65 healthy people (aged 49–83 years) were studied. To collect the dietary data, food-frequency surveys were conducted. The concentrations of Zn and Cu in serum samples were determined by atomic absorption spectrometry. The results were statistically processed using Statistica v.13 software.

Statistical analysis showed significant differences between Zn and Cu concentrations in ARC patients and healthy controls (Me_{Zn1}=0.75, Me_{Cu1}=0.81; Me_{Zn2}=0.86, Me_{Cu2}=0.99, respectively). The results of stepwise multiple regression analysis showed a statistically significant positive association of Zn concentration with the intake of 6 food groups (white bread, cured meat, fish, legumes, sweet and wholegrain bread) and a negative one for two of them (butter and potatoes) (R^2=0.44). For Cu, a significant positive relationship was noted for the milk consumption and a negative one for margarines and oils intake (R^2=0.20). In addition, for the Cu/Zn ratio, a significant positive correlation was observed for the consumption of milk and butter, and a negative one for oils and margarines (R^2=0.21).

The results indicate that there is a relationship between the dietary habits of ARC patients and the parameters studied. Identification of potential links between Zn and Cu concentrations and visual impairment could be used in ARC prevention, and should therefore be the subject of further research.

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SSbD-Oriented design of Solid Oxide Electrolyzer Cell anodes: combining Quantum Mechanical Modeling with Machine Learning approach

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Abstract:

Solid Oxide Electrolyzer Cells (SOEC) are a promising alternative to conventional energy sources, offering reversible hydrogen production and energy generation. However, efficient SOEC system design remains a challenge. This study uses a computational approach to propose lanthanum-free (REE-free) anode materials, in line with the Safe and Sustainable by Design (SSbD) strategy.

For the first time, a combined quantum mechanical (QM) and machine learning (ML) approach was used to support SOEC anode design, reducing the need for costly and resource-intensive experiments. A set of 240 doped Brownmillerite structures, modeled as 29-atom fragments, were evaluated.

Quantum mechanical calculations were carried out using DFT (MN15/LANL2DZ/6-31G)[1] in Gaussian16[2], and the resulting descriptors served as input for ML analysis. The k-means clustering method grouped the structures into five clusters and helped identify the most promising candidates for further experimental validation.

This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement N°101058784 (NOUVEAU project) and Polish Ministry of Science and Higher Education grant "Doktorat Wdrożeniowy 2023", grant agreement no. DWD/7/0321/2023

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Coordination Chemistry of Copper Ions with β-Lactam Antibiotics: A Potentiometric and Spectroscopic Studies

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Abstract:

The growing challenge of antibiotic resistance calls for innovative strategies to improve the effectiveness of existing drugs [1]. One promising approach is the formation of metal complexes with antibiotics, which can alter their chemical properties, enhance their stability, and modify their biological activity [2]. Among transition metals, copper is particularly significant due to its redox activity, coordination flexibility, and essential role in biological systems. Copper ions can interact with β-lactam antibiotics (Fig. 1.), influencing their structural conformation, reactivity, and ability to bind bacterial targets. Understanding these interactions at a molecular level is crucial for developing novel therapeutic strategies that exploit metal coordination to enhance antibiotic efficacy.

In this study, we investigate the coordination chemistry of β-lactam antibiotics (Ampicillin and Cloxacillin) with copper(II) ions using potentiometric and spectroscopic techniques. The complex formation constants were determined to evaluate the stability of the resulting species, while UV-Vis, IR, and EPR spectroscopy provided insights into their structural and electronic properties. The obtained results indicate that β-lactam antibiotics act as effective ligands for Cu(II), forming stable complexes.

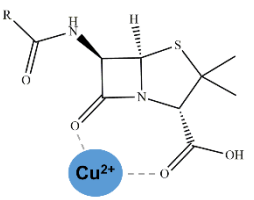

Fig. 1. Coordination model of metal-ion binding with β-lactam antibiotics

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Dual Inhibitors and Combination Drug Therapy: Designed to Overcome Resistance in Cancer Treatment

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Abstract:

Currently, there are two contrasting strategies for designing multi-targeting therapeutics, which are expected to revolutionize cancer treatment. Dual inhibitors are multi-targeting drugs that can block multiple oncogenic pathways while also improving drug resistance and side effects. In this strategy, two active molecules are combined to create new hybrid compounds. An example of this linked pharmacophore approach is cabozantinib, which has already been approved by the FDA for the treatment of medullary thyroid cancer, renal cell carcinoma, and hepatocellular carcinoma. More complex pharmacophore-based approaches, such as the fused pharmacophore or merged pharmacophore approach, are also being explored [1].

The other strategy is combination drug therapy, in which multiple drugs act on separate targets to produce an additive or synergistic effect. Several successful combination therapies have been developed, including the FDA-approved combination of dabrafenib (a BRAF inhibitor) and trametinib (a MEK inhibitor) for the treatment of metastatic melanoma with BRAF mutations. While this strategy is simpler to develop compared to dual inhibitors, it has some drawbacks, including drug–drug interactions, poor safety, and a low therapeutic index [2].

Literature:

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Disturbed vs non-disturbed wetlands: a case of bird assemblages around Lake Tana in East Africa

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Abstract:
Birds are pivotal indicators of environmental health, as they reflect alterations in habitat quality through their population dynamics and behavior. Despite the critical role birds play as ecological indicators, current conservation strategies often fall short. This study was conducted at the two sub-basin wetlands of Lake Tana to investigate and compare the assemblage of bird species between these two wetlands, one is Yiganda which is an example of minor influence of humans and other is Chimba which is under higher anthropogenic pressure. A systematic random sample technique was used, and wetland birds were recorded based on the established counting stations. In total, we recorded a total of 6,432 individuals belonging to 95 species in the two study sites in both dry and wet seasons. We found the effect of season on bird abundance differed between the two wetland types. The decrease in abundance and biodiversity from the dry to the wet season was less pronounced at Yiganda wetland compared to Chimba wetland. Overall abundance of birds and diversity differs between Chimba and Yiganda wetlands during the wet season, but not during dry season. Implementing conservation strategies in disturbed areas like Chimba can serve as a model for other regions facing similar challenges.

Key words/phrase: Anthropogenic pressure, Biodiversity, Nature protection, Wetland birds

Fig. 1. Natural Science Baltic Conference logo.

We thank the Chimba and Zege district natural resource officers for allowing us to collect these data in the study sites. We thank Ethiopian Biodiversity Institute for financing for data collection and support materials for this research.

Computational Studies of NH2-MIL-125Ti: Stability, Electronic Structure and Defects

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Abstract:

This research studies the atomic and electronic structure of the NH2-MIL-125(Ti/Cu) system—a distinct metal-organic framework (MOF) with promising photocatalytic applications. The study employs density-functional theory (DFT), which is implemented in the Vienna Ab initio Simulation Package (VASP). The theoretical simulations will consider the pristine NH2-MIL-125(Ti) and defective phases that include Cu instead of Ti sites and linker vacancies. This work will predict the MOF's stability, electronic structure, likely magnetic phases, and the effect of defects on the bandgap. Furthermore, depending on the size of the system and computational capability, this work might consider the temperature effect on the MOF's structure using molecular dynamics and machine learning. The results will be discussed in light of available experimental data.

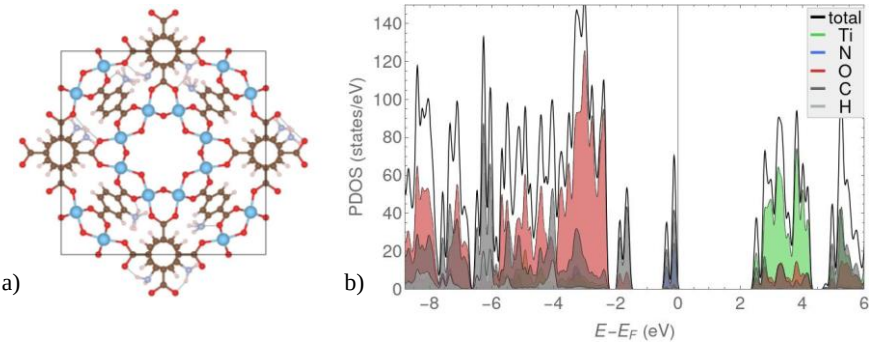

Fig. 1. (a) Atomic structure of the NH_2-MIL-125(Ti) MOF. Blue, red, brown, and white spheres represent Ti, O, C, and H atoms, respectively. (b) Partial Density of States (PDOS) obtained from DFT calculations; the Fermi level is indicated by the vertical black line.

The author thanks Dr. Henry Pinto for his guidance during this research, and is also grateful to family and friends for their continued support.

Literature:

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[2] Mancuso J.L., Mroz A.M., Le K.N., Hendon C.H. 2020. Electronic structure modeling of metal–organic frameworks. *Chemical Reviews*, 120: 8641–8715.

Antioxidant activity of 1-(azepan-1-yl)propane-1,2-dione 4-allylthiosemicarbazone and its Cu(II) and Ni(II) complexes against $ABTS^{\bullet+}$

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Abstract:

Oxidation is a vital part of aerobic metabolism, generating free radicals. While these radicals can be both beneficial and harmful, an imbalance leads to oxidative stress, contributing to diseases and neurodegenerative disorders. This has sparked interest in antioxidants, as they help protect the body from free radical damage [1].

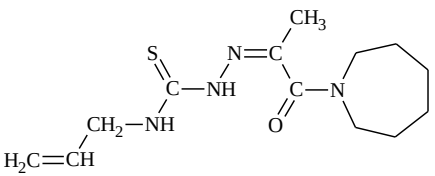

Fig. 1. The structure of HL.

The aim of this study is synthesis, characterization and study of antioxidant activity towards $ABTS^{\bullet+}$ caton radicals of 1-(azepan-1-yl)propane-1,2-dione 4-allylthiosemicarbazone (HL) and its Ni(II) and Cu(II) complexes. The HL was obtained by the reaction between 1-(azepan-1-yl)propane-1,2-dione and 4-allylthiosemicarbazide in ethanol. The complexes [Cu(L)Cl] and $[Ni(HL)_2](NO_3)_2$ were obtained by reaction between HL and metal salts, and were studied using physico-chemical methods.

The antioxidant activity was studied towards $ABTS^{\bullet+}$ caton radicals for HL and complexes. The value of IC_{50} for HL is 3.85 μg/mL, the activity of complexes is lower, for [Cu(L)Cl] is 8.16 μg/mL and for $[Ni(HL)_2](NO_3)_2$ is 10.1 μg/mL. All synthesized substances are more active than Trolox, a standard antioxidant that is used in medicine.

This work was fulfilled with the financial support of the subprogram 010602 of the institutional project.

Literature:

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Antibacterial potential of copper(II) complexes with 2-benzoylpyridine 4-norbornylthiosemicarbazone against *Acinetobacter baumannii*

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Abstract:

The increasing prevalence of infections is largely due to the reduced efficacy of antimicrobial drugs resulting from antimicrobial resistance. This resistance emerges as pathogens undergo genetic mutations in response to antibacterial treatments, leading to the formation of drug-resistant strains [1].

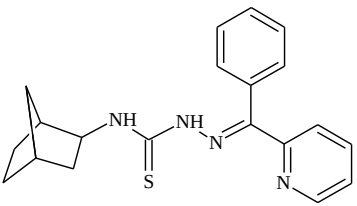

Fig. 1. The structure of HL.

The purpose of this study is study of antibacterial activity of Cu(II) complexes with 2-benzoylpyridine 4-norbornylthiosemicarbazone (HL) that contains the fragment which contains in natural product Camphor. The following complexes were obtained: $[Cu(L)NO_3]$, $[Cu(L)Cl]$ and $[Cu(L)CHCl_2COO]$.

The antibacterial activity of synthesized substances was studied towards Gram-negative microorganisms *A. baumannii* (BAA-747). The HL is not active, but its Cu(II) complexes exhibit good antibacterial activity. The value of the MIC of $[Cu(L)NO_3]$, the most active complex is 7.8 μg/mL and the value of the MBC is 15.6 μg/mL.

This work was fulfilled with the financial support of the ANCD project 24.80012.5007.14TC.

Literature:

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Steroid-Triazole Conjugates: Structural Insights and Biological Potential

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Abstract:

Steroid conjugates are a diverse class of compounds with promising applications in medicinal chemistry, offering opportunities to enhance biological activity and optimize pharmacokinetic properties [1]. Among them, steroid dimers linked by a 1,2,3-triazole ring have gained attention for their structural diversity and stability (Fig. 1) [1-2]. The triazole linker, introduced via Cu(I)-catalyzed azide-alkyne cycloaddition (CuAAC), provides a robust and efficient method for assembling these molecules [1].

The synthesized conjugates were thoroughly characterized using NMR, FT-IR, and MS techniques to confirm their structures. Their biological potential was explored through molecular docking, *in silico* pharmacological predictions, and hemolytic activity assays. These studies provide valuable insights into the structure-activity relationships of steroid-triazole hybrids, highlighting their potential as bioactive compounds and laying the groundwork for further functional optimization.

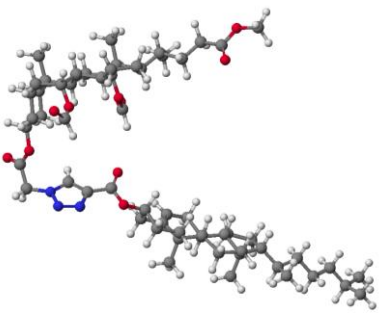

Fig. 1. Molecular model of chosen steroid conjugate connected via 1,2,3-triazole ring

Literature:

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ACYLATION REACTIONS OF METHYLCYCLOHEXYL(ARYLALKYL)PHENOLS WITH ACETYL CHLORİDE

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Alkylphenols are widely applies as intermediate products for synthesis of antioxidants, additives, plasticizers and other chemical additions to olefins, synthetic rubbers, oils and fluels.

In the article is showed the results of a study of the reaction of alkylation of phenol with 1(3)-methylcyclohexene, as well as the C_8-C_9 fraction of gasoline. The C_8-C_9 faction (130-190°C) mainly contains styrene (32.18%), α-methylstyrene (5.96%), vinyltoluene (7.37%) and indene (4.28%), which reacts with phenol as an alkylating agent.

Alkylation of phenol with methylcyclohexene and the C_8-C_9 fraction of gasoline pyrolysis was carried out on continuous laboratory setup, in the presence of modified zeolite-containing catalyst Seocar-2. The physicochemical properties of the extracted substances are as follows: para-(1-methylcyclohexyl)phenol: $T_{boil.}$= 161-164°C (10 °C / 10 mm Hg), $T_{melt.}$= 91 °C, molar mass – 190, para-(3-methylcyclohexyl)phenol: molar mass – 190, boiling temperature – 158 – 160°C/10 mmHg; melting temperature – 91°C; para-(arylalkyl)phenol based on the C_8-C_9 fraction of gasoline with characteristics: boiling temperature – 160 – 180 °C/10 mm Hg; n_D^{20} =1.5675, ρ_4^{40} =0.9736, molar mass – 200.

Acetophenones are synthesized by acylation reactions of methylcyclohexylphenols and arylalkylphenol with acetyl chloride in the presence of $ZnCl_2$.

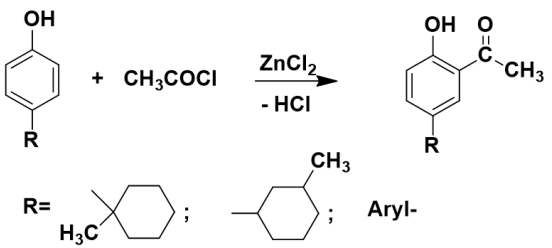

Fig. 1. Acylation rections of methylcyclohexylphenols and arylalkylphenol with acetyl chloride in the presence of $ZnCl_2$

Acetophenones have the following physico-chemical properties: 2-hydroxy-5(1-methylcyclohexyl)acetophenone: molar mass – 232, $T_{boil.}$=166-168 °C/10 mm Hg; $T_{melt.}$=114.8°C; 2-hydroxy-5(3-methylcyclohexyl)acetophenone: molar mass – 232, $T_{boil.}$=161-163°C/10 mm Hg; $T_{melt.}$=123°C; 2-hydroxy-5-arylalkylacetophenone: molar mass – 241, $T_{boil.}$=192-200°C/10mmHg. Methylcyclohexyl(arilalkyl)acetophenones are used as a photostabilizers at polyethylen.

Acknowledgements
This work was supported by the Azerbaijan Science Foundation –Grant № AEF- MGC-2024-2(50)-16/11/4-M-11

Love under the microscope: How chemicals affect our emotions

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Abstract:

Love manifests in various forms—for some, it is a tumultuous emotion full of passion, while others experience it in a calmer, less emotional manner. When we feel affection for someone, our heart rate accelerates, and blood pressure rises. During falling in love, many chemical reactions occur in the body that affect our well-being. Love is mainly perceived as an emotion; however, its biological aspect is often overlooked. Many chemical compounds control human emotions, causing us to experience euphoria, desire closeness, and better cope with pain.

Compounds responsible for these feelings include serotonin, dopamine, oxytocin, and endorphins. Dopamine makes us see our partner in an idealized way and notice positive traits in them. Endorphins cause excessive joy, reduce stress, and stimulate engagement in new and previously unknown activities. Oxytocin, also called the "love hormone," helps in building emotional bonds and strengthens the maternal instinct during contact with a newborn. In contrast, serotonin, known as the "happiness hormone," affects mood, regulates appetite, and improves sleep, and its level increases in the presence of a loved one. Thanks to these substances, love not only gives us a sense of fulfillment but also has a significantly positive impact on both body and mind. [1,2,3]

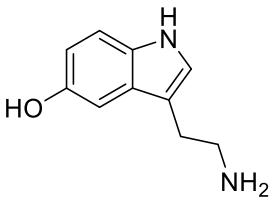

Fig. 1. Chemical formula of serotonin.

Literature:

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Comparative analysis of Organic and Non-Organic Broccoli Stems through Raman Spectroscopy

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Abstract:

Raman spectroscopy has emerged as a powerful, non-destructive analytical technique for investigating the chemical composition of vegetables such as brassica plant type, offering insights into cellular-level differences linked to cultivation practices [2]. This study applies Raman spectroscopy to compare the biochemical composition of organic and non-organic broccoli stems and cabbage residues, focusing on the identification of spectral fingerprints associated with plant metabolites, pesticide residues, and structural biomolecules.

Preliminary analyses of the spectral data reveal distinct differences in the Raman shift regions related to carbohydrates (480–1200 cm^{-1}), carotenoids (1515 cm^{-1}), and phenolic compounds (1600 cm^{-1}) between organic and non-organic samples, suggesting compositional variations likely linked to agricultural inputs and environmental stress responses.

These observations align with previous research highlighting Raman spectroscopy's sensitivity for distinguishing the chemical composition in a broccoli stem matrix [1].

The impact of this research lies in its contribution to sustainable food safety assessment by providing a rapid approach to evaluate the chemical integrity of a food product, as well as that it also determines the amount of bioactives that can positively impact our health.

Literature:

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Application of Surface-Enhanced Raman Scattering (SERS) in Breast Cancer Cell Analysis

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Abstract:

Raman spectroscopy is a powerful analytical technique used to identify the vibrational modes of molecules. When combined with nanoparticles, the intensity of the Raman bands can be significantly amplified. This enhancement arises from the interaction between the target molecule, metallic particles and light, which forms the basis of Surface-Enhanced Raman Scattering (SERS) [1].

SERS has diverse applications, including the analysis of biological specimens [2]. This study proposes that SERS is an effective method for characterizing breast cancer cells. To distinguish cancer-specific spectral signatures, Raman spectra of malignant and healthy breast cells were acquired under identical experimental conditions. The experimental approach involved the use of silver and gold nanoparticles, with the cells incubated alongside these nanoparticles for three hours before Raman spectroscopic measurements and imaging were conducted.

This study aimed to evaluate whether cancer cells generate Raman spectra that differ from those of healthy cells. Such findings could support the potential of SERS as an effective method for cancer detection.

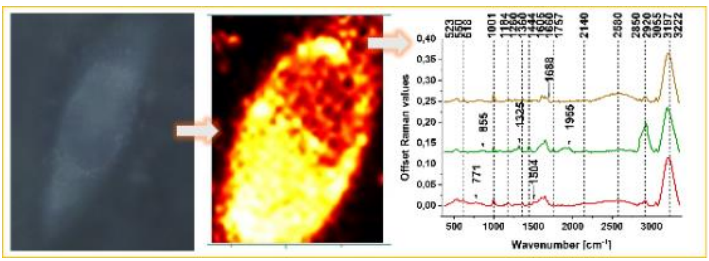

Fig. 1. Microscopy image of the cell, Raman mapping of the cell and Raman spectra of gold nanoparticles (AuNPs), MCF10A and MDA-MB-231 cells incubated with AuNPs.

The research is funded by FU²N grant 503/3-34-4-1.

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Nail polishes as an alternative to transdermal therapeutic systems

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Abstract:

Nonsteroidal anti-inflammatory drugs (NSAIDs) are widely used for treating pain, fever, and inflammation, often for common illnesses like colds. They are easily accessible, even in places lacking qualified staff to advise on proper use. Despite their benefits, NSAIDs can cause serious side effects, including gastrointestinal issues, liver toxicity, respiratory problems, allergies, and more, even when used as directed. [1]

Considering the toxicity of drugs, research has been conducted for several years to consider therapeutic nail polishes as a safe route of drug administration. Research conducted at the Krakow University of Technology to develop a nail polish containing *ciclopirox* - a drug with antifungal, antibacterial and anti-inflammatory properties has shown that the developed formulations allow for gradual release of the drug to a dose significant from the therapeutic point of view, even in the case of nails painted with a permanent cosmetic varnish. PVP-based formulations showed the best film-forming properties, with the formulation where the largest amount of *ciclopirox* was released (4.47 mg/10 ml after 24 hours) being the most noteworthy. [2]

The results of this study inspired us to investigate the development of therapeutic nail polishes that contain various drugs, especially NSAIDs, instead of ciclopirox. The tests carried out have proven that the developed therapeutic nail polish formulations can also be successfully used for the gradual release of NSAIDs such as *ibuprofen*.

The projectwas createdas part of the "DrugDesign" ScientificClub and the FutureLabPK (Project No.99. Nail polishes as an alternative to transdermal therapeutic systems)

Literature:

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What can you make out of wood, rice and egg white? The future of mobile phones in harmony with nature.

Dominika Jurkowska[1]

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Abstract:

As is well known, scientists are constantly looking for alternatives to plastic and other non-biodegradable materials. Now, Bharat Baruah of Kennesaw State University in Georgia and his colleagues have developed a process that will allow windows and smartphone screens to be made from transparent wood with the addition of egg whites, and safely composted at the end of their lives.

Wood has been turned into a transparent material before, but it was a rather complicated, time-consuming and expensive process. The new process is much simpler and cheaper, replacing synthetic epoxy with natural egg white and rice extract. It will not give us a 100% transparent material, but it will be biodegradable. Such a material also has insulating properties, so it can be used as a window.

The research is new, it was published this year, so there are certainly many issues that need to be investigated, such as the strength, thermal properties of the material and techniques to improve transparency. It is certainly a very promising material that we may all be able to use in a few years' time [1].

Literature:

[1] **Matthew Sparkes** 2025,Wood made transparent using rice and egg whites could replace windows. New Scientist.

Non-antimicrobial and Non-anticancer Properties of ZnO Nanoparticles Biosynthesized Using Different Plant Parts of Bixa Orellana

Izabela Kalisz[1]

[1]*University of Gdańsk, Faculty of Biotechnology, Department of Biophysics*

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Abstract:

One of the problems that healthcare is currently struggling with is the increase in the number of patients with cancer and infected with microorganisms resistant to commonly used drugs. Traditional methods of fighting cancer, such as chemotherapy and radiotherapy, are unfortunately toxic to both healthy and cancer-affected cells. For this reason, a search has begun for a way to target therapy at altered cells, which can be achieved with zinc oxide nanoparticles. Currently, nanoparticles are not widely used due to their lack of biocompatibility with mammalian cells. The toxicity of nanoparticles is influenced by many factors, including their size, morphology, concentration, etc. Another factor influencing the biocompatibility of nanoparticles with cells is the method of their synthesis. There are three main methods of synthesizing nanoparticles: physical, chemical, and biological, of which biologically synthesized nanoparticles are the least toxic.

The aim of this study is to produce zinc oxide nanoparticles using different plant parts (leaves, seeds, seed coats) of the *Bixa orellana*. Their antibacterial and anticancer activity was tested, showing that calcinated zinc oxide nanoparticles do not exhibit antibacterial and anticancer activity. The lack of these abilities may initially indicate their biocompatibility and thus inform about their non-toxic properties. These properties may enable the use of biosynthesized zinc oxide nanoparticles in biomedicine as an alternative treatment [1].

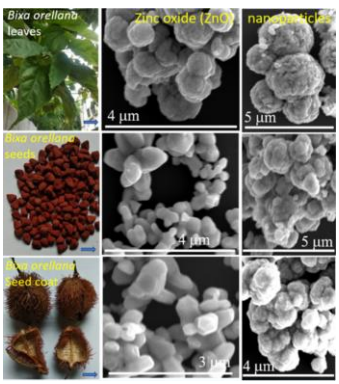

Fig. 1 Morphology of zinc oxide and its nanoparticles from different parts of Bixa Orellana

Literature:

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Photosynthetic response of microalgae to flufenamic acid and nabumetone: an IBR index-based approach

Dominika Kapuścińska[1], Agnieszka Baścik-Remisiewicz[1], Anna Aksmann[1]

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Abstract:

Nonsteroidal anti-inflammatory drugs (NSAIDs) represent a significant class of environmental micropollutants, which are increasingly found in surface waters. Their persistence and common occurrence can negatively affect the basic physiological processes of aquatic organisms, such as microalgae, which are key primary producers. For many years, green algae have been used in studies on the phytotoxicity of environmental pollutants [1]. They are also a promising tool for detoxification and removing pollutants, including pharmaceuticals and their derivatives, from the environment [2].

The presented study evaluated the impact of flufenamic acid and nabumetone on specific parameters associated with photosynthesis in the green alga *Chlamydomonas reinhardtii*. To make interpretation of the results easier and more practical, a synthetic comparison of the effects of the tested NSAIDs on microalgae, the integrated biomarker response index (IBR), was used. The biomarkers included for the analysis were the intensity of photosynthesis, the content of chlorophylls and carotenoids, and selected parameters of chlorophyll *a* fluorescence *in vivo*. The results indicate that IBR based on photosynthetic biomarkers enables a sensitive assessment of NSAID toxicity and allows for a thorough comparison of their effects on microalgae cells. This approach can serve as a valuable tool in ecotoxicological studies, helping evaluate environmental risks associated with pharmaceuticals present in aquatic environment.

This work was funded by the National Science Centre of Poland (OPUS 2019/35/B/NZ9/01567).

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Determination of the effectiveness of *Bacillus* spp. in the counteracting the effects of soil drought in yellow lupine

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Abstract:

Drought is a major abiotic stressor that significantly limits legume productivity by disrupting key developmental processes, including flowering and seed formation [1]. Yellow lupine (*Lupinus luteus* L.), a drought-sensitive legume, demonstrates a particularly strong correlation between water deficit and yield reduction, often due to premature flower abscission [2].

In the present study, we examined the biological activity of beneficial rhizosphere microorganisms - bacteria (*Bacillus subtilis* and *B. licheniformis*) and assessment their usefulness in increasing the resistance of lupine growing under soil drought stress (25% water holding capacity, WHC) [3].Plants were subjected to one of three treatments: inoculation with *Bacillus subtilis*, *Bacillus licheniformis*, or a mixture of both strains. Morphological assessments included measurements of root length, shoot length, total plant length, number of leaves, number of flowers formed, chlorophyll content, and leaf relative water content (RWC).

The results revealed notable differences in plant performance under microbial treatments, indicating that each *Bacillus* spp. variant increased flower formation compared to the control and drought conditions. These treatments also contributed to a higher RWC index in leaves and elevated chlorophyll content, which indicates improved hydration and photosynthetic efficiency during drought stress. These findings support the hypothesis that plant-associated bacteria enhance tolerance to water deficit by modulating physiological responses

This work was funded under the grant scheme of the Doctoral School of Exact and Natural Sciences at Nicolaus Copernicus University as part of the AST Minigrants editions I/2024 and III/2024.

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A comparative study of Cd(II) complexes with pyridyl-based 1,3-selen/thiazolyl-hydrazones

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Abstract:

In order to obtain biologically active compounds with (1,3-selenazol/thiazol-2-yl)hydrazine ligands, new cadmium(II) complexes $[Cd(HLSe^1)_2](ClO_4)_2$ (**1–Se**) and $[Cd(HLS^1)_2](ClO_4)_2$ (**1–S**) were synthesized and characterized (Figure 1). X-ray structural analysis revealed that both complexes crystallize in a monoclinic *C*2/*c* space group. Coordination number of Cd(II) is sixth in both cases and the ligands are coordinated in neutral form *via NNN* donor atoms set: pyridine and azomethine nitrogen atoms and nitrogen atom from selenazole or thiazole ring. For analysis of intermolecular interactions Hirshfield surfaces and 2D pseudosymmetric fingerprint plots were constructed. Crystal packings of both complexes are based on classical and non-classical hydrogen interactions. The thermal stability of the Cd(II) complex was analyzed. Based on the analysis of data obtained from spectrophotometric titration, the number of species present in the solution, the stoichiometry, and the stability of the formed Cd(II) complexes were determined. The obtained values of the cumulative stability constant indicate significant stability of the investigated compounds. The antimicrobial and antioxidant activity of the desired complexes and corresponding ligands were determined. Complex **1–S** exhibited 40 times better activity against the strains *P. aeruginosa*, *B. subtilis*, and *C. sporogenes* compared to the control antibiotic.

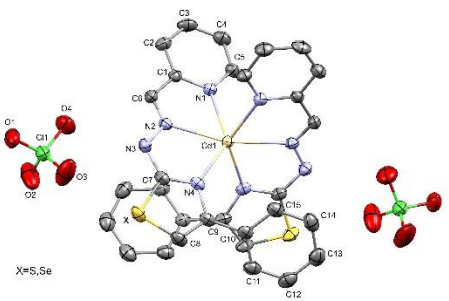

Fig. 1. ORTEP drawing of the molecular structure of **1–S** and **1–Se.** Displacement ellipsoids are shown at 30% probability level. All hydrogen atoms are omitted for clarity.

Nanomaterials: history, classification, applications and toxicity.

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Abstract:

Nanoscience and nanotechnology are among the most promising technologies of the 21st century. Nanomaterials are an emerging area of research that encompasses structures, devices, and systems with new properties and functions resulting from the arrangement of atoms on the scale of 1–100 nm [1]. The history of nanotechnology began in 1959 when Richard Feynman delivered a lecture titled "There's Plenty of Room at the Bottom," at the California Institute of Technology. Feynman's lecture was based on imagining what it would take to fit the 24-volume Encyclopedia Britannica on the head of a pin. In 2007, technologists at the Israel Institute of Technology placed the entire Hebrew text of the Old Testament in an area of just 0.5 mm^2 on a gold-coated silicon wafer. The text was etched by directing a concentrated stream of gallium ions at the wafer.

Due to its unique characteristics, nanoscale matter is a distinct form of matter from solid, liquid, gas, and plasma states. The characteristics of nanomaterials are determined mainly by their shape and size. These materials are divided into 4 types: 0D, 1D, 2D, and 3D [2]. Currently, nanotechnology is used in various fields of science, key industrial sectors, and electronics.

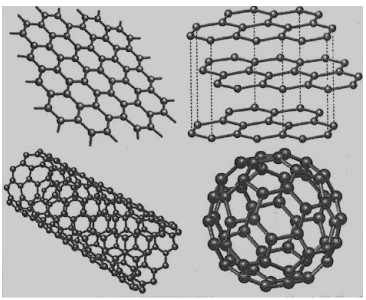

Fig. 1. The spatial structure of graphene (2D type) compared to the structures of graphite, carbon nanotube, and fullerene C_{60}

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Applications of Metal Nanoparticles in Medicine

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Abstract:
Nanoparticles have been the subject of an increasingly vast body of research. In recent years the availability and diversity of nanoparticles has increased significantly, resulting in bringing them closer to being implemented in routine applications [1]. Among many different groups of nanoparticles, metal nanoparticles stand as one of the most promising. Their unique properties, related to fascinating physical and chemical phenomena, present only at the nanoscale, make them ideal candidates for many biomedical applications. Metal nanoparticles have been proposed to function as drug delivery vehicles, facilitate new imaging modalities and as novel antibiotics to name a few [2]. As the scientific community explores the properties and capabilities of nanoparticles, there is a need to make this knowledge more accessible, in order to promote their use and further study. To this end, this presentation compiled a selection of metal nanoparticles that have found potential use in medicine. As with any newly emerged area of study, there is a need for research that could translate laboratory findings into applicable solutions. This is especially difficult in the case of nanoparticles due to many conflicting results of safety studies [3]. This presentation strives to make nanoparticles more approachable through a digestible form factor, tailored to a wide audience.

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Multifaceted effect of metabolites and EVs secreted by probiotic strains on Candida albicans pathogenic activity and host-microbe dynamics

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Abstract:

The microbe balance plays a critical role in maintaining host homeostasis. Health-promoting bacterial strains, particularly those from genera *Lactobacillus* and *Bifidobacterium*, regulate microflora composition through a variety of secreted bioactive molecules, preventing from overgrowth of opportunistic pathogens, including fungi *Candida albicans*. Within this array of bioactive compounds, probiotic bacteria produce bilayered structures that enclose diversified cargo, known as extracellular vesicles (EVs). Due to their nanometer-scale size and ability to protect vesicular cargo, they serve as effective long-distance mediators and interkingdom communicators, as they are secreted by the majority of kingdoms, including bacteria and eukaryotic cells [1].

The aim of this study was to determine the effect of metabolites secreted by selected probiotics bacterial strains (*Lactoplantibacillus plantarum*, *Lacticaseibacillus rhamnosus* and *Streptococcus salivarius*) on *C. albicans* cells, with the focus on the role of bacterial EVs in modulating biofilm formation ability and adhesion to host epithelial cells.

Cell-free supernatants (CFS) derived from probiotic cultures contributed to *C. albicans* growth reduction and increased cell disruption, while isolated EVs fraction exhibited more ambiguous results. The 4.5h co-incubation with *C. albicans* cells promoted fungal cell death, similarly to CFS; however, EVs also strongly increased yeast filamentation essential for further biofilm development. Simultaneously, EVs appeared to alter the structural organization of the biofilm, as microscopic observations revealed that the biofilms consisted of loosely connected clusters of yeast cells. Moreover, EVs did not exhibit cytotoxic effects on human epithelial cells. Adhesion tests indicated that *C. albicans* retained the ability to adhere to epithelial monolayers in the presence of EVs. However, a tendency of yeast cells to aggregate was observed without an enhancement of their filamentation.

Taken together, these results highlight the complex and multifaceted roles of probiotic derived metabolites and their influence on fungal pathogenesis.

This research was supported by the National Science Centre, Poland (no. 2021/43/D/NZ6/01464 to J.K.K)

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Double and multi-metal cyanides: tools to minimize environmental impacts

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Abstract:

The aims are to develop efficient, cost-effective adsorbents for the rapid sorption of heavy and radioactive metal ions in wastewater as well as CO_2 adsorbents that simultaneously act as catalysts for the controlled ring-opening copolymerization of epoxides with captured CO_2 to produce polypropylene carbonate.

Key research question: What is the fate of natural waters and the atmosphere if heavy and radioactive metal and CO_2 pollution is not immediately eliminated?

Mean idea: Highly efficient adsorbents of CO_2 and heavy metal ions can minimize the environmental damage. Hexacyanoferrate family is of particular interest in this respect due to (i) high ability to bind heavy and radioactive metal ions, (ii) adsorb CO_2, and (iii) act as a catalyst to provide controlled reaction between adsorbed CO_2 and epoxides. This study focuses on colloidal structures. The creation of new structures offers a wide range of rational choices for various applications. The research is quantitatively substantiated by Dynamic Light Scattering, Laser Doppler Velocimetry, and Infrared Spectroscopy.

The synthesized structure of double metal cyanides corresponds to micelle (A): coordination polymer in aggregate with an amorphous part. The role of potential determining ions is played by $[Fe(CN)_6]^{y-}$. The K^+ ions of the Stern layer have relatively lower kinetic energy and cannot be detected potentiometrically. The counter-ions of the diffuse layer are a part of the bulk solution due to osmotic force.

$$\overbrace{[m\mathrm{Zn}_a[\ \widetilde{\mathrm{Fe}}\ (\mathrm{CN})_6]_b}^{\substack{\text{aggregate}\\ \text{II or III}}}\ \overbrace{n[\mathrm{Fe(CN)}_6]^{y-}}^{\substack{\text{potential-}\\ \text{determining}\\ \text{ions}}}\ \overbrace{y(n-x)\mathrm{K}^+]}^{\substack{\text{counter-ions}\\ \text{of Stern layer}}}\ \overbrace{y{\cdot}x-}^{\substack{\text{charge}\\ \text{of}\\ \text{particle}}}\ \overbrace{y\cdot x\mathrm{K}^+}^{\substack{\text{counter-ions}\\ \text{of diffuse}\\ \text{layer}}} \quad \text{(A)}$$

The colloidal nanostructure (A) is rich in Lewis basic centers determined by the σ-donor capacity of the weakly antibonding 5σ nitrogen orbital of M-C≡N-. Zeta potential is –53 mV for ferrocyanides and –35 mV for ferricyanides by laser Doppler electrophoresis. Lewis basic centers represent the coordination site for heavy and radioactive metal cations.

The synthesized structure of multi-metal cyanides corresponds to micelle (B):

$$[m\mathrm{Zn}_a[\mathrm{Fe(CN)}_6]_b\ \overbrace{n[\mathrm{Fe(CN)}_6]^{y-}}^{\substack{\text{potential-}\\ \text{determining}\\ \text{ions}}}\ \overbrace{x\mathrm{T}^{2+}c\mathrm{K}^+}^{\substack{\text{counter-ions}\\ \text{of Stern layer}}}\ ]^{2x+c-y\cdot n}\ \overbrace{(y\cdot n-2x-c)\mathrm{Ion}^{(l)}}^{\substack{\text{counter-ions}\\ \text{of diffuse}\\ \text{layer}}} \quad \text{(B)}$$

Adsorbed “T” corresponds to transition cations coordinated as "innocent" cation. These particles have small positive zeta values and are colloidal unstably. The electron-deficient incomplete coordination sphere of adsorbed “T” cations acts as the Lewis acid center.

The findings should be considered in the strategy of controlled ring-opening copolymerization of epoxides with CO_2 to give polycarbonates. The proposed structures of catalyst micelles provide an opportunity to focus careful attention on every detail of their catalytic activity.

Artificial intelligence tools to improve the diagnosis of artificial stone silicosis

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Abstract:

Silicosis is a progressive and incurable lung disease caused by the inhalation of respirable crystalline silica (RCS). It is one of the most important occupational diseases worldwide [1] and has recently re-emerged due to the increasing use of artificial stone, a popular material primarily used in the manufacture of kitchen and bathroom benchtops.

High levels of RCS are generated during the processing of this material, as it is composed of over 90% silica. This has led to an increase in the incidence of artificial stone silicosis (ASS), which affects younger workers and progresses more rapidly and severely than traditional silicosis from mining [2].

Early diagnosis is crucial for implementing preventive measures; however, current radiological techniques, such as chest X-rays and high-resolution computed tomography, have limitations in early detection and lead to discrepancies in diagnoses among radiologists. Artificial intelligence (AI), especially convolutional neural networks (CNNs), has shown potential in medical image analysis to improve disease detection and diagnosis [3]. However, the lack of annotated image sets and the need for explainable and interpretable models for healthcare professionals represent challenges for its practical clinical implementation.

Within the framework of the PEOPLE project, we have developed a clinical decision support tool based on explainable artificial intelligence, designed to assist clinical experts in the diagnosis and classification of silicosis in patients exposed to artificial stone. This tool also allows for annotation of images and labeling of radiological signs of the disease, generating data sets that can feed into and continuously improve predictive models. The platform is ready to integrate new diagnostic features as new architectures and models are developed. This research allows us to harness the potential of AI in the clinical field, aligning it with the current needs of modern medicine.

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Comparative Characterization of Oils Extracted from Milk Thistle Seed Cakes: Physicochemical, Chromatographic, Spectrophotometric, and Thermal Analyses.

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Abstract:

Milk thistle (*Silybum marianum*) seed cakes, obtained as by-products of oil extraction, are rich in bioactive lipophilic compounds [1]. The aim of the study was to compare the physicochemical, thermal, and antioxidant properties of oils extracted from two different seed cake samples, each obtained from different Polish sources.

Soxhlet extraction was conducted for 6 hours using two solvents: hexane (H) and dichloromethane (DCM). The resulting oils were analyzed for acid and peroxide values, fatty acid profile, total phenolic content (TPC), antioxidant activity (DPPH assay), and oxidative stability using Pressure Differential Scanning Calorimetry (PDSC). Additionally, before oil extraction, the calorific value, antioxidant activity and phenolic content of the pomace were analyzed.

Fatty acid analysis revealed similar profiles across all samples, with oleic and linoleic acids as dominant components. Notably, hexane-extracted oil from Cake-1 showed a significantly higher polyunsaturated fatty acid content compared to its counterpart. Acid values ranged from 8.77 to 11.26 mg/g, and peroxide values from 7.8 to 9.7 meq O_2/kg. DCM-extracted oils showed slightly higher acid values but lower peroxide values, indicating increased oxidative resistance. TPC in oil samples ranged from 1.45 to 1.55 mg GAE/g, and antioxidant activity varied from 4.8% to 6.9% inhibition of DPPH, with DCM-extracted samples generally performing better. PDSC analysis provided oxidation induction times (τ_{int}) and maximum oxidation times (τ_{max}). Hexane-extracted oils from Cake-1 and Cake-2 showed τ_{int} of 60.33 and 54.81 min, respectively, while DCM-extracted oils demonstrated enhanced stability with τ_{int} values of 114.93 and 119.36 min. τ_{max} followed similar trends. Cake residues retained higher levels of phenolics (2.25–12.50 mg GAE/g) and antioxidant activity (29.2–44.7% DPPH inhibition). Bomb calorimetry revealed energy content of 23 224 J/g in Cake-1 samples, with Cake-2 determined at 22 700 J/g.

Overall, oils extracted using DCM demonstrated better oxidative and antioxidant performance, while slight compositional differences were observed between cakes. These findings provide insight into the valorization potential of milk thistle seed cakes as sources of functional oils and bioactive compounds for nutraceutical and food applications.

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The influence of impact modifier on properties of biodegradable polymer compositions

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Abstract:

There are ongoing changes in the polymer market. Instead of using fossil-based, non-degradable polymers such as polyethylene or polypropylene in the production of single-use products, containers, and packaging, more and more companies look for natural-origin substitutes. The global market for natural polymers—such as starch, proteins, polypeptides, and polysaccharides—was valued at USD 9.3 billion in 2023 [1]. However, bio-based polymers are still limited by their higher cost and lower mechanical properties compared to fossil-based polymers [2, 3].

We focused on developing a biodegradable and compostable composite material by combining starch with bio-polyester and an impact modifier in varying ratios. The objective was to identify formulations that retain functional properties while providing optimal mechanical performance.

The research methodology involved the preparation of composite samples with impact modifier using a twin-screw extruder, followed by injection molding of test samples and characterization tensile and impact strength, and also melt flow index (MFI).

This study demonstrates the potential of low-cost and sustainable materials. The research was conducted in collaboration with Bio Plast Pom Company [4], highlighting its potential for industrial application.

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[4] https://bioplastpom.pl

The Role of the Natural Anastomosing Narew River in Mitigating Microplastic Flow

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Abstract:

Water pollution by microplastics (MP) is a well-known environmental issue, although research in Poland remains limited. This study assessed the level of MP pollution in the unique, highly natural, anastomosing Narew River and its tributaries, with a particular focus on the Narew National Park (NNP). The analysis included both the quantity and quality of MPs in water samples from regulated and natural sections of the rivers. Environmental samples were collected during the growing season in July 2025. Microscopic observations were made to count and visually inspect the particles' shape, color, and size. The average concentration of MPs was 496 particles/m³. Blue and black were the dominant colors, accounting for 29% and 27% of the samples, respectively. Fibers and fragments were the most common types, comprising 41% and 57%, respectively. The majority of particles were smaller than 2 mm, with an average size of 745 μm. We conclude that assessing the extent of pollution in undisturbed, protected areas is essential, as it may play a significant role in reducing the flow of MPs into the Baltic Sea.

Cu/Co-Doped ZIF-8 as a visible light-activated photocatalyst for dye degradation

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Abstract:

Zeolitic imidazolate frameworks (ZIFs), a subclass of metal-organic frameworks composed of metal ions and imidazolate linkers, have emerged as promising candidates for wastewater treatment.[1] However, the wide band gap of pristine ZIF-8 limits its photocatalytic efficiency. To address these challenges, metal doping has been widely explored as a strategy to enhance the light-harvesting ability, charge separation efficiency, and catalytic performance of ZIF-based photocatalysts.[2] This study presents the synthesis and characterization of novel trimetallic ZIF material, where Zn(II) sites in the ZIF-8 structure are partially substituted by Cu(II) and Co(II) ions, enhancing their photocatalytic properties. The material was synthesized using reaction-diffusion framework method utilizing a hydrogel agar medium to promote controlled incorporation of metal ions. The structural and compositional features of the Cu/Co-doped ZIF-8 were investigated using powder X-ray diffraction (PXRD), scanning electron microscopy with energy-dispersive X-ray spectroscopy (SEM-EDS), UV-Vis and FTIR spectroscopy, along with inductively coupled plasma mass spectrometry (ICP-MS) for elemental analysis of digested samples. The photocatalytic efficiency of these materials was evaluated by studying the degradation of Mordant blue 9 dye under visible light irradiation, without requiring additional oxidant, demonstrating their potential for sustainable wastewater remediation.

Acknowledgment: This work has received funding from the European Union's Horizon Europe Widening Participation program under grant agreement No 101059534 (PFAStwin).

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Chemical characterization and pharmacological potential of essential oils of *Senecio vulgaris Vahl* and *Salvia corrugata L.* from the Ecuadorian Andean region

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Abstract:

Salvia corrugata Vahl (Lamiaceae) is a plant endemic to the mountainous regions of Ecuador, whereas *Senecio vulgaris L.* (Asteraceae) is an invasive weed with worldwide distribution. Both species have traditional uses but scarcely from chemical and pharmacological perspectives. This study provides an initial chemical characterization of essential oils and plant extracts obtained by steam distillation and extraction organic solvent extraction.

The preliminary chemical characterization was carried out using specific instrumental techniques: gas chromatography coupled with mass spectrometry (GC-MS) to assess the chemical composition of the essential oils, and infrared spectroscopy (FTIR) and ultraviolet-visible spectroscopy (UV-Vis) to analyze the vegetable extracts. These techniques confirmed the presence of terpenoids, phenols, flavonoids, and alkaloids, highlighting the presence of sesquiterpenes in *S. vulgaris* and diterpenes in *S. corrugata*, linked to antimicrobial, antioxidant, and potentially neuronal effects.

The results support the therapeutic potential of these plants and provide a foundation for further biological testing against microbial strains and cell cultures. This study also highlights the pharmacological value of species often considered harmful or ornamental, emphasizing the importance of exploring unconventional plants as natural health resources.[1-3]

I would like to thank the Department of Chemistry and the Bioproducts Plant of the Universidad Técnica Particular de Loja (UTPL) for their support in the extraction and characterization of essential oils and plant extracts.

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The use of benzimidazole derivatives to increase plant tolerance to soil salinity

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Abstract:

Water is the most abundant compound on Earth's surface and a fundamental element for the functioning of living organisms. Various environmental factors can lead to water deficits in plants, resulting in either physical drought due to soil water shortage or physiological drought in saline soils. High salt concentrations hinder or prevent water uptake by plant roots. Moreover, excessive soil salinization is exacerbated by the global rise in average temperatures, which intensifies soil water evaporation and increases the frequency of agricultural irrigation.

This study aims to evaluate the effectiveness of the benzimidazole derivative omeprazole (OM) in enhancing plant tolerance to soil salinity. The impact of soil application of OM solutions at 5 and 10 μM concentrations on mitigating salt stress—induced by sodium chloride (NaCl) application—was analyzed in lettuce (*Lactuca sativa* var. *crispa* L.) and sweet basil (*Ocimum basilicum* L.). The plants were cultivated as *baby leaves* and *microgreens* and included both green- and red-leafed cultivars differing in protective pigment accumulation.

Non-invasive assessments included the leaf greenness index (SPAD), spectrophotometric analysis of chlorophyll *a* and *b*, carotenoids, and leaf proteins. Additionally, photosynthetic activity was examined using modulated chlorophyll *a* fluorescence analysis, and leaf protein profiles were assessed via SDS-PAGE with densitometric evaluation. Intracellular accumulation of the osmoprotectant proline was also quantified.

The results demonstrated that OM application alleviates salt stress effects in lettuce and basil; however, this response is species- and cultivar-specific. An increase in chlorophyll content was observed in the red-leaf lettuce cultivar Lollo Rossa and the green-leaf basil cultivar Sweet Large. In the red-leaf basil cultivar Dark Opal, OM stimulated leaf protein accumulation despite salinity stress. Across all cultivars, OM treatment enhanced photosynthetic activity and reduced non-photochemical quenching of absorbed light energy. Additionally, OM-treated plants exhibited a decrease in intracellular proline levels.

This study confirms that the benzimidazole derivative omeprazole exerts a beneficial effect in mitigating salt stress in crop plants and may serve as a potential tool for improving crop yields in saline-affected agricultural areas.

The workshop is co-financed by the Minister of Science (Poland) under the "Regional Excellence Initiative" program (project no.: RID/SP/0015/2024/01)

Direct recycling of graphitic anodes from spent lithium-ion batteries

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Abstract:

The accelerated growth of the lithium-ion batteries (LIBs) market, which are being utilised in an increasing number of electric vehicles (EVs), portable electronics and renewable energy storage systems, has given rise to the pressing need to address the end-of-life management of spent cells. According to analyses and projections by the International Energy Agency (IEA), announced global recycling capacity is projected to exceed threefold the supply of batteries that could potentially be recycled in 2030, as EVs reach the end of their operational life within the Announced Pledges Scenario. However, EV battery retirement is expected to grow rapidly from the second half of the 2030s [1]. This massive volume of spent LIBs represents a valuable secondary source of critical materials, including graphite.

One of the most promising approaches for graphite recovery is direct recycling, which enables the immediate reuse of the recovered anode material in new battery cells without extensive chemical processing. The aim of this study is to investigate two direct recycling methods for spent graphitic anodes and to evaluate the electrochemical performance and structural characteristics of the recovered graphite. The recycled materials were compared with pristine commercial graphite in terms of electrochemical performance as well as structural features to assess the feasibility of each recycling approach.

Financial support from the National Science Centre, Poland, under the SONATA BIS programme, grant No. UMO-2022/46/E/ST8/00395 is gratefully acknowledged.

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Ab initio study of the electronic properties and magnetic phases of thermoelectric oxide material $Ca_3Co_4O_9$

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Abstract:

Thermoelectric materials can be used as an alternative sustainable energy source, as they can convert waste heat into power. We performed density-functional theory (DFT) calculations to study the layered calcium cobaltite ($Ca_3Co_4O_9$). We model this system using the generalized gradient approximation (PBE) functional and meta-generalized gradient approximation (meta-GGA) R2SCAN functional. A rational approximation for the supercell was considered to determine the structural and electronic properties and the magnetic phases. The initial magnetic phases are expected to relax to ferromagnetic, antiferromagnetic, and ferrimagnetic phases. Considering the energy, we select the most likely phases, compute the band structure, and discuss it in light of the available experimental data. These results are important for future work, as further calculations are expected to determine the thermoelectric properties of calcium cobaltite [1].

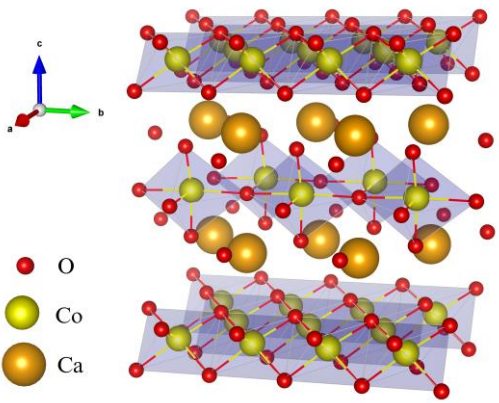

Fig. 1. Layered calcium cobaltite $Ca_3Co_4O_9$ supercell (3/2) with CoO_2 octahedra highlighted.

Literature:

[1] Lemal, S., Varignon, J., Bilc, D. I., & Ghosez, P. (2017). Thermoelectric properties of layered calcium cobaltite Ca 3 Co 4 O 9 from hybrid functional first-principles calculations. *Physical Review B*, *95*(7), 075205.

Ozempic and the Rise of GLP-1 Drugs: Benefits, Controversies, and Public Health Risks

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Abstract:

Glucagon-like peptide-1 (GLP-1) receptor agonists, including semaglutide (Ozempic), were originally developed for the treatment of type 2 diabetes. These drugs mimic the natural hormone GLP-1, which helps regulate blood sugar by increasing insulin release, reducing glucagon secretion, and slowing down digestion. In addition to improving blood sugar control, GLP-1 receptor agonists promote weight loss by reducing appetite through their effects on the brain and increasing feelings of fullness [1]. Ozempic, in particular, has gained attention for its off-label use in weight management, leading to high demand and shortages that have affected diabetic patients. Although these drugs are effective, they also come with safety concerns. Reported side effects include nausea, vomiting, pancreatitis, gallbladder disease, and possible cardiovascular risks. Additionally, data from the UK Medicines and Healthcare products Regulatory Agency (MHRA) have linked GLP-1 receptor agonists to 82 deaths, raising concerns about their long-term safety [2]. This poster examines the risks of uncontrolled use of GLP-1 receptor agonists, the controversies surrounding Ozempic, and the necessary future directions in regulation and research.

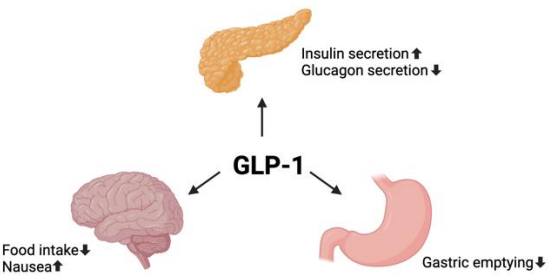

Fig. 1 Metabolic effect of GLP-1 on different organs.

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Crystal structures of new polycarboxylate coordination compounds based on VO(IV) and VOO(V) ions and catalytic properties in olefin co(polymerization) processes

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Abstract:

Contemporary research is focused on the development of new, economical and simple methods for the synthesis of transition metal ion-based catalysts with high activity and thermal and thermodynamic stability. Of particular interest is the "green" and one-step synthesis of oxovanadium(IV) and dioxovanadium(V) coordination compounds, which can provide an alternative to the currently used catalytic systems in (co)polymerization and olefin metathesis processes [1].

As part of the research conducted, new VO(IV) and VOO(V) coordination compounds containing dipicolinate, thiodiacetate, oxydiacetate, iminodiacetate and *N*-methyliminodiacetate anions were obtained. Their crystal structure was determined and their thermodynamic stability was analyzed. The obtained (di)oxovanadium(IV/V) complexes were used as catalysts in the polymerization of ethylene and copolymerization of ethylene with oct-1-ene, using Et_2AlCl (diethylaluminum chloride), $EtAlCl_2$ (ethylaluminum dichloride) and MMAO-12 (modified methylaluminoxane) as cocatalysts. In addition, the molar masses, dispersity, thermal properties and microstructure of the obtained (co)polymers were studied.

The project is funded by the Ministry of Education and Science under the Pearls of Science Program Project No. PN/01/0137/2022.

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Searching for pharmacophores of the L1-binding loop of platelet-derived growth factor PDGF-BB

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Disturbances in the physiological process of wound healing can lead to chronic wounds - a significant medical, social and economic problem that affects a growing number of patients, especially those suffering from civilization diseases such as diabetes. Classical therapies often prove insufficient, prompting the search for new treatment strategies, including the use of growth factors, i.e. those that regulate healing processes [1]. One of these is the platelet-derived growth factor PDGF-BB, which has already found clinical application in the treatment of neuropathic wounds. However, peptides capable of mimicking the function of proteins while retaining their favorable characteristics, such as biocompatibility, non-toxicity and ease of synthesis, are attracting increasing attention from researchers. This is no different for PDGF-BB, whose short fragments, containing regions responsible for binding to the receptor, also show biological activity. The Pdgf2 peptide designed on this basis (the L1 loop of the PDGF-BB protein) not only stimulated proliferation of human fibroblast and keratinocyte lines, but also accelerated wound healing in a mouse model [2].

Despite its promising therapeutic properties, the key amino acid residues responsible for its activity remain unknown. In order to identify them, an alanine scan - a systematic substitution of consecutive amino acids with an alanine residue - was performed. Peptides were synthesized by microwave solid support synthesis (MW-SPPS).

The resulting compounds were tested for affinity to the PDGFRβ receptor using a ELISA based system. In parallel, circular dichroism measurements were performed to assess the effect of individual substitutions on the secondary structure of the peptides. The results of the study allowed the selection of amino acids critical for the binding of the Pdgf2 peptide to the receptor and potential sites for further structural modifications. The identification of these key residues represents an important step towards the design of therapeutic peptides with optimized pro-regenerative activity, which may find future applications in the treatment of chronic wounds.

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Computational studies of topological defects on transition-metal dichalcogenide NbS_2 monolayer superlattice

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Abstract:

Two-dimensional (2D) transition metal dichalcogenides (TMDs) have attracted considerable interest due to their versatile electronic properties and promising applications in nanotechnology. Niobium disulfide (NbS_2), a metallic TMD, distinguishes itself from semiconducting counterparts such as MoS_2 through its unique electronic and structural characteristics. NbS_2 typically crystallizes in layered polytypes, such as the 2H phase, where niobium atoms occupy octahedral sites between sulfur layers, stabilized by weak van der Waals forces. Unlike conventional semiconducting TMDs, NbS_2 displays intrinsic metallic behavior, high electrical conductivity, and strong electron-phonon interactions, which give rise to superconductivity in its bulk form with a critical temperature. While thickness-dependent studies confirm the retention of metallic properties in monolayer NbS_2, superconducting transitions in the 2D limit remain poorly understood. These attributes position NbS_2 as a compelling candidate for advanced conductive materials. [1]

This study employs ab initio density-functional theory (DFT) calculations implemented in the Vienna Ab initio Simulation Package (VASP) to investigate the electronic structure of 2D NbS_2 superlattice formed with topological defect. The results shed light on the material's thickness-dependent properties, offering insights into its potential as a 2D conductor. Key findings will be analyzed to bridge gaps in understanding 2D NbS_2 behavior at the atomic scale, with implications for its application in nanoscale electronic devices.

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E water pipes as a significant source of microplastics in drinking water

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Abstract:
Drinking water is supplied to consumers via extensive distribution networks (DWDS) that have been developed over many years. For more than 40 years, susceptible to corrosion metal alloy pipes, have been gradually replaced by plastic pipes, mainly made of polyethylene (PE). As reports show, plastic pipes quickly degrade under operating conditions, becoming a source of secondary drinking water pollution with microplastic (MP) particles. The presence of microplastics (MP) in drinking water is a growing problem due to their chemical diversity, small size and increasingly well-documented adverse effects on human health. The aim of this study was to assess the potential for MP release from PE drinking water transmission pipes. The experiments, which were carried out on a semi-technical scale model and under real conditions, included an analysis of the degree of MP contamination of the distributed water, with an emphasis on PE fragments, and an examination of the course of PE degradation under operating conditions. The tests showed that the number of MP particles increases during water distribution, with the smallest particles being the most prevalent. The particles identified in the distribution network water (DWDS) were predominantly PE fragments, and their number was higher than in the treated water (DWTP). On the other hand, tests on a semi-technical model showed that PE pipes degrade quickly under operating conditions, causing cracks and peeling of their surface, and consequently the release of numerous PE particles into the water. It was observed that the ageing of PE pipes is rapid, and its effects are clearly visible after a short period of operation in DWDS. The studies confirmed that under operating conditions, PE fragments are released into drinking water, becoming its secondary pollution, and their concentration depends on the share of PE pipes in the DWDS material structure.

Long range theoretical study on LiH_2

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Abstract:

Lithium chemistry has received great attention in recent years due to the importance that LiH molecules and its ionic variants can have in the primordial universe [1,2]. The reaction LiH + H → Li + H_2 is considered to contribute to LiH depletion, while the hydrogen-exchange reaction LiH + H → LiH + H leads to the retention of LiH in this process.

In this work we report our recent studies on the long-range interactions between the reactants of those reactions. For the LiHH system, the main contribution for long-range interactions is the dispersion interaction. To model the dispersion interaction, the parallel and perpendicular values of the polarizabilities, for the diatomic (H-H and Li-H) have been calculated and fitted (see figure 1).

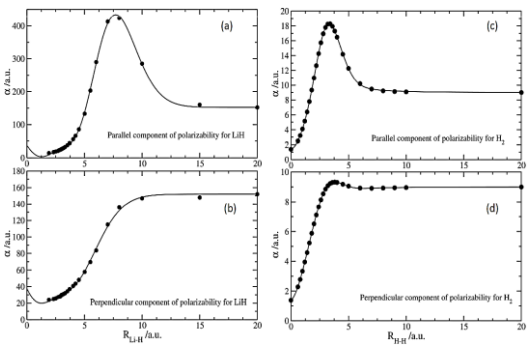

Fig. 1. Parallel and perpendicular components of polarizabilities, for LiH ((a) and (b)) and H_2 ((c) and (d)). Solid lines are the functional form fit to the ab initio calculations (solid dots).

The dispersion interaction coefficients C_6 have been computed as C_8 and C_{10} have been semiempirical estimated from C_6 using a universal correlation. The total dispersion interaction was obtained as a function of C_n and inter-atomic distances [3]. The dynamical correlation energy has been obtained for the interaction between H-LiH and Li-HH.

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First principles studies of 7x7 graphene superlattices with topological defects and transition metal adatoms

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Abstract:

Graphene's unique properties have made it a promising material for many emerging areas. However, the absence of a bandgap and magnetic attributes restricts its potential for application in nanoelectronics and spintronics. These properties can be significantly altered by topological defects, such as Flower-Like Defects (FLD) (Fig. 1), which can also offer insights into their efficient applicability in those fields [1]. Previous studies show that FLD in 5x5 and 6x6 supercells remove the characteristic Dirac cone, while in 7x7 supercells, the Dirac cone is recovered [2]. Consequently, these findings prompt inquiries regarding the significance of defect size and symmetry in the electronic structure of graphene.

This study examines the impact of FLD in 7x7 supercells on the electronic properties of graphene and the additional modification of these properties by transition metal adatoms. Using density functional theory (DFT), we analyze changes in band structure, density of states, and magnetic properties.

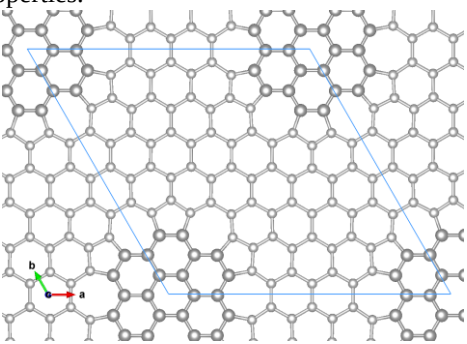

Fig. 1. FLD in 7x7 graphene supercell.

The authors acknowledge the School of Physical Sciences and Nanotechnology

Literature:

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Optimization of ultrasonic-assisted extraction of pomegranate seed oil

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Abstract:

The purpose of this study was to optimize the ultrasound-assisted extraction (UAE) process for pomegranate seed oil (PSO) in order to maximize the extraction efficiency and evaluate its effect on the oil composition. Based on previous studies on pomegranate seed oil optimization [1,2], a three-factor, three-level Box-Behnken experimental design was used, with ultrasound amplitude (30–90%), sonication time (6–12 min), and liquid/solid (L/S) ratio (10–20) as selected variables. The extraction efficiency was assessed based on the oil yield (%) and maximum oxidation time (T_{max}), determined by differential scanning calorimetry. Among the factors tested, only the L/S ratio had a statistically significant ($p < 0.05$) effect on the oil yield, with the optimal extraction efficiency being 12.85% at higher L/S ratios. Compared to the Soxhlet method, UAE showed significantly higher extraction efficiency. In addition, PSO extracted using UAE showed a significantly longer oxidation time (T_{max}), suggesting better oxidative stability. It has been shown that pomegranate seed oil is characterized by a high content of conjugated linolenic acids (CLnA), which constitute 70–80% of all fatty acids found in this oil. However, PSO extracted using the Soxhlet method had significantly higher polyunsaturated fatty acid content and lower polyphenol content. These results highlight the advantages and trade-offs of UAE in PSO extraction and provide insights into optimizing extraction parameters to improve oil recovery and quality. Furthermore, the study highlights the potential of UAE as a sustainable and efficient alternative to conventional extraction techniques. The results may contribute to the development of greener extraction processes for bioactive compounds, which will benefit both the food and pharmaceutical industries.

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Study of complexation reaction in the system of copper(II) ions and uridine-5’-diphosphoglucuronic acid

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Abstract:

The objective of the study is to investigate the complexation reaction involving copper(II) ions and uridine-5'-diphosphoglucuronic acid. Based on the results, the protonation constants of the ligand were determined, along with a comprehensive characterization of the resulting complex compounds. This characterization encompassed the evaluation of overall stability constants (logβ), the formation reaction equilibrium constant (logK_e), and the pH at which the complexes predominate. Furthermore, spectroscopic analyses were conducted to elucidate the coordination mode of the studied complex compounds.

Uridine-5'-diphosphoglucuronic acid (UDP-GluA) (Fig. 1), a compound derived from the combination of uridine-5'-diphosphate and glucuronic acid, plays a crucial role in the detoxification processes within the body. These processes are catalyzed by the enzymes known as UDP-glucuronyltransferases, which facilitate the removal of potentially harmful and carcinogenic metabolites, such as cannabinoids, thyroxine, certain bile acids, morphine, and acetaminophen, from the body [1,2].

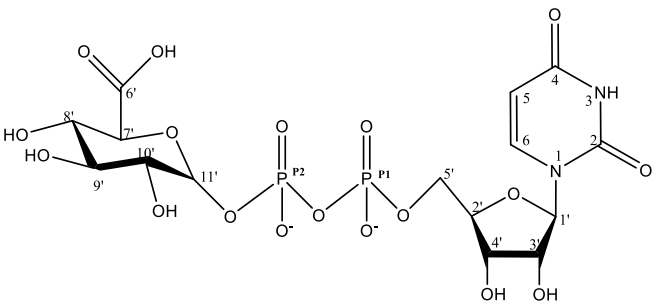

Fig. 1. Formula of the uridine–5′-diphosphoglucuronic acid [1].

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Learning by experimenting: an IBSE approach to chemistry education at the high school level

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Abstract:

Modern science education calls for innovative teaching methods that actively engage students in the learning process. A key objective in teaching science is the development of scientific thinking based on inquiry, analysis, and evidence-based reasoning. One of the most effective ways to develop this skill is through practical laboratory work, where students independently go through the research cycle — from formulating a hypothesis, conducting the experiment, to analyzing the results and drawing conclusions [1].

This approach aligns with the Inquiry-Based Science Education (IBSE) methodology, which emphasizes student-centered learning through experimentation. Such activities not only support the understanding of scientific concepts, but they also help develop analytical skills, methodological awareness, and motivation to learn [2].

As part of laboratory workshops held at the Faculty of Chemistry, Adam Mickiewicz University in Poznań, high school students took part in experimental classes focused on the precipitation and filtration of copper(II) hydroxycarbonate. Participants formulated their own research questions, hypotheses, and objectives, and then carried out the experiment independently. They documented their observations, analyzed the results, and compared their conclusions with their initial assumptions. This process supported the development of critical thinking skills and a deeper understanding of chemical reactions.

These activities serve as a practical example of implementing the IBSE framework in chemistry education, where students become active investigators rather than passive recipients of knowledge. The integration of theoretical content with hands-on experimentation not only increases knowledge retention but also makes learning more meaningful and engaging. Experiences like these show how inquiry-based approaches can effectively support the development of scientific reasoning — a foundational skill for further education in science and technology.

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Diagnostic potential of fluorescently labeled isothiocyanate derivatives

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Abstract:

Every year, approximately 20 million new cancer cases are recorded. WHO data indicate that the drastic increase in cancer incidence is caused by significant changes in the surrounding environment as well as human lifestyle. This necessitates the search for new, more effective drugs, as well as increasingly advanced diagnostic and research tools that can accelerate or facilitate an efficient diagnostic process, especially since WHO highlights early diagnosis as a key factor in increasing survival rates. [1]

Theranostics, which combines diagnostics with therapy, aligns with these research efforts, addressing patient needs and enabling the initiation of treatment during the diagnostic process. This project aims to investigate the application potential of selected fluorescently labeled isothiocyanate (ITC) derivatives as theranostic tools. These compounds exhibit high and selective activity against prostate cancer cells (PC3 cell line) and breast cancer cells (T47D cell line), highlighting their therapeutic potential.

The combination of an anticancer ITC with a fluorophore creates an ideal dual-function molecule, where one part is responsible for anti-cancer activity, while the other enables visualization, which is essential for the diagnostic process.

The spectroscopic properties of the obtained derivatives were measured in three solvents: methanol, acetonitrile, and cyclohexane. Their spectral and photophysical properties strongly depend on the polarity of the used solvent. The diagnostic potential of the obtained anticancer derivatives was initially determined using cellular models - GUV's liposomes and cancer cells such as PC3 cells (prostate cancer cells), T47D cells (breast cancer cells).

Personalized medicine, which includes theranostics, significantly enhances effectiveness, safety, and quality while also potentially reducing treatment costs. The current situation and the continuously rising number of cancer cases, it is essential to seek new tools with more selective and multifunctional effects.

Acknowledgements and more

The research was partially funded by the Young Scientists' Research (BMN no. 539-T070-B218-25)

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Rational design of enzyme-responsive fluorescent organoruthenium prodrug for real-time tracking of cargo release and cytotoxicity

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Abstract:

Stimuli-responsive controlled delivery and real-time release monitoring are crucial for metallo-chemotherapeutics to overcome the obstacles they face during (pre)clinical development [1-3]. In this study, we structurally modified a conventional half-sandwich Ru(arene) complex into a single-component fluorogenic as well as esterase-responsive nanosystem via functionalizing the NN-bidentate ligand with 10,12-pentacosadiynoic acid (PCDA) derivative, thereby designing amphiphilic complex and further adopting the co-assembly strategy. Prior to obtain the nanoassembly, in an attempt to infer the benefits of functionalizing the ligand, a series of four organoruthenium complexes including the amphiphilic complex were prepared and characterized well. This nano-assembly is found to release the Ru complex in the presence of porcine liver esterase in concomitant with the four-fold increase in its fluorescence intensity. Such a stimuli-responsive behaviour is exploited for real-time release monitoring of Ru complex and understanding its functionality to induce cell death in THP-1 cancer cells. Compared to free Ru complex, this nanosystem exhibited higher cytotoxicity towards HeLa cells and lower toxicity in non-cancerous GM-5756 cells. Zebrafish embryo toxicity analysis confirmed its biocompatibility and uptake for further possible *In vivo* studies. GSH-binding could be a possible mechanism of cytotoxic action of released Ru complex.

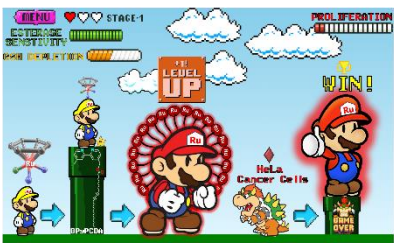

Fig. 1. Graphical abstract

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ENGINEERING SILICA NANOCARRIER USING POLYDIACETYLENE FOR pH-RESPONSIVE RELEASE, ENHANCED ANTICANCER ACTIVITY AND REDUCED INVIVO TOXICITY

Chezhiyan Sumithaa,[1] Przemyslaw Gajda-morszewski,[2] Marappan Velusamy,[3] Malgorzata Brindell,[2] Olga Mazuryk,[2*] and Mani Ganeshpandiana[1*]

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Abstract:

Despite the enormous efforts made over the past two decades to develop metallodrugs and nanocarriers for metallodrug delivery, the precise strategies that aim to optimize the design of both metallodrug and metallodrug carriers jointly in a concerted effort are still uncommon.[1,2]Addressing this, we synthesized and evaluated three half-sandwich ruthenium(II) complexes bearing pyridylimidazo[1,5-a]pyridine ligands functionalized with polycyclic aromatic moieties (Ru(nap), Ru(ant), Ru(pyr)) as potential anticancer agents. Among these, Ru(pyr) exhibited superior cytotoxicity against HT-29 colorectal cancer cells compared to the other complexes and cisplatin. To enhance its delivery, we engineered amino-functionalized mesoporous silica nanoparticles (AMSNs) coated with polydiacetylene (PDA) as a functional nanocarrier. Notably, the PDA gatekeepers facilitated cellular uptake of Ru(pyr) and enabled its sustained release from the nanoformulation. Furthermore, zebrafish embryo toxicity assays indicated the potential of these PDA-coated nanocarriers for in vivo applications.

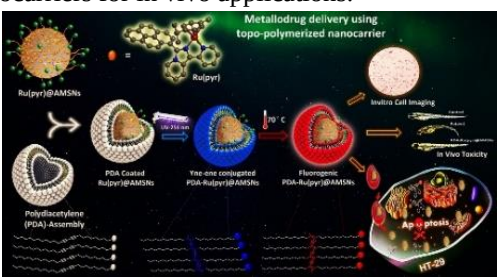

Fig. 1. Nanoformulation of Ru(arene) complex

The author is sincerely grateful to the SRM IST and CSIR-Direct SRF (File.No.09/1045(18594)/2024-EMR-I),

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NATURE RESPONSE TO PLASTIC

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Abstract:

We live in a world built on plastic. Every year production keeps growing — yet only a fraction is recycled. PET makes up just 5% of global plastics, but dominates packaging and textiles. It persists. It accumulates...

In 2016, scientists discovered Ideonella sakaiensis a bacterium capable of digesting PET using two enzymes: PETase and MHETase. Together, they break PET into EG and TPA, which can be fed into the Krebs cycle like any other carbon source.

This poster explores a biological strategy to fight plastic pollution — not by collecting waste, but by breaking it down at the molecular level. Through enzyme engineering and microbial design, we envision scalable, sustainable biodegradation.

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Multiprocess Reaction Dynamics Program (MReaDy) and Applications

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Abstract:

MReaDy[1] is a program for studying reactive dynamic systems using a global potential energy surface (gPES).

Potential Energy Surfaces (PES), based on ab initio calculations, is a powerful tool to study the rate of elementary reactions and their dynamics. It is indicated to compute state-to-state rate constants. In a more complex mechanism, we will be in the presence of different and simultaneous elementary reactions, corresponding to all the possible reactive and non-reactive collisions between the species present and leading to the respective products. Attempting to build a traditional PES for such a system quickly becomes impossible. To circumvent this problem, a global Potential Energy Surface (gPES) can be defined by integrating various PESs, each representing an elementary reaction expected to play a role in the chemical process. MReaDy is built in such a way that it performs reactive dynamic calculations based on such gPES.

We have already used MReaDy to study the combustion dynamics of hydrogen and oxygen mixtures with success[2,3]. Recently, MReaDy has been adapted for studying hydrogen and oxygen combustion confined within carbon nanotubes, as well as H + O2 + M three-body reaction systems.

Acknowledgements: FCT under the PTDC/QUI-QFI/31955/2017 research project, co-financed by the European Community Fund, FEDER and the COST Action CA18212 "Molecular Dynamics in the GAS phase".

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