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Novel Trends in Chemistry, Research and Education 2025

Mgr. Soňa Király (ed.)

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Novel Trends in Chemistry, Research and Education 2025

Book of Abstracts

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Design and properties of multi-target agents based on quinoline scaffold

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An innovative strategy in modern drug discovery involves the design of multi-target compounds, also known as multi-target directed ligands (MTDLs) or "promiscuous drugs". Multi-target agents are single chemical entities designed to interact simultaneously or sequentially with two or more biological targets that are key to the mechanism or progression of a disease. This strategy contrasts with the traditional "one drug, one target" paradigm of drug discovery [1,2]. This approach is based on the concepts of privileged structures, polypharmacology and multifactorial diseases [3,4]. It appears to be a useful tool in the design of anti-invasive drugs, as the therapeutic agents designed in this way interact with multiple targets, thereby preventing resistance or being able to destroy resistant pathogens/cells [5-7]. Similarly, multi-target drugs can be designed for the simultaneous treatment of autoimmune and inflammatory diseases [2,4].

Quinoline-based compounds have a wide range of promising biological properties, which is why they are receiving special attention in drug design and medicinal chemistry [8,9]. The quinoline scaffold can be easily and rapidly synthesized, indicating the importance of this privileged structure [10,11]. Furthermore, this simple structural element has unique physicochemical properties and allows for a large number of targeted modifications [12-18].

This contribution focuses on the design and investigating several series of ring-substituted hydroxy- and/or aminoquinolines.

Acknowledgements

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Breaking Amyloid with Light: Azobenzene Derivatives as Photo-Responsive Agents Against Aβ Aggregation

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Amyloid fibrils formed by amyloid β (Aβ) peptides are a defining neuropathological hallmark of Alzheimer's disease (AD), a rapidly growing and currently incurable neurodegenerative disorder. Developing new strategies to modulate and eliminate these aggregates remains a critical challenge.

In this work, we harness the reversible photo-induced isomerization of azobenzene molecules—switching between cis (nonplanar, metastable) and trans (planar, thermodynamically stable) conformations—to mechanically disrupt Aβ fibrils. We designed and evaluated azobenzene-based compounds containing one or two azobenzene moieties linked by DTPA, integrating in vitro, in silico, and cellular approaches.

The DTPA-linked azobenzene dimer DTPA-$(AZB)_2$ demonstrated potent fibril-dissociating activity at low micromolar concentrations, with approx. 10-fold enhancement upon light-induced isomerization. These compounds converted fibrils into non-cytotoxic species, highlighting their therapeutic potential. Our *in silico* analyses suggest that photo-switching imposes mechanical stress on β-strands, facilitating fibril disruption. Furthermore, we show that both light and calcium ions significantly amplify the dissociation efficiency, and experiments performed in artificial cerebrospinal fluid confirm activity under physiologically relevant conditions. Together, these findings establish DTPA-$(AZB)_2$ as a promising photo-switchable modulator of amyloid structures and lay the groundwork for future development of light-controlled therapeutic strategies for AD and related neurodegenerative diseases.

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Chemistry Teacher Training

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University teacher training is a key link in the chain connecting social expectations, education policies, and the actual learning of students in schools. The quality of teachers has long been identified as one of the most important factors influencing student outcomes and the overall success of school systems. International OECD reports and European Union documents systematically point to the need to strengthen teacher training, their continuous professional development, and the link between theory and practice.
The aim of this contribution is to analyse the university education of chemistry teachers as a complex system shaped by a normative framework (Bologna Process, European Higher Education Area), national policies, academic traditions, and the dynamics of the school environment.

Teacher and the professionalization of the teaching profession
Most empirical studies in the field of education agree that teachers are the most important school factor influencing student outcomes, apart from family and socioeconomic background. This consensus is also reflected in the well-known OECD report Teachers Matter: Attracting, Developing and Retaining Effective Teachers, which systematically analyses the policies of 25 countries and emphasizes that the quality of the school system cannot exceed the quality of its teachers in the long term. [1]
Teacher training is therefore not just a technical process of "supplying" graduates to the labour market, but a strategic investment in the future of society. The way universities prepare future teachers has a fundamental impact on whether they will be able to respond to the challenges of the 21st century – globalization, digitalization, the climate crisis, growing classroom diversity, inclusive education, and increasing social inequalities.
The professionalization of the teaching profession encompasses three basic dimensions. The first is professional competence – a deep understanding and knowledge of the subject matter in connection with the scientific discipline to which the subject is linked, and the ability to transform the scientific system into a didactic system (subject didactics). The second is pedagogical-psychological competence – knowledge of learning processes, motivation, development, and classroom social dynamics. The third is the ethical-reflective dimension – the ability to critically analyse one's own practice, reflect on values, and make decisions in accordance with professional ethics and moral character. An important part of professionalization is also the concept of professional standards for teachers, which in many countries serves as a reference framework for designing the content and structure of study programs in higher education teacher training or educational programs as part of their lifelong learning and professional development.

In Europe, two basic models of approach to the construction of teacher training program content can be identified: concurrent/integrated and sequential/consecutive. The integrated model combines subjects in the field of study, teaching fundamentals, and subject didactics from the very first years of study, with students identifying with the teaching profession from the outset and teaching practice also being included from the beginning of their studies. The consecutive model, on the other hand, assumes that students first complete subjects in their field of study and then subjects in teaching fundamentals and subject didactics, including teaching practice.
Chemistry teachers are currently trained at seven universities in Bratislava, Komárno, Trnava, Nitra, Banská Bystrica, Ružomberok, and Košice. The content and structure of these study programs vary, but all are designed as bachelor's and master's degrees. Based on the analysis, it can be concluded that universities have approached the creation of programs differently within their internal accreditations. Following the publication of the new description for the field of study of teaching and pedagogical sciences, it can be stated that the concurrent model prevails.

The quality of teacher training is also linked to the status and professional development of university educators who train teachers. If future teachers are expected to use innovative, student-centered, and inclusive approaches, it is essential that they encounter such approaches during their own university studies. This requires systematic support for the development of the pedagogical and didactic competencies of university teachers.

References
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MXene-based materials: Novel catalysts for wastewaters treatment

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General participation rules

Wastewater treatments are a crucial challenge worldwide as their treated effluents are released into the natural environment. This point is a big concern since the current technologies are not 100% efficient, thus leading to pollution. With the release of new regulations, especially the European Directive No. 2024/3019 related to municipal wastewater treatments [1], the quality of the treated wastewaters should be addressed and MXenes (and particularly nanomaterials derived from MXenes) can potentially shape the future of wastewaters treatment. MXenes have found plenty of applications although they are currently investigated as cocatalysts in remediation processes [2,3]. In this presentation, I introduce first the environmental context along with scientific context of MXenes. Then, their used in the preparation of innovative catalysts for wastewaters treatment is highlighted where the example of oxidized MXenes is discussed for the degradation of pharmaceutical contaminants in water [4]. Mechanistic elucidations during the degradation process is also explained, as they are important parameters to consider for potential scale-up applications. The take-home message is that MXenes are promising catalysts that can contribute significantly to the EU Water Framework Directive [5].

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Modified pyridinium oximes in the fight against organophosphate poisoning

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Organophosphorus compounds (OPs) are widely used in agriculture as pesticides (e.g., dichlorvos, diazinon, chlorpyrifos, and parathion), in industry and technology as softening agents and lubricant additives, and in the medical and veterinary fields as therapeutic agents. Some OPs are identified as chemical warfare agents (CWAs), nerve agents, or both. sarin, tabun, VX, or so-called A-agents ("Novichoks") are well-known members of the OP nerve agent family, and are associated with terrorist attacks. The history of nerve agents began prior to World War II in Germany. The first-known nerve agent, tabun, was synthesized in the laboratories of IG Farben in Germany by Dr. Gerhard Schrader in 1936. A few decades later, the nerve agent VX was developed in the United Kingdom. Further developed nerve agents include intermediate volatile agents, an example of which are A-agents, known as Novichoks. During the Cold War, nerve agents were stored and prepared for potential military use, but were not used in military conflicts. However, they were misused by Saddam Hussein in Iraq in the Kurdish village of Birjinni (1988) and by the Japanese Aum Shinrikyo sect in Matsumoto (1994) and Tokyo (1995). More recently, sarin was several times misused within the Syrian conflict (2013-2018) and an agent from the Novichok family was proposed to be the cause of the intoxications of Sergei and Yulia Skripal in the UK (2018) and Alexei Navalny in Russia (2020) [1].

Nerve agents phosphonylate serine Ser203 at the esteratic part of the active site of human acetylcholiesterase (*h*AChE; UniProtKB: P22303; EC: 3.1.1.7). AChE plays a key role in termination of the action of a neurotransmitter acetylcholine in the peripheral nervous system and central nervous system, and prolonged inhibition of AChE can lead to lifethreatening consequences. The causal treatment of OP poisoning are oxime reactivators (e.g. pralidoxime, obidoxime, asoxim). Oxime reactivators restore function of cholinesterase through nucleophilic attack of oxime to the phosphorus of OP in the catalytic active site of the inhibited cholinesterase [2]. Studies done by our research group show that the nucleophilicity of oxime reactivators can be modified by the substitution of halogens in close proximity of the oxime moiety [3]. Such modifications lead to increased formation of the oximate ion followed by higher reactivation of inhibited cholinesterases. It is important to also consider the position of the substituents and the oxime group in reactivator as it has a direct impact on its efficiency. While reactivators with oxime group in position C2 on pyridinium moiety (e.g. asoxime) are better reactivators of soman inhibited AChE, they are weak for reactivation of tabun inhibited AChE. On the other hand, reactivators with oxime group in position C4 on pyridinium moiety (e.g. obidoxime) are better reactivators of tabun inhibited AchE [4]. These findings provide an important basis for further detailed research on modified oxime reactivators useful for the treatment of intoxication by OPs. Our research group synthesized and evaluated the physicochemical and reactivation properties of a series of novel modified pyridinium oximes [3]. Some of the tested compounds significantly surpassed the reactivation efficacy of clinically used reactivators and are suitable candidates for *in vivo* studies.

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Dual Education in the Field of Testing and Recycling of Lithium Battery Manufacturing Waste

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This work introduces an innovative dual education model developed through collaboration between FECUPRAL, s.r.o. and the Secondary Industrial School of Electrical Engineering in Prešov. The program focuses on practical training in the field of testing recycled materials from lithium battery production, reflecting current trends in circular economy, environmental sustainability, and technological innovation. The primary goal is to bridge vocational education with real-world practice in the rapidly growing sector of battery material processing.
During their practical lessons, students engage in the full process of manufacturing NMC based lithium pouch cells using recycled materials from lithium cell production waste, including preparation, weighing, processing, and testing of the final cells by cycling. The program utilizes recycled active powder outputs from the patented WALCH Dry Impact Refine® technology, co-developed by FECUPRAL and its German partner WALCH Recycling. The practical training takes place in a dedicated laboratory space built within the company's premises. Students work under the supervision of a professional mentor and a school representative, with emphasis placed not only on manual skills but also on understanding the underlying chemical and technological principles. The curriculum includes theoretical instruction in electrochemistry, materials science, and industrial automation. Each student is expected to independently produce and test their own lithium cell, and to prepare a report based on the test results. This approach enhances the quality of vocational education, fosters deeper student engagement in technical disciplines, and prepares them for real-world challenges in industry and environmental engineering.

A novel approach to the spectrophotometric determination of gold using its halide/pseudohalide ionic associates

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The present study investigates the interaction between halide and pseudohalide substituted chloroaurates and a symmetric carbocyanine dye, 1,3,3-trimethyl-2-[5-(1,3,3-trimethyl-1,3-dihydroindol-2-ylidene)-penta-1,3-dienyl]-3H-indolium chloride (DIDC). The work focuses on optimizing the formation and subsequent semi-microextraction of the Au–DIDC ionic associates for spectrophotometric gold determination at 647 nm. Substitution of ligands in chloroaurates was found to significantly improve both the sensitivity and selectivity of the method. The molar absorptivity of the formed ion associates ranged from (10.7 – 15.6) × 10^4 L mol^{-1} cm^{-1}, depending on the ligand. A novel analytical system was developed under optimized conditions: azide ligand (N_3^-), pH 5.0, 5 × 10^{-5} mol L^{-1} DIDC, and amyl acetate as the extraction solvent. The achieved limit of detection (LOD) and limit of quantification (LOQ) were 0.10 µg mL^{-1} and 0.31 µg mL^{-1} of gold, respectively. The proposed method was successfully applied to the determination of gold in artificial and pharmaceutical samples, providing accurate and reproducible results. Quantum Theory of Atoms in Molecules (QTAIM) analysis of the electron density for DIDC-chloroaurate complexes, calculated at the CPCM(water)-B3LYP/ma-def2-SVP level of theory, enabled the construction of a selectivity sequence that correlated well with the experimental findings. The developed system thus offers a sensitive and selective approach for spectrophotometric determination of gold based on ion-pair formation and semi-microextraction.

Keywords: gold determination; ion associate; carbocyanine dye; semi-microextraction; QTAIM.

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Beyond the Double Helix: Artificial Circular Construct for Non-B DNA Research

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In addition to the well-known B-form, DNA molecule is capable of adopting a variety of noncanonical secondary structures. Examples of such non-B DNA motifs include Z-DNA, four-stranded G-quadruplexes, i-motifs, hairpins, triplexes (H-DNA), and numerous other alternative DNA conformations. The formation of these structures is determined by the primary DNA sequence but is also strongly influenced by environmental factors such as temperature, pH, pressure, the type and concentration of ions, the presence of ligands or molecular crowding agents [1,2]. The biological significance of non-B DNA structures lies in their direct impact on cellular processes, including the regulation of gene expression at both transcriptional and translational levels, epigenetic modulation of chromatin architecture and DNA recombination. These structures are formed in repetitive genomic regions mostly. Recent studies increasingly indicate that the dynamic formation of non-B structures can modulate the expression of genes associated with specific diseases, including neurodegenerative disorders. In addition, these structures can contribute both to the onset of diseases and to evolutionary changes driven by mutagenesis and selection [1,3,4]. Moreover, the unique conformations and relative stability of non-B DNA structures make them attractive elements for DNA-based nanotechnology. Their ability to reversibly change conformation in response to environmental factors has been exploited in the design of smart nanomachines, biosensors, molecular switches, and aptamers [5,6].

We have prepared and characterized an artificial construct based on circular DNA molecules. Structural properties of the resulting DNA minicircles were assessed using circular dichroism spectroscopy, atomic force microscopy and gel electrophoresis. The overall architecture is assembled from strategically designed single-stranded DNA sequences that serve as building blocks for the formation of double-stranded circular scaffold. The system also allows the formation of non-B DNA structures within the central region of the circular construct [7]. We examine non-B structures in the central region, ds-DNA linkers, and the overall minicircle architecture, evaluating how local structural changes and environmental factors affect the system. Our current efforts also focus on the incorporation of structural modules directly into plasmid DNA using restriction endonucleases. This approach opens new avenues for the study of their physicochemical characteristics and biological functions in a biologically relevant context.

Acknowledgements

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The 20th anniversary of the synthesis and study of ordered nanoporous materials at KACH PF UPJŠ in light of the Nobel Prize in Chemistry in 2025: we were part of the story

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Twenty years ago, the story of the Laboratory of Synthesis of Ordered Nanoporous Materials and the Laboratory of Adsorption and Thermal Analysis at KACH ICHV PF UPJŠ began. Over the past two decades, the laboratories have undergone dynamic development and achieved significant scientific success, becoming recognised centres of excellence in the field of nanomaterials and the research and development of adsorption technologies. During this period, the research team working in the laboratories has become one of the best in Slovakia and is recognised abroad.

Initially, the laboratories focused on the adsorption of technologically important gases, but their research portfolio gradually expanded to include magnetism, drug carriers and delivery, and catalysis. In terms of the materials studied, the laboratories focus on synthesising and researching the applications of metal-organic frameworks (MOFs) and mesoporous silica-based nanomaterials (MSN). The laboratories currently focus on carbon-based materials and their composites with MOFs, as well as applications involving the use of MOFs in the design of electrodes for lithium batteries and ecological topics.

In 2025, the Nobel Prize in Chemistry was awarded to scientists Omar Yaghi, Susumu Kitagawa and Richard Robson in recognition of their research on metal-organic frameworks (MOFs). This event was very encouraging for our team and confirmed the direction in which we were heading. We have been part of the MOF story from the beginning, following the growth and development of the topic. We did not just stand on the sidelines or jump into the topic for the sake of it; our expertise stems from our department's long-term research into zinc carboxylates. We are proud to say that similar research, for which the Nobel Prize in Chemistry in 2025 was awarded, is also being conducted at KACH PF UPJŠ.

The lecture will present the key milestones in the research and development of the KACH PF UPJŠ laboratory of nanoporous materials, as well as examples of our research on MOFs and MSN.

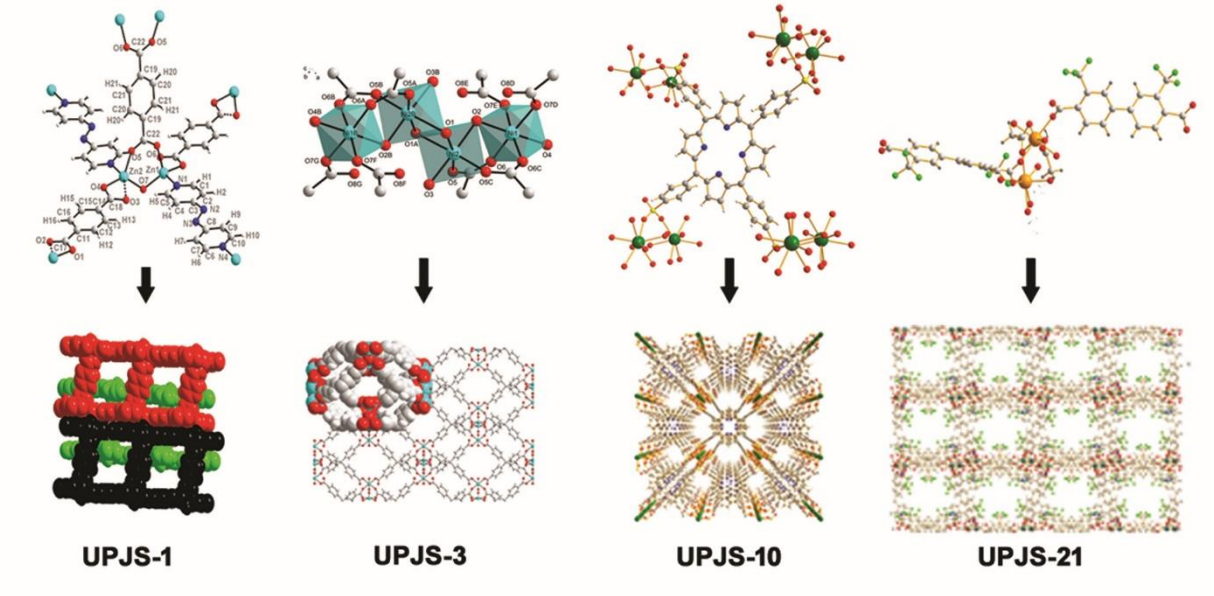

Figure 1 Examples of some MOF types prepared at KACH PF UPJŠ.

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Electrochemical Mechanism of Insulin Oxidation on Cu-Enhanced Carbon Paste Electrodes

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In this study, the insulin oxidation mechanism on two previously prepared copper-modified carbon paste electrodes (CPEs) was studied. The electrode modifications were prepared from carbon powder obtained from waste sources combined with coconut oil, which served as a natural binder. Thereafter copper particles were deposited onto the electrode surface using two different methods: cyclic voltammetry (CV Cu/CPE) and pulsed electrodeposition carried out in fifteen cycles (15pCu/CPE).

To study the insulin oxidation mechanism on unmodified and both modified electrodes cyclic voltammetry method was performed. Measurements were realized in pure PBS and in a 5 µM insulin in PBS with pH 9. The oxidation sequence on this electrode can be interpreted through the following steps (Eq. 1-2):

$$Cu^0 + H_2O \rightarrow Cu_2O + 2H^+ + 2e^- \quad \text{(approx. 0.0 V)} \quad (1)$$

$$Cu_2O + H_2O \rightarrow CuO + 2H^+ + e^- \quad \text{(approx. 0.2 V – 0.5 V)} \quad (2)$$

The scan-rate-dependent voltammograms for both modified electrodes were recorded. For each system, higher scan rates generate proportionally larger anodic and cathodic peak currents. The anodic peak shifts positively and the cathodic peak negatively as the scan rate increases, behaviour characteristic of quasi-reversible or irreversible charge-transfer processes. For the CV Cu/CPE a linear dependence of anodic peak current on the scan rate was observed. This linearity indicates that the process is dominated by adsorption. This is reasonable, as insulin can bind to Cu(II) species and form complexes on the electrode surface.

The electron-transfer parameters were estimated using Laviron's approach (Eq. 3):

$$E_P(V) = E^{0'} - \frac{RT}{\alpha nF} ln \frac{RTk_s}{\alpha nF} + \frac{RT}{\alpha nF} \ln v \quad (3)$$

From the *Ep* vs. *v* plot, the formal potential was determined as 0.089 V. The first oxidation step involves approximately 1.3 electrons, consistent with the proposed mechanism, and the heterogeneous rate constant was calculated to be 0.505 cm s^{-1}. These results suggest a quasi-reversible reaction in which one electron is exchanged in the initial step. The second oxidation wave does not follow a linear dependence on ln v, so Laviron's model cannot be applied to it reliably.

For the 15pCu/CPE log *Ipa* vs. log *v* the slope of 0.19 is far below the expected values for diffusion- (0.5) or adsorption-controlled (1.0) systems, indicating that the rate is primarily limited by electron-transfer kinetics. This interpretation is also supported by the growing peak separation at higher scan rates. In this case, the first oxidation peak overlaps strongly with the second one, especially at elevated scan rates, which complicates the analysis and prevents a clean application of Laviron's theory to extract accurate kinetic parameters.

Based on obtained results we can conclude that copper-modified carbon paste electrodes prepared from waste-derived carbon enabled the study of insulin oxidation, with the CV Cu/CPE showing an adsorption-controlled process and a quasi-reversible initial one-electron step. The 15pCu/CPE was limited mainly by electron-transfer kinetics, as indicated by the low log Ipa vs. log v slope and increasing peak separation. Overall, the results show that the copper deposition method strongly affects the insulin oxidation mechanism and the ability to extract reliable kinetic parameters.

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Applications of Liquid Chromatography for Direct Chiral Separation of Drugs

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Chiral separations play an important role in the chromatographic analysis of various bioorganic compounds as well as drugs. Chiral drugs currently represent almost 50% of the total market, covering a wide range of therapeutic areas. Currently, the development and production of enantiomerically pure drugs is increasingly important because they provide higher efficacy and safety compared to racemates. Enantiomers may differ significantly in their pharmacological properties, therefore their separation is necessary.
Various separation methods such as chromatography and capillary electrophoresis are used to separate racemic mixtures. Separation of racemic mixture into individual enantiomers can be achieved by using a derivatizing reagent or either a chiral stationary or chiral mobile phases. High-performance liquid chromatography on chiral stationary phases with various kinds of chiral selectors is applied as the method of first choice for direct chiral separation.
The aim of this work was to provide a brief review of direct chiral separations of racemic pharmaceuticals using liquid chromatography that have been published in the last period.

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Mixed Micelles Cloud Point Extraction for Sensitive Spectrophotometric Determination of Two Transition Elements

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Vanadium and molybdenum belong among transition metals. Vanadium is used in various industries while molybdenum is an essential element, playing a role in enzyme production. Both of them have a positive effect on human organism, therefore they are available in the form of dietary supplements. They also occur naturally in several types of food or water sources. However, in higher concentrations, they are toxic. Because of both negative and positive effects, it is important to monitor vanadium and molybdenum levels in samples of their source.
In cloud point extraction (CPE), a non-ionic surfactant serves as an extraction reagent. Under certain conditions, surfactant creates micelles that have the ability to encapsulate the analyte and separate it from the aqueous solution. Mixed micelles cloud point extraction (MM CPE) is a variant in which an additional ionic surfactant is used. The ionic surfactant possesses the ability to bind to the ionic complex containing the analyte, resulting in the creation of a ternary complex. For V(V) analysis, an ionic surfactant cetylpyridiniumchloride was added into the solution, for the determination of Mo(VI), Aliquat® 336 was used.
MM CPE for the determination of V(V) and Mo(VI) was performed using 4-nitrocatechol as a complexing reagent with the addition of the respective ionic surfactant. The solutions were first incubated and then kept in a freezer to ensure micelles formation and separation in the form of a surfactant rich phase (SRP) at the bottom of the solution. After the aqueous phase was disposed of, the SRP was diluted with ethanol and distilled water. In this state, it was suitable for spectrophotometric detection. Absorbance measurements at 670nm for V(V) and 435nm for Mo(VI) were performed. The limit of detection values reached 0.6 and 3.2 mg L^{-1} for V(V) and Mo(VI), respectively. V(V) and Mo(VI) were determined in real samples of mineral water, dietary supplements, catalyst (V(V)), and steel (Mo(VI)). The implementation of the ionic surfactant for the MM CPE resulted in higher absorbance signals and therefore a more sensitive determination [1, 2].

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Monitoring of polyphenolic compounds in berry fruits

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Polyphenols are secondary plant metabolites that contain at least one aromatic ring and one or more hydroxyl groups. They are considered important dietary antioxidants, often exhibiting higher efficacy than vitamins C or E. These compounds may exert strong protective effects against cellular oxidative damage, and act both directly and indirectly against oxidative stress. Studies suggest that a diet rich in polyphenols may offer protection against coronary heart disease and lung cancer. Dietary intake of flavonoids has been shown to reduce the incidence of prostate cancer. Berry fruits are known to have the highest content of polyphenols, with a wide range of phenolic subclasses, primarily flavonoids and phenolic acids [1, 2].

In this work, the content of polyphenolic compounds will be determined in selected types of berry fruits: chokeberry, blackcurrant, lingonberry, elderberry, blueberry, cornelian cherry and pokeweed. Two forms of fruit will be compared – fresh berries and berries dried at 40 °C. Ultrasound-assisted extraction will be used, carried out for 30 minutes in an ultrasonic bath at laboratory temperature. Samples will be extracted using 50% methanol, then filtered using a vacuum pump or centrifuged for 10 minutes at 9000 rpm.

The analysis will focus on selected phenolic acids – chlorogenic acid, gallic acid, caffeic acid, trans-ferulic acid – and one flavonoid, catechin. High-Performance Liquid Chromatography (HPLC) with UV detection at a wavelength of 254 nm will be used for quantification. Separation of analytes will be performed on an ACE C18 column (250 x 4,6 mm; 5 µm). The mobile phase will consist of acetonitrile-water-acetic acid in a ratio of 10:89:1 (v/v/v). Elution will be carried out in isocratic mode with a flow rate of 1.0 $ml.min^{-1}$.

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SESSION 1 ANALYTICAL CHEMISTRY

Fluorescent Determination of Perchlorates Using Vortex-Assisted Liquid–Liquid Microextraction

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Perchlorate (ClO_4^-) represents a significant endocrine disruptor and an emerging environmental contaminant that can threaten both human health and ecosystems [1]. Due to its extensive industrial applications-particularly in solid rocket fuels, fireworks, explosives, pyrotechnics, batteries, and paints-perchlorate ions are released into the environment from multiple sources [2,3]. Their high solubility in water and improper disposal of materials containing perchlorate salts contribute to widespread contamination of surface and groundwater, as well as to accumulation in plants and the food chain. Human exposure to perchlorate mainly occurs through water, food, and plants. It competes with iodide for thyroid uptake via the sodium-iodide symporter, disrupting hormone synthesis and potentially causing hypothyroidism [4–6]. Despite growing knowledge about the global occurrence of perchlorate, legislative frameworks for its regulation remain insufficient in many countries [7]. These facts highlight the need for developing effective methods to limit the presence of perchlorate in the environment and reduce its negative impact on health.

The main objective of this study was to develop a new, highly sensitive, and selective method for the fluorescent determination of perchlorate based on vortex-assisted liquid–liquid microextraction (VALLME). The dye 1,1′,3,3,3′,3′-hexamethylindodicarbocyanine iodide (HIDC) was used as a complexing agent. In the initial phase of the research, the possibility of forming an ion associate (IA) between perchlorate and the dye 1,1′,3,3,3′,3′-hexamethylindocarbocyanine chloride (Astrafloxine) was also investigated; however, experimental results showed that this dye was not suitable under the selected experimental conditions, and further optimization was therefore carried out using HIDC.

The developed method is based on the formation and extraction of an IA between the perchlorate anion and HIDC dye, with the fluorescence signal recorded at an excitation wavelength of 640 nm and an emission maximum of 666 nm. During the method development, both chemical and physical parameters of the experiment were optimized to achieve maximum fluorescence signal intensity and extraction efficiency.

The optimized conditions included an HIDC concentration of 1.5×10^{-6} M, 0.5 mL of buffer at pH 6, 500 µL of n-amyl acetate as the extraction solvent, a vortexing time of 15 s at 1600 rpm, and centrifugation for 2 minutes at 3000 rpm. Under these conditions, a linear signal response was obtained in the range of 8–150 µg L^{-1} ($R^2 = 0.9977$), with a detection limit (LOD) of 2.53 µg L^{-1}. The efficiency of the microextraction process was characterized by a preconcentration factor (PF = 10).

The proposed method is characterized by high sensitivity, selectivity, simplicity, and low consumption of organic solvents, making it suitable for environmental analyses in accordance with the principles of green analytical chemistry.

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Analytical evaluation of PAH degradation during the cultivation of hydrocarbon-utilizing bacteria with bioremediation potential

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Polycyclic aromatic hydrocarbons (PAHs) are persistent environmental pollutants characterized by high toxicity and low biodegradability [1]. In this study, bacterial strains capable of utilizing PAHs [2,3] were isolated from various extreme environmental habitats. The isolates were cultivated in mineral media supplemented with selected PAHs (specifically fluorene and phenantrene) as the sole carbon source and exposed to a range of concentrations to determine the maximum levels that the bacteria were able to utilize. The degradation efficiency was assessed by monitoring the residual concentrations of the target compounds using high-performance liquid chromatography with diode array and fluorescence detection (HPLC-DAD/FLD). The results revealed that several bacterial strains exhibited a remarkable ability to degrade specific PAHs even at elevated concentrations, highlighting their potential application in bioremediation of contaminated environments.

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Decoding the Structural Signatures Driving Amyloid Modulation

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Protein aggregation into amyloid fibrils represents a hallmark of numerous human disorders, including Alzheimer's disease ($A\beta_{42}$ peptide) and systemic amyloidosis. Despite differences in their amino acid sequences and native conformations, these fibrils share a characteristic cross-β-sheet structure, making them compelling targets for small-molecule modulators [1]. Coumarins derivatives exhibit diverse biological activities, including anti-amyloid, antioxidant, and enzyme-inhibitory effects [2]. Understanding which structural motifs drive these activities can accelerate the development of potent derivatives and inform rational design strategies.

In this study we performed structural and functional analysis of six synthetic compounds (M1–M6) and compare their activity with previously investigated coumarin derivatives - namely bis-coumarins - connected via 4- and 7-carbon alkyl linkers (BCD4 and BCD7), and the mono-coumarin derivative - umbelliferone (MCD). The goal was to identify structural motifs underlying the inhibitory potential of studied compounds against $A\beta_{42}$ peptide amyloid aggregation by combining machine learning analysis together with experimental assays.

Thioflavin T (ThT) fluorescence assays revealed diverse effects among M-compounds: while M3 inhibited $A\beta_{42}$ peptide amyloid fibril formation, M1, M2, M4, and M5 displayed modest inhibition, and M6 unexpectedly promoted aggregation. These findings were confirmed by atomic force microscopy (AFM). Computational analysis linked the observed activities to specific structural features. Although M1, M2, and M3 all contained the key structural motifs previously associated with inhibitory potential, their effects on $A\beta_{42}$ peptide aggregation differed markedly. These suggest that the mere presence of these motifs is not sufficient for activity, rather, their special arrangement, linker flexibility, and electronic properties determine whether a compound effectively interferes with fibril formation. M3, combining optimal orientation of polar substituents and aromatic moieties, exhibited inhibitory activity, while M1 and M2, despite containing similar motifs, showed only weak effects.
Conversely, halogenated and less polar motifs in M6 might facilitate fibril nucleation and possibly stabilize β-sheet stacking, consistent with its aggregation promoting behaviour observed in ThT assays, and atomic force microscopy.

When compared with the previously characterized bis-coumarin derivatives BCD4 and BCD7, which exhibited strong anti-amyloid activity, the new M-series compounds follow a similar structure–activity pattern. Compounds retaining optimal linker length and balanced polarity, such as M3, maintained high inhibitory potential comparable to BCD7, whereas others deviating from this motif (e.g. M6) lost activity or even promoted aggregation.
By integrating motif-level analysis with ThT fluorescence data and AFM imaging, this study provides valuable insights into the structure–activity relationships governing coumarin-based modulators of amyloid aggregation and highlights structural features that can guide the design of more potent inhibitors.

Acknowledgements

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Development of LOV2 domain as genetically encoded photosensitizer

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Flavin mononucleotide (FMN) belongs to a group of efficient photosensitizers with a high quantum yield of singlet oxygen ($^1O_2$) production [1]. However, due to its lack of selectivity toward diseased tissue, FMN needs to be attached to a specific carrier that can be targeted. One such protein containing FMN is the Light-Oxygen-Voltage (LOV) domain 2 from *Avena sativa*. Previous studies have revealed that when FMN is incorporated into a protein, its surroundings strongly affect the efficiency of $^1O_2$ production [2].

Our approach to design new genetically encoded photosensitizers relies on FMN dissociation caused by the oxidation of amino acids at the FMN binding site. An important part of this approach was to propose mutations that, upon irradiation with light and subsequent oxidation, increase the volume of the mutated amino acids and trigger FMN dissociation without destabilizing the protein structure. After analyzing the FMN binding site, we designed, expressed, and purified three different LOV2 domain mutants: V416C, T418C and V416CT418C. We measured their $^1O_2$ phosphorescence and the results demonstrated an increased efficiency of $^1O_2$ production, supporting our approach. Results from fluorescence measurements confirmed that after irradiation, FMN was effectively released into the solution [3].

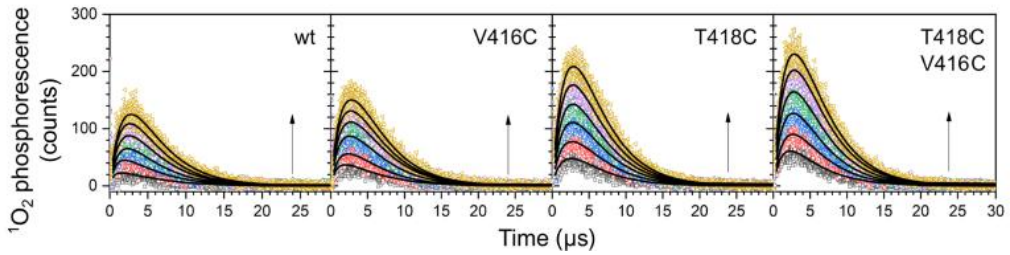

Figure 1 Time-resolved singlet oxygen phosphorescence of the LOV2 domain of *Avena sativa* (AsLOV2) variants, with the same scaled y-axis for all plots. The color scheme represent the following accumulated incident energy: black open squares 0.2 J, red open circles 0.8 J, blue triangles 1.4 J, green reverse triangles 2 J, purple diamonds 2.6 J, and yellow ochre left triangles 3.2 J [3].

Acknowledgements

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Interaction of a quinacrine analog with different polynucleotides: A noticeable preference towards a triplex RNA structural motif

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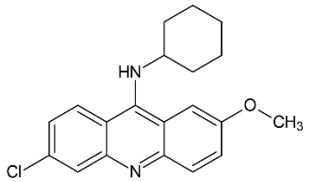
Low-molecular-weight ligands represent some of the most promising drug candidates in modern chemotherapy due to their broad spectrum of pharmacological effects. Acridine derivatives belong to such molecules and are known for their ability to interact with all sorts of biomolecular targets, including various DNA and RNA structural motifs [1]. In the past years, long non-coding RNA (lncRNA) have gained considerable attention due to their crucial, yet mysterious role in gene expression and associated disease modulation. Some of these lncRNAs contain short triplex sequences, which are essential for their stability, catalytic activity or ligand binding [2]. Targeting these structural motifs with small molecules in order to destabilize them and disrupt their biological function could therefore prove to be a viable therapeutic strategy. A recent study of an acridine derivative revealed its ability to bind and destabilize poly(UAU) triplex structure [3], implying that such compounds represent promising candidates for further research of RNA triplex motifs and their interaction with small molecules.

The present work has been focused on the interactions of a quinacrine analog **A1** (Figure 1) with different DNA and RNA structural motifs, including double-stranded calf thymus DNA (ctDNA), single-stranded polyriboadenylic acid (polyA), double-stranded polyriboadenylic-polyribouridylic acid (polyAU) and a triplex poly(UAU) motif composed of a Watson-Crick poly(AU) duplex and a Hoogsteen poly(U) single strand. We have employed spectroscopic methods to probe whether the studied compound forms a complex with the tested polynucleotides and to determine the corresponding binding constants (K_b). Our results have proven that **A1** binds to all four DNA/RNA motifs, as implied by the formation of isosbestic points in the absorption titration spectra and the associated hypochromic and bathochromic shifts typical for the interaction of small molecules with nucleic acids. Interestingly, we observed notable differences in the binding constants (Figure 1), implying a binding preference of **A1** towards the poly(UAU) triplex motif (K_b = 6,40 × 10^4 $mol^{-1}.dm^3$) as opposed to the other polynucleotides (K_b = 0,66 – 2,37 $mol^{-1}.dm^3$). These findings provide basic foundations for further research of the compound's ability to selectively interact with triplex RNA structures in the hope of discovering novel triplex-binding ligands.



A1

Polynucleotide	K_b ($mol^{-1}.dm^3$)
ctDNA	1,32 ± 0,38 × 10^4
poly(A)	2,37 ± 0,25 × 10^4
poly(AU)	0,66 ± 0,02 × 10^4
poly(UAU)	6,40 ± 0,17 × 10^4

Figure 1 Chemical structure of compound **A1** and K_b values for its interaction with tested polynucleotides.

Acknowledgements

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Nanofibrous delivery system for hydrophobic compounds encapsulated in self-assembled amphiphilic hyaluronan

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This study focuses on the development of a biodegradable nanofibrous drug delivery system designed to encapsulate a hydrophobic compound within a hydrophilic matrix, aiming to enhance its solubility and optimize its pharmacokinetic properties while ensuring strong stability.
Hyaluronan, a highly biocompatible natural polymer, serves as a unique substrate for nanofiber production [1]. The hyaluronan-based nanofibers were fabricated from a polymer solution via 4SPIN LAB® electrospinning device. Considering the various applications of the resulting fibers, natural pullulan, synthetic polyvinyl alcohol (PVA), and polyethylene oxide (PEO), were tested as the fiber-forming components. High-molecular-weight synthetic polymers were used, as they generally do not penetrate the skin when applied dermally. Non-toxic solvents such as demineralized water and isopropanol (IPA) were selected, both evaporated during the electrospinning process, leaving only the active compound and polymers in the resulting fibers.
The model compound, ubidecarenone (CoQ10), an essential constituent of cell membranes with highly hydrophobic nature due to its lipophilic isoprenoid chain [2], was incorporated into water-soluble nanofibers. The process involved pre-encapsulating of the hydrophobic compound within a self-assembled amphiphilic derivative of hyaluronan [3]. The nanoparticle size suitability was confirmed via dynamic light scattering (DLS) analysis of the particle-size distribution. Electrophoretic light scattering (ELS) confirmed the zeta potential values indicative of a well-stabilized colloidal system prior to electrospinning. To improve CoQ10 incorporation efficiency, several modifications to the solution formulation were explored.
The study systematically evaluated the impact of various parameters and physicochemical factors on the fibers' morphology. For each spinning solution, conductivity, surface tension and dynamic viscosity were measured [4]. To obtain defect-free and homogeneous fibers, processing parameters such as applied voltage, flow rate, emitter-to-collector distance, as well as environmental conditions including temperature, humidity, pressure, and air flow [4], were adjusted and monitored. The resulting fibers were examined using scanning electron microscopy (SEM) and the fiber diameter was measured. Fibers with a diameter of less than 100 nm were successfully fabricated.
The CoQ10 content in the nanofiber samples was analysed using high-performance liquid chromatography (HPLC), preceded by thermogravimetric analysis (TGA) of the fiber dry matter, to obtain accurate values.
The structural integrity of the CoQ10 under the high electric field conditions of electrospinning, was assessed using Raman spectroscopy. To mimic the electrospinning process conditions for obtaining the pure substance, a CoQ10 sample was electrosprayed under high voltage onto a collector without fiber formation. Raman spectral shifts were used to identify any potential molecular alterations induced during the process.
Furthermore, as the most suitable form of application, the transdermal penetration profile of CoQ10 encapsulated in nanofibers, was evaluated on porcine ear skin using the FDA approved Franz diffusion cells. The CoQ10 content in skin extracts after transdermal penetration was analysed by liquid chromatography-tandem mass spectrometry (LC-MS/MS).

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SESSION 2 BIOCHEMISTRY

Photodynamic therapy using UiO-66-based metal-organic frameworks (MOF) as photosensitizer carriers for breast cancer and antibacterial applications

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Antibacterial resistance is a global health concern, and conventional chemotherapy often damages healthy cells alongside cancerous ones. Photodynamic therapy (PDT) is an emerging treatment that employs light-activated compounds, known as photosensitizers, to selectively destroy target cells. This approach offers the potential to eliminate bacteria without promoting antibiotic resistance and to kill cancer cells while sparing healthy tissue. In this study, the MOF, UiO-66 was utilized as a carrier for various drugs, including photosensitizers. The photosensitizer tested in this research was methylene blue (MB), a heavily studied molecule in photobiology.

The nanoparticles were functionalized with amination (UiO-66-NH_2) and histidine (UiO-66-His) to enable better interaction with plasma membranes of cells and bacterial walls. The therapeutic efficacy of MB loaded in UiO-66, UiO-66-NH_2 and UiO-66-His was evaluated on SK-BR-3 breast cancer cells (Figure 1) and *S. epidermidis* and *E. Coli* bacterial strains. *S. epidermidis* exhibited a stronger inhibition response to known bacterial inhibitors (5-fluorouracil, chloramphenicol) than MB. However, *E. Coli* showed resistance to all tested treatments, except chloramphenicol. The results indicate weaker efficacy of PDT in bacterial cultures under the studied conditions in comparison with higher efficacy against SK-BR-3 breast cancer cells.

Overall, this study is demonstrating its greater potential for cancer treatment under the tested conditions.

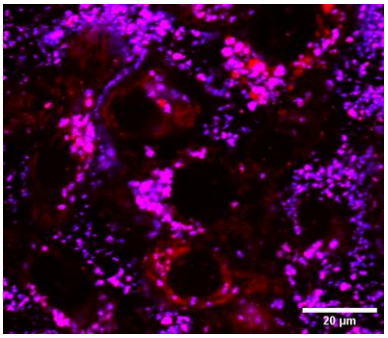

Figure 1 Representative images of cancer cells (SKBR3) exposed to UiO-66-NH_2 (blue) loaded with MB (red). MB in the particles is presented in pink.

Acknowledgements

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SESSION 2 BIOCHEMISTRY

Application of Functionalized UiO-66(Zr) Metal–Organic Frameworks for Raman-Based Analysis of Cellular Models

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Raman spectroscopy (RS) is a non-invasive, label-free analytical technique that identifies molecular vibrations, with each spectrum serving as a unique molecular fingerprint. Due to the weak scattering of water, RS is particularly suitable for biological and biomedical samples. When combined with microscopy, it enables high-resolution spectral and chemical imaging, allowing precise molecular characterization of cells and tissues. Additionally, the combination of RS with methods like fluorescence microscopy or optical coherence tomography (OCT) allows for multimodal bioimaging by combining the molecular specificity of RS with other structural and functional information. This approach is becoming increasingly relevant in oncology, where it supports precise diagnosis, targeted therapy, and improved safety. A key focus lies in the design and characterization of functional modular nanoparticles, particularly micro- and mesoporous metal–organic frameworks (MOFs), which offer high drug-loading capacity, excellent stability, biocompatibility, and tunable surface properties for advanced bioimaging and drug delivery applications. Among them, UiO-66(Zr) nanoparticles (NPs), based on zirconium ions and terephthalate ligands, exhibit outstanding robustness, tunable particle size, low cytotoxicity, and facile surface functionalization.

This study illustrates the utilization of UiO-66(Zr) NPs and their derivatives (UiO-66(Zr)-NH_2, UiO-66(Zr)-FA, UiO-66(Zr)-NH-CH_2-FA) as prospective carriers for the chemotherapeutic agent 5-fluorouracil (5FU) and their application in Raman-based analysis of cellular models. The porous structure of these materials enables efficient entrapment of hydrophilic drug molecules, while their distinct vibrational fingerprints allow label-free optical detection. Raman microspectroscopy was employed to record reference spectra, identify spectral markers, and evaluate the structural integrity and modular functionality of the NPs. Characteristic Raman bands confirmed the high crystallinity of UiO-66(Zr), while surface functionalization caused distinct spectral shifts and fluorescence backgrounds, which added to the contrast in the images. In addition, UiO-66(Zr)-NH_2 NPs were detected within human dermal fibroblast (HDF) cells, confirming cellular uptake and reproducible Raman responses. The obtained results demonstrate that functionalized UiO-66(Zr) MOFs can serve as versatile platforms for multimodal Raman-based bioanalysis, offering promising potential for both targeted drug delivery and optical diagnostics.

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BSA binding properties of hybrid indole derivatives

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Albumins are one of the most used transport proteins in blood plasma. Bovine serum albumin (BSA) is a protein that is up to 76% structurally similar to human serum albumin. It consists of a single polypeptide chain composed of 583 amino acid residues and is organized into three homologous helical domains – I, II and III. They are further divided into two subdomains, A and B [1]. Due to its high similarity to human serum albumin, BSA has been extensively studied as an *in vivo* carrier of both endogenous and exogenous drugs [2].

In this study, we focused on investigating the interaction between BSA and three newly synthesized hybrid derivatives of indole L1 – L3 (Figure 1). Several indole derivatives have been shown to have antitumor and antimicrobial effects [3]. The interactions between studied ligands and BSA as their potential carrier were studied using spectroscopic methods such as UV-Vis absorption spectroscopy, fluorescence spectroscopy and circular dichroism (CD) spectroscopy. Through the application of these techniques, we determined the binding mode, thermodynamic parameters and binding sites of the ligands within BSA.

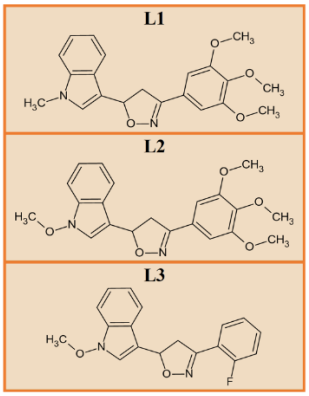

Figure 1 Molecular structure of studied compounds

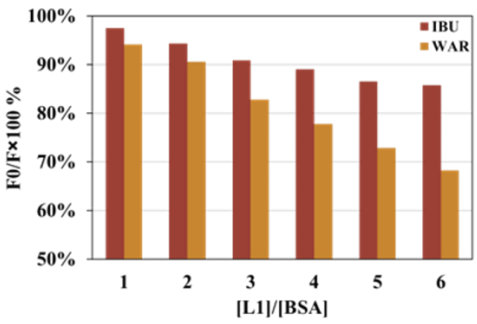

Figure 2 Displacement of Ibuprofen (IBU) and Warfarin (WAR) from the BSA by compound L1.

The spectroscopic analysis revealed notable binding interactions between the ligands and BSA. Fluorescence spectroscopy showed the highest binding constant ($K = 58{,}5 \times 10^5\ M^{-1}$) for L1 at 35 °C. The thermodynamic parameters ($\Delta H > 0$, $\Delta S > 0$) suggest hydrophobic binding between protein and ligands, and $\Delta G < 0$ indicates spontaneous process. Competitive fluorescence displacement experiment with Ibuprofen and Warfarin (Figure 2) confirmed that all compounds L1 – L3 bind at Sudlow's site I in subdomain IIa. Circular dichroism analysis showed that increasing concentration of compound altered BSA's secondary structure, with the greatest α-helix reduction observed for L3 and the smallest one for L1.

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Fluorescence Spectroscopic Characterization of Binding Interactions between Silver (I), Zinc (II), and Gallium (III) thiophene-2-carboxylates and Human Serum Albumin

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Human serum albumin (HSA) is the most abundant protein in blood plasma and plays a crucial role in maintaining colloidal osmotic pressure. Owing to its capacity to bind various ligands, it also serves as a transport protein for both endogenous and exogenous compounds [1-3]. The binding property of albumin reduces the toxicity of many drugs and prolongs their half-life, as drugs compete for binding at specific sites. Consequently, albumin plays a significant role in the pharmacokinetics and pharmacodynamics of numerous drugs [4].
This study characterizes the binding interaction between three 2-thiophenecarboxylate (Tio2c) complexes with various central metal atoms Ag(I), Zn(II) and Ga(III), $[Ag(Tio2c)]_2$ (AgTio2c), $\{[Zn_2(Tio2c)_4]_2\}_n$ (ZnTio2c) and $[Ga(Tio2c)_3]\cdot H_2O$ (GaTio2c) and HSA using fluorescence spectroscopy. Fluorescence quenching experiments were conducted at four different temperatures, and the binding constant (K_b), Stern–Volmer quenching constant (K_{SV}), bimolecular quenching constant (K_q), and thermodynamic parameters (ΔH, ΔS and ΔG) were calculated for each complex. The results indicate that all studied complexes bind spontaneously to a single site on HSA with moderate affinity ($K_b \sim 10^4\ M^{-1}$). The K_{SV} for the investigated complexes (AgTio2c, ZnTio2c, GaTio2c) were determined, with values observed to be on the order of $10^4\ M^{-1}$, indicating significant quenching efficiency. AgTio2c exhibited dynamic fluorescence quenching, which indicates that the quenching process occurs mainly through collisional interactions between the fluorophore and the quencher in the excited state [5]. In contrast, ZnTio2c showed static quenching behaviour, suggesting the formation of a non-fluorescent ground-state complex between the fluorophore and the quencher before excitation [5]. Analysis of the thermodynamic parameters revealed that the binding process is endothermic and largely driven by hydrophobic interactions. These results suggest that these complexes can efficiently bind to HSA, influencing their biological transport and activity. Among them, the AgTio2c complex appears to be the most suitable and promising candidate for biological applications. However, additional studies are required to fully assess its bioavailability.

Acknowledgements

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SESSION 2 BIOCHEMISTRY

Folate receptors as promising targets for photosensitive drug delivery using upconverting nanoparticles

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Cancer remains a serious issue that requires ongoing attention and improvement of established treatment methods. One reason for this is the resistance of tumour cells, which often develops during the treatment process. Nanoscience offers innovative strategies to reliably deliver drugs to their target, overcome resistance, and thus bypass the defence mechanisms of tumour cells. Given the rapid progress in chemical methods, several strategies exist for constructing suitable transport systems that can also actively participate in the treatment process.

Photodynamic therapy is an innovative cancer treatment that uses light, photosensitizers, and molecular oxygen to trigger destructive photochemical processes in tumour cells. The production of reactive oxygen species during this process causes the selective destruction of tumour cells. Photon-upconverting nanoparticles, which convert infrared light into visible light, enable the application of photodynamic therapy even in deeper tumours.

These particles consist of a core and a shell, which can be doped with lanthanide ions to ensure that the emission of radiation matches the requirements of a given photosensitizer. The most common activators are Er^{3+}, Tm^{3+}, while the sensitizer ions in the particles are Yb^{3+} and Nd^{3+}. As infrared light penetrates deeper into tissue, photodynamic therapy can be used in antitumour treatment even when conventional light sources are ineffective.

The effectiveness of the treatment can be improved by targeting nanoparticles to cell receptors. For this reason, upconverting nanoparticles were modified with folic acid (FA) to enable targeting of folate receptors (FAr) on cancer cells. Confocal fluorescence microscopy was used to identify changes in cancer cells before and after treatment with upconverting nanoparticles and photodynamic therapy. Fluorescence immunostaining (Figure 1) revealed changes in tubulin, FAr, and the Golgi complex in U87MG cells after photodynamic therapy with orange LED light at 590 nm. These results demonstrate that FA modification is an effective approach for targeted nanodelivery in the photodynamic therapy of cancer cells.

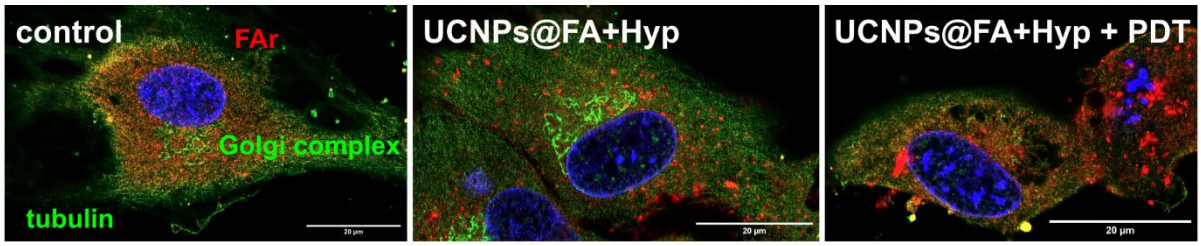

Figure 1 Representative images of cancer cells (U87MG) exposed to upconverting nanoparticles (UCNPs) modified by folic acid (FA). Nanoparticles were transported hypericin (Hyp) – photosensitizer and activated by photodynamic treatment (PDT) - 590 nm light (2 Jcm^{-2}). Tubulin, Golgi complex and Folate receptors (FAr) were immunostained.

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Study of new disubstituted diphenylamine derivatives with albumin and its antioxidant activity

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Diphenylamine (DFA) derivatives exhibit a wide range of biological activities and hold a special place in pharmacology, especially as nonsteroidal anti-inflammatory agents (NSAID). Evidence indicates that the bioactivation of haloaromatic drugs into reactive quinone metabolites is a key factor contributing to hepatotoxicity. Predictions suggest that DFA may also undergo bioactivation, resulting in the formation of reactive quinone metabolites [1].
Their structure consists of two aromatic rings connected by a secondary amine [1]. This determines their pronounced anti-inflammatory [1], antimicrobial [2] and antitumor [3]. DFA derivatives possess strong fungicidal, insecticidal, acaricidal, rodenticidal, and/or herbicidal effects [4]. They may also exhibit antifosphorylating [5] and antioxidant activity [6]. DFA are largely capable of binding to serum proteins, such as human serum albumin (HSA) [7]. HSA functions as a carrier of metabolites and xenobiotics in human blood. Studying the binding of this transport protein with DFA can provide insight into its bioavailability [8].
The study focuses on the investigation of disubstituted DFA derivatives and their antioxidant and antibacterial activities. Emission spectra confirmed the binding of the examined diphenylamine derivatives to HSA.

Acknowledgements

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Destruction of Insulin Amyloid Fibrils by Phytoalexins with Added Antioxidant Benefit

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Insulin is a peptide hormone that regulates blood glucose levels. It is an essential therapy for type 2 diabetes. However, long-term injections may result in insulin localized amyloidosis. The disease is characterized by the accumulation of insulin amyloid fibrils at the injection site and can disrupt glucose regulation [1]. Phytoalexins are chemical compounds produced by plants under stress, resulting from exposure to pathogens or physical damage. Their synthesis is a crucial element of the plant's built-in immune system. Several studies revealed antioxidant, anti-inflammatory, anticancer, metabolic, neuroprotective and antimicrobial actions of phytoalexins, making them an attractive topic of interest [2].

The objective of our study was to investigate the destructive effects of nine indole-based phytoalexins (Phy) and their synthetic derivatives on pre-formed human insulin amyloid fibrils *in vitro*. The destruction effect was examined using Thioflavin T (ThT) and Nile Red fluorescence assays, atomic force microscopy (AFM), and circular dichroism (CD) spectroscopy. Initial screening performed by the ThT and Nile Red fluorescence assays identified three phytoalexins — Phy 7, Phy 9, and Phy 11 — as strong fibril-destructors. The results of concentration-dependent studies showed that Phy 7 was the most potent compound with the highest destruction potential. The DC_{50} value (concentration of phytoalexins that decreases the fluorescence intensity of amyloid fibrils by 50 %) was below 22 μM, followed by DC_{50} values determined for Phy 11 (91 μM) and Phy 9 (157 μM). A treatment of pre-formed insulin fibrils with Phy 7, Phy 9 and Phy 11 resulted in a significant reduction in β-sheet content, as confirmed by far-UV CD spectroscopy. AFM confirmed the destructive activity of Phy 7, Phy 9 and Phy 11, where fewer and smaller amyloid fibrils were observed after treatment with the Phy. Importantly, cytotoxicity assessment revealed that Phy 7 and Phy 11 showed no toxicity toward HEK-293 cells at the tested concentrations (10 μM, 100 μM, 200 μM). On the other hand, Phy 9 showed cytotoxicity already at 100 μM. In the DPPH assay, all three effective Phy exhibited lower radical-scavenging capacity than gallic acid (used as a standard) at equivalent concentrations. Phy 9 and Phy 11 showed the significant antioxidant activity among the tested derivatives, corresponding to ~ 45% (Phy 9) and ~ 33 % (Phy 11) of the activity of gallic acid. Phy 7 exhibited only ~ 16 % of the antioxidant activity of gallic acid.

In conclusion, this study identified several promising phytoalexin candidates, particularly Phy 7 and its bis-indolyl derivative, Phy 11, as potent, non-cytotoxic agents for disrupting insulin amyloid fibrils and exhibiting significant antioxidant effects. These findings demonstrate that indole phytoalexins offer a promising strategy to modulate effects associated with long-term insulin therapy.

Acknowledgements
This work was funded by the EU Next Generation EU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V02-00039, and by research grants from the Slovak Research and Development Agency under the Contract No. APVV-22-0598, and Slovak Grant Agency 02/0164/22, 02/0141/25, 01/0347/23, 1/0037/22.

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Functional targeted delivery of flavin mononucleotide by DARPin and AsLOV2 C450A protein to breast cancer cells

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One of the major challenges in modern oncology is to develop therapeutic strategies that selectively target cancer cells while minimizing damage to healthy tissues. A promising approach involves receptor-specific targeting, such as the HER2 receptor frequently overexpressed on the surface of breast cancer cells [1]. Our research focused on developing protein conjugates for potential use in photodynamic therapy (PDT). This is a minimally invasive treatment that uses light-activated photosensitizers to destroy cancer cells. As a core component, we employed the genetically modified variant AsLOV2 C450A, which produces singlet oxygen upon blue-light illumination and binds its flavin mononucleotide (FMN) cofactor more tightly than the wild-type protein [2]. To achieve specific binding to HER2 receptors, AsLOV2 C450A was fused with Designed Ankyrin Repeat Proteins (DARPins). The recombinant fusion proteins were expressed in E. COLI. Conjugates were purified by HPLC and their molecular mass was confirmed using SDS-PAGE. Differential scanning calorimetry showed melting temperature and thermal stability of proteins. FMN was detected by its absorption and emission maxima with UV/VIS spectroscopy. Results provided by confocal microscopy indicate selective binding of the DARPin–AsLOV2 C450A conjugate to HER2-positive cells, highlighting its potential as a targeted photosensitizing platform for future use in photodynamic treatment of breast cancer.

Acknowledgements

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Stability effect of FMN on flavin proteins miniSOG and SOPP3

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MiniSOG (Mini Singlet Oxygen Generator) is flavoprotein derived from LOV-domain of phototrophin 2 in *Aradopsis thaliana* [1]. It is monomeric protein composed from 106 amino acids, Mw 15,3 kDa, containing strongly bound flavin mononucleotide (FMN). MiniSOG belongs to genetically encoded photosensitizers, which were developed for precise spatio-temporal control of ROS production withing living cells and organisms. SOPP3, variant of the miniSOG, was made for improving their photosensitizer properties [2]. Genetically encoded photosensitizers are promising tool for selective non-invasive photodynamic therapy of cancer due to the spatial selectivity and locality of destructive action compared to other methods of oncotherapy.
In the present study we use differential scanning calorimetry (DSC) to analyze effect of FMN on stabilization of miniSOG and SOPP3 as well as their T100C mutants. Ongoing studies show that miniSOG, which is known as less potent photosensitizer, has higher thermal stability (T_m = 52 °C) compared to its variant SOPP3 (T_m = 45 °C). The introduction of the T100C mutation into these proteins was shown to have an even greater destabilizing effect according to spectrometric and DSC measurements and affected the binding of FMN to the protein itself. By adding FMN in DSC thermal stability measurements of the proteins and mutants at different ratios, it was shown that the FMN increases the stability of proteins (Figure 1).

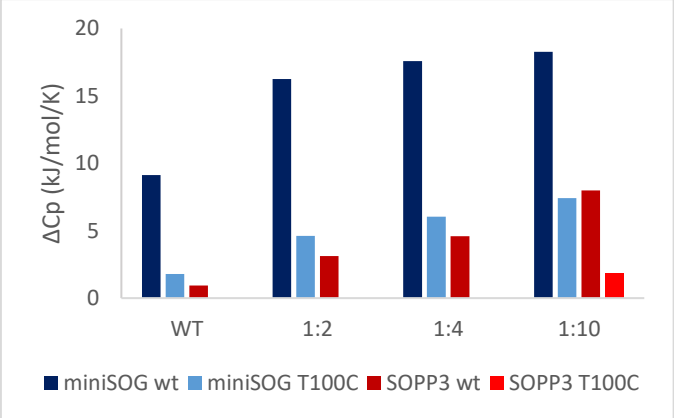

Figure 1 DSC analysis of effects of FMN on miniSOG, SOPP3 and their T100C mutants. Rations 1:2, 1:4 and 1:10 are rations of protein:FMN.

According to our study, the ability to more easily release the FMN group due to mutations to create a more potent photosensitizer has a significant impact on protein stability. At the same time, stability of flavin proteins itself depends on the affinity of FMN to the polypeptide chain. These results are in accordance with previous results with LOV2 domain (Felčíková et al., 2023).

Acknowledgements

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Visualization HER2 positive cells with NanoLuc

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Oxidation of the luciferin substrate leads to the emission of light called luminescence. The catalysis oxygenation of the luciferin pigment allows oxidoreductases, named luciferases. Very innovative and structurally optimized type of luciferase is NanoLuc. The NanoLuc luciferase technology has been successfully utilized for several applications, including the investigation of protein – protein and protein – ligand interactions, exploring gene regulation and cell signaling, monitoring protein stability, utilization as BRET-based biosensors, and bioluminescence imaging [1, 2]. One of most problems which are discussed is limited light penetration into tissues. The application of internal light sources, based on chemiluminescence or bioluminescence of some molecules in the presence of a suitable substrate or catalyst, represents approach which can resolve problem with light penetration.

Very elegant delivery system, which allows increasing of specificity, are DARPins. DARPins are specifically designed ankyrin repeat proteins that typically exhibit high binding affinity to the targeted protein/receptor. A DARPin-Luciferase complex (NanoLuc) has been designed and created with high specificity for the HER2 receptor.

The HER2 is a protein/receptor localized on the surface of some cancer cells and has tyrosine kinase activity. HER2 can initiates signaling cascades that lead to cell growth and proliferation after activation. This receptor is a significant therapeutic target for anticancer treatments designed to inhibit its signaling pathways. A tumor is considered "HER2-positive" if it has an amplification of the HER2 gene, overexpression of the HER2 protein, or certain mutations in the gene, which all result in overly active HER2 signaling. Traditional treatments for HER2-positive cancers aim to block HER2 signaling by using monoclonal antibodies, tyrosine kinase inhibitors, or antibody-drug conjugates.

Our results suggest that it is possible to use specifically modificated DARPin with NanoLuc for visualization of “HER2 positive “ cells.

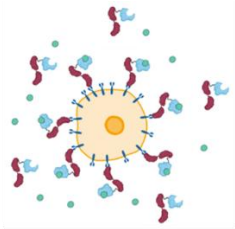

Figure 1 Schematric binding luminiscence substrate coletrasine to DARPin NanoLuc complex on the surface HER2 positive cells.

Figure 2 Luminescence HER2 positive cells after addition substrate coletrasine to preincubated DARPin NanoLuc cells.

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Determination of biologically interesting substances from natural materials using UV/Vis and HPLC methods

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Recently, a great interest has been focused on the use of anthocyanins in the nutraceutical industry as functional food sources for their sorts of potential health benefit, including anti-inflammation, anticancer, anti-mutagenesis, and anti-bacterium. Anthocyanins also possess the effect on reducing the risks of heart disease, preventing Alzheimer's disease, decreasing blood glucose and DNA damage, as well as regulating the immune system and improving visual. These above health contributions mainly attribute to the antioxidant activity and free radical scavenging property of anthocyanins [1]. UV/Vis spectrophotometry is a quantitative analytical technique that measures the amount of light a chemical compound absorbs in the ultraviolet and visible ranges of the electromagnetic spectrum. This method is widely used across various fields like chemistry, biology, environmental science, and material science due to its sensitivity and versatility. An HPLC method is an analytical technique that separates, identifies, and quantifies components in a liquid mixture. High-performance liquid chromatography (HPLC) is the standard method for analyzing anthocyanins, a class of flavonoid pigments responsible for red, purple, and blue colors in plants. Due to their poor stability, analysis requires careful preparation and optimized HPLC conditions to prevent degradation [2, 3].
The aim of the study was to determine the anthocyanin content using UV/Vis spectrophotometry and HPLC analysis of blackberry (*Rubus fruticosus L.*) and fresh grapevine (*Vitis vinifera L.*) fruits. An ethanol solution acidified with 1% phosphoric acid was used as the extraction agent in the preparation of extracts from blackberries and grapevines. The prepared extracts were purified using Amberlite XAD-7 with distilled water acidified with hydrochloric acid and followed by ethyl acetate as the mobile phase. When measuring UV/Vis spectra, the absorbance of the samples was measured at wavelengths of 520 nm and 700 nm. Distilled water was used as a blank sample. Cyanidin-3-glucoside was determined to be the basic component of anthocyanins. At a wavelength of 520 nm, the change in pigment absorbance is directly proportional to the concentration of these pigments. The absorbance of diluted samples was measured using an Agilent Technologies Cary 60 UV/Vis spectrophotometer. The anthocyanin (cyanidin-3-glucoside) content of the prepared grape and blackberry extracts was determined using a UHPLC Ultimate 300 (Thermo Scientific) instrument. The measurement was performed on a Polaris 5 C18-A column with dimensions of 250×4.6 mm. The mobile phase flow rate (acetonitrile with 0.5% formic acid) was set to 1 ml/min. and the thermostat to 20°C. The sample injection volume was 20 µl and the pressure was 150 bar. The UV detector (DAD) was set to a wavelength of 528 nm.

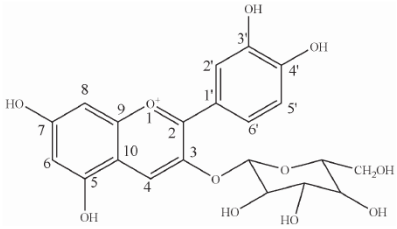

Figure 1 Cyanidin-3-glucoside, a type of natural pigment called an anthocyanin, found in many dark-colored fruits and vegetables, which acts as a powerful antioxidant and anti-inflammatory agent [4].

The anthocyanin content in grapevine was 30.84 mg·dm^{-3} in purified extract. In wild blackberries, the anthocyanin content in the purified extract was 66.63 mg·dm^{-3}. Based on qualitative HPLC analysis, it was confirmed that cyanidin-3-glucoside is present in extracts of grapevine and wild blackberries.

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Basic hydrolysis of chiral menthyl ester of (4*S*,5*S*)-5-(acridin-4-yl)-3-(2,4,6-trimethylphenyl)-4,5-dihydro-1,2-oxazole-4-carboxylic acid

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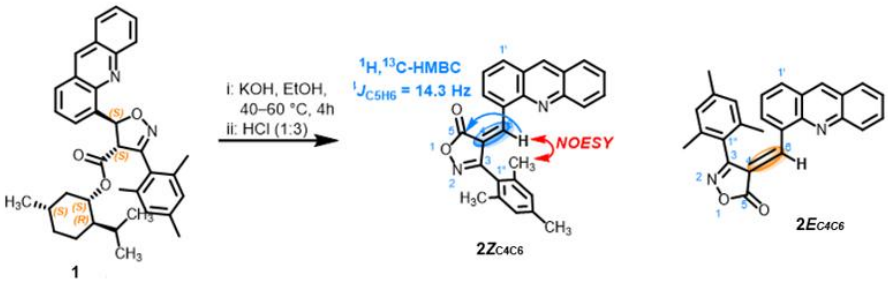
During this period, organic chemistry continued to develop, thanks to advances in technology and the need for new compounds, which led to their synthesis and applications in medicine, materials and many other areas. This field of chemistry also develops thanks to new experiments that result from the study of reaction mechanisms. Also in this work, a seemingly simple hydrolysis of an ester was studied, which, however, did not lead to the expected product, but provided completely new heterocyclic compounds.
Basic hydrolysis of the acridine derivative **1** was carried out to probe their stability under strongly nucleophilic conditions, validate the proposed intermediate structures through conversion to predictable products, assess the retention or loss of stereochemical information during ring opening and rearrangement, and generate complementary derivatives for comparative stereochemical and mechanistic studies. The reaction of **1** with KOH released (1*S*,2*R*,5*S*)-(+)-menthol and furnished, not the carboxylic acid, but instead the corresponding isoxazolone derivatives as mixtures of the **2*Z*$_{C4C6}$** and **2*E*$_{C4C6}$** isomers in ratio 3.8:1.0 (based on ^{1}H NMR spectrum of reaction mixture), as described previously [1]. Recrystallization from methanol afforded the mixture of the **2*Z*$_{C4C6}$** and **2*E*$_{C4C6}$**, which were fully characterized by NMR spectroscopy.



Derivative	Selected ^{1}H NMR chemical shifts [δ, ppm]							
	H6	H1'	H2'	H3'	H5'	H3'',5''	*p*-H7''	*o*-H8''
2Z$_{C4C6}$	9.14	8.23	7.72	9.56	7.98	7.10	2.44	2.37
2E$_{C4C6}$	9.56	7.94	6.86	7.02	8.31	6.75	2.27	2.03

Derivative	Selected ^{13}C NMR chemical shifts [δ, ppm]										
	C3	C5	C6	C1'	C2'	C3'	C5'	C1''	C2'',6''	*p*-C7''	*o*-C8''
2Z$_{C4C6}$	165.5	168.8	149.2	134.8	125.5	136.2	129.8	123.6	137.8	21.4	20.1
2E$_{C4C6}$	160.7	170.6	149.7	132.9	123.9	133.7	130.1	126.0	136.9	21.1	19.9

Figure 1 Basic hydrolysis of **1** leading to the formation of **2*Z*$_{C4C6}$** and **2*E*$_{C4C6}$**isomers. The double bond at C4=C6 is the site of *E*/*Z* isomerism. Structural elucidation of **2*Z*$_{C4C6}$** and **2*E*$_{C4C6}$** using NMR spectroscopy. Selected key ^{1}H and ^{13}C NMR chemical shifts are summarized in the tables.

The ^{1}H NMR spectra of **2*Z*$_{C4C6}$** and **2*E*$_{C4C6}$** reveal notable differences attributable to the anisotropic effects of the acridine and phenyl rings, as well as substituent shielding. The relatively high chemical shift of H6 arises from the anisotropy of the acridine ring. In the **2*E*** isomer (across the C4=C6 double bond), H1' and H2' exhibit decreased chemical shifts relative to the **2*Z*** isomer, reflecting shielding by methyl groups and the phenyl ring, whereas H3' in **2*Z*** is deshielded by the carbonyl group. H5' in **2*Z*** experiences lower chemical shift due to methyl shielding. The *E*/*Z* assignment was confirmed via the $^{3}J_{C5H6}$ coupling constant measured from ^{1}H,^{13}C-HMBC spectra.

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Topologically Constrained DNA, Embedding and Visualizing Non-Canonical Structures in Minicircles

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Despite the fact that more than 10 % of the human genome is potentially capable of forming non-canonical DNA structures (NCS), their emergence within classical B-form duplex segments is generally thermodynamically disfavoured. However, accumulated experimental evidence demonstrates that such motifs do exist and contribute to regulatory processes in cells [1]. Their formation is strongly influenced by sequence context, DNA topology and external environmental factors. In addition to the linear configuration, DNA may assume a circular topology. DNA minicircles are small covalently closed double-stranded DNA loops that occur naturally in kinetoplast mitochondrial DNA and serve as model systems in structural biology. By eliminating free ends, minicircles impose topological constraints, enabling researchers to mimic nucleosomal or supercoiled DNA and to probe DNA structural dynamics. These constructs have been instrumental for studying NCS DNA conformations beyond the standard B-form. Such structures include G-quadruplexes (G4) four-stranded helices formed by G-rich sequences stabilized by K^+ ions, i-motifs (iM) intercalated four-stranded C-rich DNA favored at acidic pH, and hairpin/cruciform extrusions from palindromic repeats. NCS are biologically significant, with evidence of their formation *in vivo* and roles in regulating replication, transcription, and genome stability [2, 3].
DNA minicircles provide a unique platform to embed and stabilize NCS in a duplex context. The topological strain and local base-pair mismatches together promote the emergence of these structures that would be thermodynamically unfavorable in an unconstrained helix. Polyacrylamide gel electrophoresis (PAGE) and circular dichroism (CD) spectroscopy have been used to confirm structural conversion in such minicircles. G4 forming circles display anomalous electrophoretic mobility and a CD signature characteristic of [4]. Thermal analyses indicate that an intramolecular G4 embedded in a minicircle remains stable under physiological salt conditions. Likewise, C-rich minicircles fold into iM structures at acidic pH, causing compaction of the DNA and faster migration on gels. The presence of iM is corroborated by pH-dependent CD spectral changes and a biphasic melting profile for the iM core. Palindromic inserts can similarly extrude hairpins within a circle, relieving bending strain and showing distinct melting behavior [4, 5].
Importantly, the visualization of these DNA architectures by atomic force microscopy (AFM) has directly confirmed the formation of NCS in minicircles. By "trapping" non-B DNA structures in a constrained yet observable setting, minicircle systems allow detailed characterization of the folding topology and stability of G4, iM, and related motifs under near-physiological conditions. The ability to detect an iM within a DNA circle by AFM, or to observe a robust G4 signal in the presence of KCl, provides direct evidence that such exotic DNA conformations can persist in duplex DNA when appropriately facilitated. This not only supports their proposed regulatory roles in gene expression, but also informs the design of DNA-based nanodevices [1, 3].
Overall, the integration of NCS into minicircles combined with analysis by PAGE, CD, and AFM – illuminates how DNA sequence and topology cooperate to yield structural polymorphism. Visualizing embedded bridges the gap between biochemical assays and real-space morphology, enhancing our understanding of DNA's conformational diversity and paving the way for applications in nanotechnology and molecular medicine.

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Mass photometry as a tool to assess K_d for homodimeric enzyme glucose oxidase

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Glucose oxidase (GOX, EC 1.1.3.4) is an oxidoreductase that catalyzes oxidation of β-D-glucose to a D-glucono-δ-lactone. It exists as a homodimer (D) that is in dynamic equilibrium with its monomer (M) subunits (eq. 1). According to experimental evidence, only the dimeric form of GOX is active [1]. To understand the relationship between its structure and function, it is essential to know the value of the dissociation constant K_d, which quantifies the equilibrium between the D and M forms (Figure 1). Using a revolutionary mass photometry method [2], we were able to determine the K_d for homodimeric GOX to be 24 nM (in PBS, pH 7.4, 24 °C). This is a simple, time-saving and effective procedure that will also serve as a guide for determining the K_d for any other oligomeric protein. On the other hand, it should be noted that the calculation of the K_d may be subject to error related to the measurement methodology. At higher GOX concentrations (e.g. 5 nM), the number of landing particles is too large and could affect particles distribution.

$$\mathbf{D} \underset{}{\overset{K_d}{\rightleftharpoons}} \mathbf{2M} \qquad \text{(eq. 1)}$$

$$K_d = \frac{[M]^2}{[D]} \qquad \text{(eq. 2)}$$

$$C_T = [M] + 2[D] \qquad \text{(eq. 3)}$$

$$[M] = \frac{-K_d + \sqrt{K_d^2 + 8K_d C_T}}{4} \qquad \text{(eq. 4)}$$

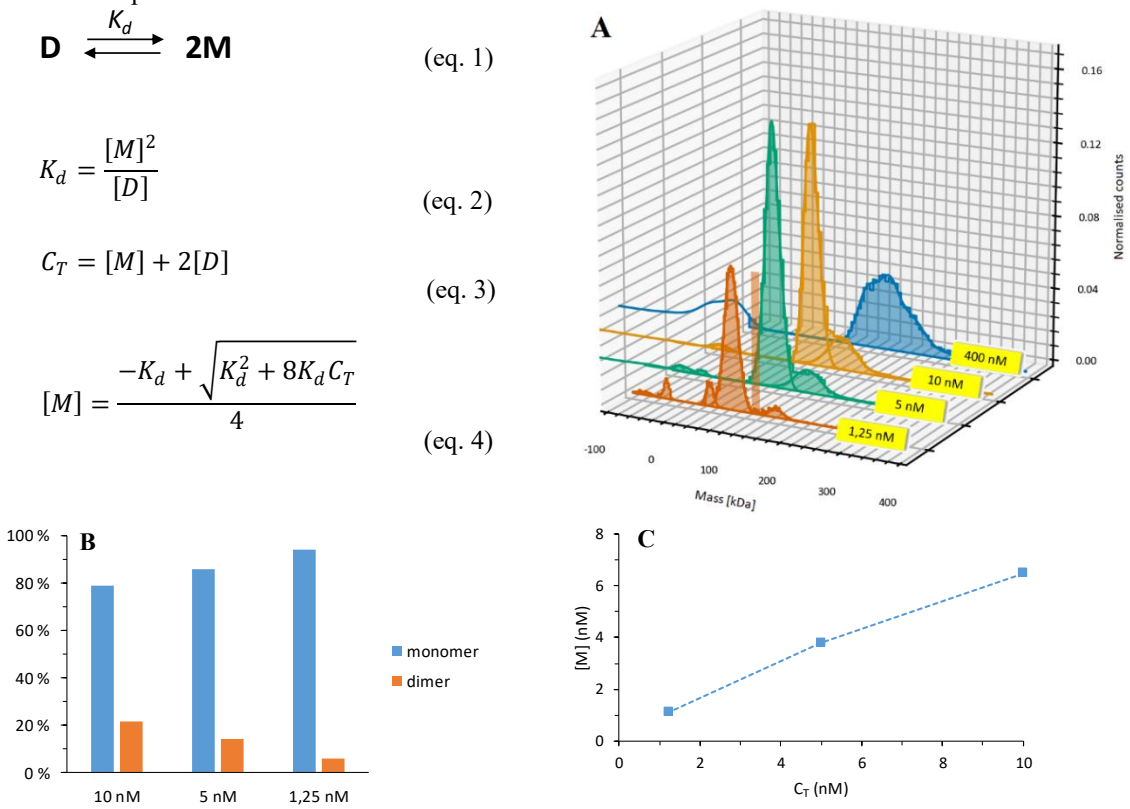

Figure 1 Output from mass photometry (Refeyn TwoMP) showing molecular mass and populations of GOX at its various total concentrations, C_T, depicted in yellow boxes (**A**), a dependence of monomer (M) and dimer (D) distribution of GOX on C_T (**B**) and a plot of molar concentration of M on C_T (**C**). Dashed line in (**C**) is the best fit according to equation 4. Equations 2 and 3 express relationships between K_d, C_T, and M, D concentrations.

Acknowledgements

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Supporting Chemistry Teachers in Integrating Artificial Intelligence into Teaching through Innovative Training

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The use of artificial intelligence (AI) by teachers has become a key topic in contemporary education, as the emergence of generative AI is fundamentally reshaping how teachers plan, design, and implement instruction [1]. The growing availability of AI tools simultaneously offers new opportunities to support, personalise, and enhance both teaching and learning. This contribution reports the results of research aimed at identifying and assessing the impact of the innovative training programme Teaching Chemistry in Secondary Schools: Fostering Digital and Scientific Literacy (TCDSL) on the development of chemistry teachers' digital competences, with particular emphasis on strengthening competences relevant to the DigCompEdu framework-specifically Area 2 (Digital Resources), Area 3 (Teaching and Learning), and Area 4 (Assessment)-in relation to the pedagogically meaningful use of AI. The training programme was explicitly aligned with the requirements of DigCompEdu [2] and aimed to support teachers in integrating activating methods, digital technologies, digital assessment tools, and AI applications into chemistry teaching. The content of the TCDSL programme, including all educational materials, was transferred to the MS Teams environment. Instruction was organised into six modules with a total of 50 hours, delivered in a combined present (25 h), online (15 h), and distance (10 h) form. The training was provided by experts in chemistry didactics from three Slovak universities: the Faculty of Science at Pavol Jozef Šafárik University in Košice, the Faculty of Education at Trnava University in Trnava, and the Faculty of Science at Comenius University in Bratislava. The research sample comprised secondary school chemistry teachers (N=15) from three Slovak regions. The research was conducted during the first term of the 2024/2025 school year using a one-group pre-test–post-test design. A self-constructed questionnaire, completed before and after the training, served as the research instrument. Items were conceptually linked to DigCompEdu competence descriptors, focusing on teachers' perceived readiness to select, adapt, and create digital and AI-supported resources (Area 2), to use AI to design and implement digitally enhanced learning activities (Area 3), and to apply AI-based or AI-supported tools in summative and formative assessment (Area 4). The analysis of results in the area of AI use indicated an overall improvement in teachers' level of knowledge in AI following the training. Teachers demonstrated a clearer understanding of the concept and pedagogical potential of chatbots and became more proficient in independently using a broader set of AI tools. The most frequently used tools included ChatGPT, Copilot, Gemini, Canva, Magic School, and Midjourney. Teachers reported a more frequent use of AI during lesson preparation, particularly to streamline their work, generate or adapt teaching materials, and personalise the content provided to students-corresponding to improvements in DigCompEdu Area 2 and Area 3. Teachers also expressed expectations for stronger institutional support in implementing AI meaningfully within DigCompEdu Areas 3 and 4, especially in relation to securing licences, ensuring appropriate technical infrastructure and organisational support, and providing sustained opportunities for further professional development focused on AI integration in teaching and assessment.

Acknowledgements

This contribution was supported by the National project "Digital Transformation of Education and School " (DiTEdu). This project is financed by the European Social Fund Plus through the Programme Slovakia 2021-2027; grants VEGA No. 1/0051/25 "Development of the Digital Competence in Future Science Teachers", KEGA No. 001UPJŠ-4/2023 "Implementation of Formative Assessment in Primary School Teaching with the Focus on the Digital Form", and VVGS IPEL 2025-3464 "Designing Summative and Formative Assessment Tools for the Special Practice of School Experiments I Course".

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Contemporary Approaches in Chemistry: Mesoporous Silica for Efficient Anticoagulant Drug Delivery

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The investigation of mesoporous silica in the context of anticoagulant therapies shows promising results. The particular anticoagulant analysed herein is intended to prevent blood coagulation due to irregular clotting that can lead to serious health issues, including stroke, heart attack, or venous thromboembolism. The large surface and uniform pore structure of mesoporous silica allows the amount of drug to be absorbed inside the pore, whether the drug is poorly soluble in water, like anticoagulant drug apixaban (APX) and often stabilises drugs in the amorphous form to increase their solubility [1]. The mesoporous silica, like SBSA-15, has channels that regulate drug diffusion, enabling to control, sustained drug release and enhanced bioavailability. Additionally, SBA-15 is amenable to functionalization with ligands or pH-sensitive groups for targeted delivery [2]. In our study, we successfully synthesised the SBA-15 and functionalized it with the aminopropyl, chloropropyl, and mercaptopropyl ligands, followed by wet impregnation performed twice with apixaban in chloroform solvent to observe the surface area capacity. The characterisation of the samples is investigated by FTIR, TGA-QMS, SAXS, XRD, SEM, elemental analysis and nitrogen adsorption at 77 K. The illustrative sample present for FTIR, TGA and Nitrogen asaorption of SBA-15, SBA-15-SH, SBA-15-APX I, SBA-15-APX II in first and second impregnation which contain APX (Figure 1). Figure 1 (a) shows the presence of the mercaptopropyl ligand (-SH) and the APX after impregnation which confirm in TGA Figure 1 (b) that observed more weight loss than pure SBA-15 and supported by surface area of pure SBA-15 is 652 m2/g decrease to 156 m2/g for SBA-15-SH-APX II.

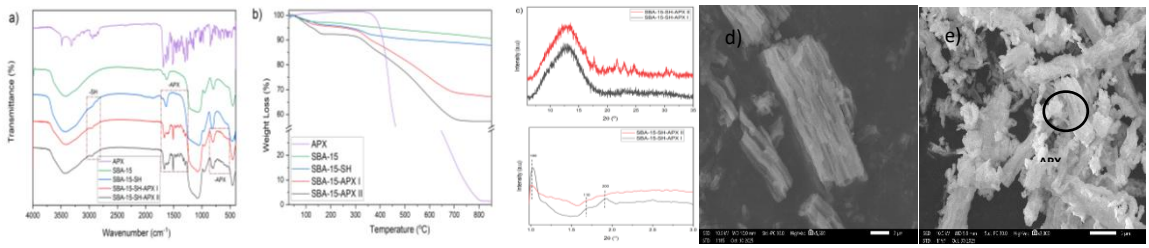

Figure 1 Results of a) FTIR, b) TGA c) XRD d) SEM of SBA-15 and e) SEM of SBA-15-SH-APX II.

Upper Figure 1(c) is the XRD profiles of SBA-15-SH-APX I that indicated amorphous silica and lack of crystalline drug and show broad humps at 13–18°, in 2θ. The absence of sharp apixaban peaks suggests the drug is molecularly dispersed or amorphous within the mesoporous matrix. However, SBA-15-SH-APX II with the second impregnation displays crystallisation with small peak at 20-25° in 2θ, revealed the drug is outside the internal surface area which is confirmed by the SEM result in Figure 1(e) and SAXS showed the structure changed after the second impregnation in lower Figure 1 (c). The SBA-15 SEM without ligand and drug showed the rod-shaped. Conclusion: This result confirms successful encapsulation of APX in the SBA-15-SH matrix, where the amorphous form increases potential solubility and supports a sustained release profile. For the next research, we will study drug release at different pH.

Acknowledgements

This work was supported by the Slovak Research and Development Agency under Contract APVV-23-0097 and by VEGA Project 1/0442/25. The SAXS measurements were realised in the frame of EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. No. 09I03-03-V04-00722 and 09I03-03-V03-00034.

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Adsorption of Toxic Volatile Organic Vapors on HKUST-1: Structure–Property Correlations and Application in Gas Mask Filters

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Volatile organic compounds (VOCs) are a chemically diverse group of carbon-based molecules that readily evaporate at ambient temperatures and arise from industrial production, fuel combustion, solvent use, and everyday household activities. Their ubiquitous presence in indoor and outdoor air poses serious environmental and health risks, contributing to tropospheric ozone formation and causing respiratory or carcinogenic effects. Therefore, efficient VOC abatement remains a global priority.

Conventional adsorbents such as activated carbon or zeolites, though widely used, often suffer from limited selectivity, poor adsorption of highly volatile molecules, and low regenerability. In contrast, metal–organic frameworks (MOFs) have emerged as next-generation sorbents due to their crystalline nature, tunable pore structure, and high surface area. Among them, HKUST-1 (Cu-BTC, or MOF-199) is particularly attractive for VOC capture because of its robust Cu paddle-wheel structure, large pores (6–9 Å), and high surface area (600–1600 $m^2\ g^{-1}$). Its low-cost synthesis and good thermal stability (up to 350 °C) make it a realistic candidate for scalable filtration technologies.

In this work, the adsorption behaviour of HKUST-1 toward a representative set of VOCs: methanol, formaldehyde, benzene, toluene, pyridine, aniline, benzaldehyde, benzyl bromide, and salicylaldehyde, was systematically investigated to assess its potential for gas-mask filter applications. Activated HKUST-1 (150 °C, vacuum) was exposed to saturated vapors under static conditions, and adsorption capacities were determined gravimetrically after 3, 24, and 48 h to evaluate both fast and equilibrium uptake.

The results revealed strong dependence on molecular size, polarity, and volatility. Rapid adsorption occurred within the first three hours, followed by stabilization or slight desorption. The framework displayed exceptionally high affinity for small, polar molecules: methanol uptake reached 1897 mg g^{-1} (≈ 2 g adsorbate per g adsorbent) at 25 °C, and formaldehyde exhibited comparably strong sorption. In contrast, bulky VOCs such as benzyl bromide and salicylaldehyde showed limited diffusion into the pores, resulting in significantly lower capacities. Increasing temperature (35–45 °C) reduced uptake due to the exothermic nature of adsorption, but substantial sorption persisted, indicating good performance under realistic operational conditions.

Overall, HKUST-1 demonstrates high capacity, stability, and partial selectivity toward low-molecular-weight polar VOCs, outperforming conventional carbons in terms of tunability and structural control. These results highlight HKUST-1 as a promising candidate for personal protective filters and broader air-purification applications. Future research should address cyclic regeneration, humidity tolerance, and composite design to further enhance its applicability in environmental protection and occupational safety.

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Reinventing HKUST-1 Synthesis: A Comparative Insight into Sonochemical and Solvothermal Routes

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HKUST-1 (also MOF-199 or CuBTC) is a metal-organic framework, that was first synthesized by Williams and co-workers in 1999. This material is well-known for its microporous structure containing Cu(II) paddle-wheel cluster and a favorable specific surface area. It is commonly used for CO_2 capture, hydrogen storage, water purification and so on. A wide variety of synthetic routes for HKUST-1 have been developed. The solvothermal method remains the standard and most widely used approach. However, some methods are more energy-efficient, less time-consuming, and still deliver quality results. To illustrate, the mechanochemical method minimizes solvent usage, while the sonochemical method reduces energy consumption compared to its solvothermal counterpart.

In this study, the synthesis of HKUST-1 is carried out using different methods while maintaining the same reaction mixture and reactants. The purpose is to compare the obtained materials in terms of their structural and textural properties and to evaluate their adsorption performance in the following experiments. In all HKUST-1 syntheses, the same reaction mixture was used. Specifically, 0.444 g of 1,3,5-benzenetricarboxylic acid was dissolved in 13.333 mL of a 1:1 DMF/ethanol mixture and added to 6.667 mL of an aqueous solution of 0.924 g of copper (II) nitrate trihydrate in a 30 mL glass vial. Depending on the type of synthesis, the resulting mixture in the vial was then processed under different conditions.

Two different syntheses of HKUST-1 were carried out, namely solvothermal (ST) and sonochemical (SC) preparation. Both methods yielded crystalline HKUST-1 materials. The sonochemical route produced a higher amount of material. Although the solvothermal synthesis typically requires about 8 hours, shortening the reaction time to 160 minutes resulted in a significantly lower yield compared to the sonochemical method performed for the same duration (Figure 1).

Based on the promising results of the solvothermal and sonochemical syntheses, a third route — microwave-assisted synthesis (MW-HKUST-1) — is planned to be explored. This approach is expected to further reduce the reaction time and energy consumption while providing uniform crystal formation. The synthesized materials will undergo adsorption experiments aimed at evaluating their sorption capacities toward selected adsorbates. The experiments will be conducted in a static system, monitoring mass changes to determine adsorption capacity and kinetics.

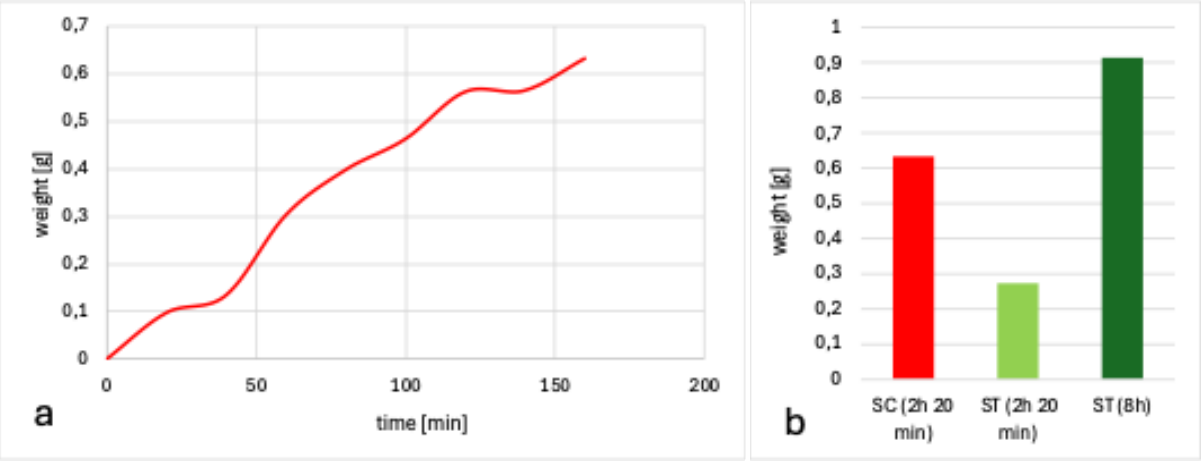

Figure 1 a) Graphical representation of HKUST-1 sonochemical synthesis by time, b) Comparison of HKUST-1 sonochemical and solvothermal synthesis performance.

Acknowledgements

This work was supported by: VEGA 1/0058/25, VEGA 1/0442/25, EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the Project No. 09I02-03-V01-00022 (SUNFLOWERS), No. 09I03-03-V03-00034 (MASS-PRAM) and No. 09I03-03-V05-00008 (VVGS-ESGV-2923).

Mesoporous Silica Nanoparticles for Sustained Oral Delivery of Apixaban

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Mesoporous silica nanoparticles (MSNs) are attractive materials for controlled drug delivery because of their large surface area, tunable pore structure, and biocompatibility. In this study, spherical mesoporous silica nanoparticles (SMS) were synthesized and evaluated as carriers for the antithrombotic drug apixaban, a direct factor Xa inhibitor with poor aqueous solubility and short half-life [1].
The nanoparticles were prepared by a sol–gel process and functionalized with organic ligands (–SH, –NH_2, –Cl) to tailor surface interactions with the drug. TEM analysis confirmed uniform spherical morphology (~300 nm) and a well-ordered porous structure. N_2 adsorption–desorption isotherms displayed Type IV behaviour with a clear hysteresis loop, confirming mesoporosity. The BET surface area ranged from 300 to 600 $m^2 \cdot g^{-1}$ with pore sizes of 3–5 nm, while TGA analysis verified successful surface modification and was used to estimate apixaban loading of 150–200 $mg \cdot g^{-1}$ depending on functionality.
Apixaban was incorporated using the wet impregnation method in methanol, which enabled efficient pore filling. In vitro release studies performed at pH 2 and pH 7.4 demonstrated sustained release over 72 hours, followed by a plateau. The release rate was slower in acidic conditions due to reduced drug solubility and stronger electrostatic interactions with the protonated silica surface. When a second portion of drug-loaded nanoparticles was added after 72 hours, the release process restarted, confirming the reproducibility of the system.
These results highlight the potential of SMS mesoporous silica nanoparticles as effective carriers for poorly soluble antithrombotic drugs, capable of sustained release that could reduce dosing frequency and improve therapeutic safety.

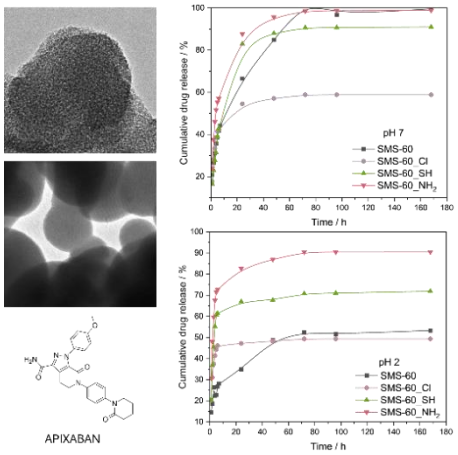

Figure 1 TEM images of SMS nanoparticles (average size: 300 nm) and release profiles of apixaban from nanoparticles in pH 7 and pH2.

Acknowledgements

This research was supported by the Recovery and Resilience Plan for Slovakia, project No. 09I03-03-V04-00722.

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Engineering MOF-Based Cathodes for Enhanced Stability and Capacity in Lithium–Sulfur Batteries

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Energy remains one of the most essential human needs and is the cornerstone of technological and societal progress. Since their commercialization in the early 1990s, rechargeable lithium-ion (Li-ion) batteries—featuring energy densities of approximately 200–400 Wh kg^{-1} and 500–1300 Wh L^{-1}—have dominated the global market. Continuous advances in Li-ion technology have brought performance close to theoretical limits; however, current energy demands for electric vehicles, portable electronics, and large-scale storage systems already surpass the achievable capacities of Li-ion cells. This has accelerated the search for alternative energy-storage technologies with higher energy density, lower cost, and improved environmental compatibility.

Lithium–sulfur (Li–S) batteries have emerged as one of the most promising next-generation systems. Unlike Li-ion batteries, which rely on the intercalation and deintercalation of lithium ions within layered structures, Li–S batteries operate via a multi-step conversion mechanism. During charge and discharge, elemental sulfur is electrochemically reduced to lithium polysulfides (Li_2S_n, $4 \leq n \leq 8$), which are then converted to insoluble Li_2S. The reaction occurs at an average potential of approximately 2.1 V versus Li/Li^+, corresponding to a high theoretical energy density of 2500 Wh kg^{-1} and 2800 Wh L^{-1}—nearly an order of magnitude greater than that of conventional Li-ion systems.

Despite these advantages, practical implementation of Li–S batteries faces several intrinsic challenges. Sulfur possesses extremely low electronic conductivity (~5×10^{-30} S cm^{-1}), which limits charge transport and active material utilization. Furthermore, sulfur undergoes substantial volume expansion (~80%) upon lithiation, causing mechanical stress and electrode instability. The most critical issue is the polysulfide "shuttle effect," where soluble lithium polysulfides migrate between the cathode and anode, leading to self-discharge, capacity fading, and poor Coulombic efficiency.

To overcome these limitations, porous host materials capable of immobilizing sulfur species and maintaining electrical contact are being intensively investigated. Among them, metal–organic frameworks (MOFs) have attracted particular attention due to their tunable pore structure, high surface area, and chemical versatility. MOF-based cathodes can effectively confine polysulfides through physical adsorption and chemical interactions while providing conductive pathways for charge transport.

Several representative MOFs, including MIL-101(Fe)-NH_2, MOF-76(Gd), and STAM-1, have been systematically studied as sulfur hosts. The amino-functionalized MIL-101(Fe)-NH_2 with a surface area of ~3500 m^2 g^{-1} delivered an initial discharge capacity of 705 mAh g^{-1} at 0.5 C and retained 476 mAh g^{-1} after 200 cycles, corresponding to a low capacity fading rate of 0.162% per cycle. Similarly, carbonized MOF-76(Gd) exhibited an initial capacity of 658 mAh g^{-1} and maintained 93% of its capacity after 200 cycles. The copper-based STAM-1 framework achieved a discharge capacity of 452 mAh g^{-1} at 0.5 C and retained 430 mAh g^{-1} after 100 cycles with a Coulombic efficiency of 97%.

These results demonstrate that well-designed MOF architectures can efficiently stabilize the sulfur cathode, accommodate volume changes, and accelerate the conversion of sulfur intermediates. By improving electron/ion transport and suppressing polysulfide diffusion, MOFs substantially enhance the overall reversibility, rate capability, and long-term cycling stability of Li–S batteries.

In summary, this study confirms that MOF-based sulfur hosts represent a viable strategy for developing high-capacity, durable, and cost-effective next-generation energy-storage systems. The insights gained here may further guide the rational design of multifunctional MOF composites tailored for advanced electrochemical applications.

Acknowledgement

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SESSION 4 INORGANIC CHEMISTRY

Half-sandwich type coordination compounds of ruthenium and osmium with 8-hydroxyquinoline derivates

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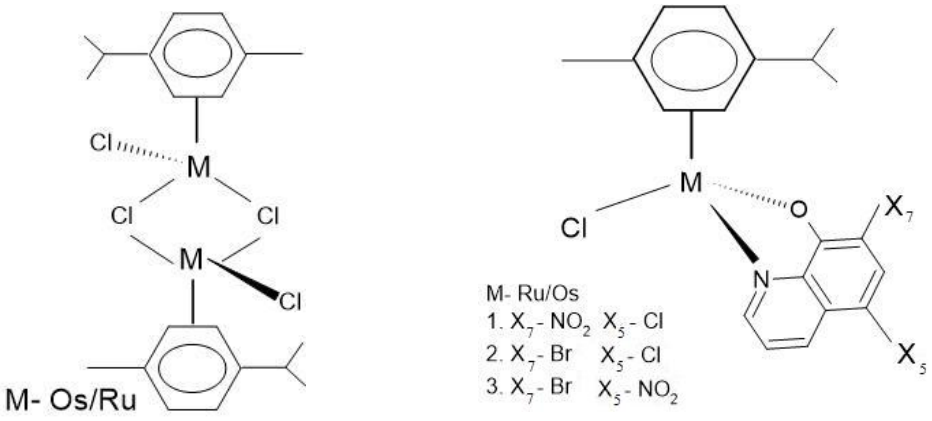
P-cymene is a naturally occuring compound as the major component of essential oils of plants of species *Protium heptaphyllum* and a biological precursor of carvacrol. It´s included in the group of monoterpens with known antioxidant effect. Coordinating chemical compounds including *p-cymene* with a ruthenium center represent a new group of compounds with possible antitumor activity. The reason behind this statement lies in the discovery of the complex [(η^6-*p-cymene*)Ru(*pta*)Cl_2] (*pta* - 1,3,5-triaza-7-fosfaadaamantane) also known as RAPTA-C, which exhibits lower toxicity and a different action mechanism as traditional platinum based anticancer drugs. Based on the structural type of this compound, many other compounds with various types of ligands have been prepared and studied with similarly promising properties.[1] Synthesis of these half-sandwich type compounds starts from the [Ru(η^6-*p*-cymene)(μ-Cl)Cl]$_2$ dimer shown in **Figure 1 a.)**, which can be obtained in different halogenated forms such as bromine an iodine but also with different central atoms such as osmium. Based on the result of our research in the CSD database we found that we would like to prepare new compounds including 8-hydroxyquinoline derivates. The derivates include 5-chloro-7-bromo-8-hydroxyquinoline; 5,7-dijodo-8-hydroxyxyquinoline; 5-chloro-7-nitro-8-hydroxyxyquinoline and 5-nitro-7-bromo-8-hydroxyxyquinoline. From the ruthenium and osmium dimers we prepared six compounds shown in **Figure 1 b.)** by adding the corresponding ligands to dichlormethane in the Monowave 300 microwave reactor. [2] The structure of **[Ru(*5-Cl,7-NO_2Q)(cym)*Cl], [Ru(*5-Cl,7-BrQ)(cym)*Cl], [Ru(*5-NO_2,7-BrQ)(cym)*Cl], [Os(*5-Cl,7-NO_2Q)(cym)*Cl], [Os(*5-Cl,7-BrQ)(cym)*Cl]** and **[Os(*5-NO_2,7-BrQ)(cym)*Cl]** has been confirmed using infrared spectroscopy, CHN elementar analysis, mass spectrometry and ^{1}H NMR spectroscopy. [3]



a.) **b.)**

Figure 1 Structures of the a.) dimers and b.) compounds.

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SESSION 4 INORGANIC CHEMISTRY

Use of silver compounds with potential biological activity in local therapy using creams and gels

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Silver compounds represent a promising alternative for the treatment of infections caused by pathogenic microorganisms in view of the growing problem of bacterial resistance. The toxicity of silver toward bacterial cells has long been recognized, whereas its toxicity to humans appears to be relatively low, which is one of the main advantages of silver compared to other medically relevant metals [1]. Moreover, in recent decades, silver complexes have attracted considerable attention as potential anticancer agents, since complexes containing various types of ligands have demonstrated selective activity against different cancer cell lines [2]. The most common pharmaceutical dosage forms designed for topical application to the skin or mucous membranes are semisolid formulations, such as gels and creams. Their advantages include self-administration, non-invasiveness, and a reduced incidence of adverse reactions compared to other dosage forms. At the same time, they provide a suitable environment for the penetration of active substances into the skin [3].

In our experimental work, we prepare stable complexes of selected ligands with silver ions, which are expected to exhibit structural and other physicochemical properties suitable for the evaluation of biological activity, particularly antibacterial and anticancer effects. For characterization of prepared complexes infrared spectroscopy and X-ray analysis are used. These complexes are subsequently incorporated into semisolid pharmaceutical formulations, such as creams and gels, intended for topical application to the skin, with the aim of utilizing their biological activity directly at the site of action. The evaluation of these prepared creams and gels includes organoleptic assessment (colour, odor) and phase separation. Spreadability testing and pH measurement are evaluated at three different time intervals to assess their stability: on the day of preparation, after two weeks, and after one month. As a next step in our research, we will focus on evaluating the biological activity of prepared creams and gels, with emphasis on their potential antibacterial and anticancer effects for local therapeutic applications.

Acknowledgements

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Enhancing CO_2 and H_2 Adsorption in MIL-101(Cr) via Polyethyleneimine Functionalization

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Various porous materials are studied nowadays across many fields of research to offer a solution to the modern world problems such as energy storage, fossil fuels replacement, the greenhouse gas effect and many more. Among them, one of the most extensive groups includes metal-organic frameworks (MOFs). MOFs can deal with all the mentioned above and other issues due to their special structure, which generally includes metal ions or clusters linked with an organic segment creating pores. Once synthesized, MOFs can undergo modification to improve their sorption capacity or other features. One of the possibilities, dealing with gas adsorption, is finding a substance capable of adsorbing gas well and covering a pore surface of the MOF with the substance e.g. with a polyethyleneimine (PEI). This polymer shows very good ability for CO_2 capture even at low pressures or ambient temperature[1]. PEI also enhance pore structure and increases surface polarity, which is useful for H_2 adsorption.

In our work, we focused on one specific type of MOF - the MIL (Materials Institute Lavoisier) group and its post-modification to improve sorption capacities for H_2 and CO_2. We synthesized seven different MIL-101 materials with a structure of a 3D lattice and chose one of them for further study according to their sorption capacities. The one with the best overall results was MIL-101 containing chromium(III) ions in its metal clusters, and we modified it by PEI with three different monomeric units – 800, 1300 and 2000. The original material was modified by all three PEI polymers in four weight percentages 25%, 50%, 75% and 100% of PEI using methanol as a solvent.

All the materials prepared, and the original MIL-101(Cr) were characterised by IR spectroscopy, powder X-ray diffraction, volumetric N_2 adsorption @77 K, H_2 adsorption @77 K and CO_2 adsorption @273 K (see Figure 1). The results show that among the twelve modified samples, those containing 25 wt% PEI showed the best overall performance. In particular, the material modified by PEI 1300 at 25 wt% exhibited the highest surface area (S_{BET} = 1567 m^2/g). As can be seen in Figures 1d), e) and f), all 25 wt% samples demonstrate higher CO_2 sorption capacities than the unmodified material (see blue (d), orange (e) and light green (f) curve in Figure 1) and for 50 wt% the capacities are similar to the original material. Figures 1a), b) and c) show that modified materials with 25 wt% exhibited similar (PEI 1300) or worse (PEI 800 and 2000) H_2 sorption capacities. Other samples with MIL-101(Cr) modified by PEI with higher wt% exhibited sorption capacities worse than the original material in both cases.

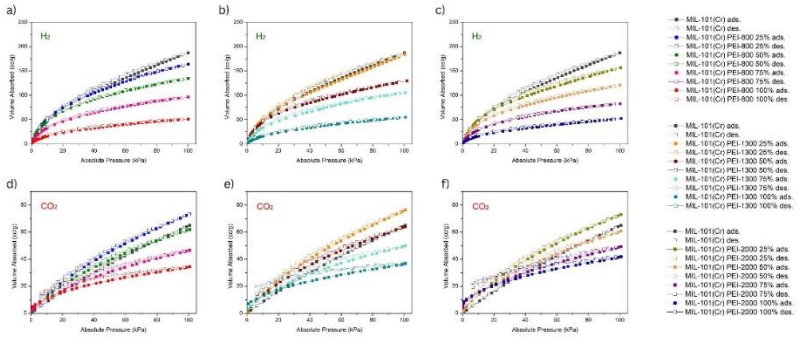

Figure 1 a) b) c) H_2 and d) e) f) CO_2 adsorption isotherms of prepared MIL-101(Cr) PEI modified materials.

Acknowledgements

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UiO-66-NH_2 as an adsorbent of anionic xenobiotics from aqueous environments

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In recent years, there has been growing interest in developing metal-organic frameworks (MOFs) for environmental applications. These porous structures represent a promising approach in battling pollution of aqueous matrices [1]. MOFs, also known for high porosity and large surface area, are networks that can be modified for specific applications. Our work focuses on applying zirconium-based MOF, UiO-66-NH_2, for heavy metal adsorption in water systems.

The UiO-66-NH_2 was synthesized via the solvothermal method and applied for metal ions adsorption from aqueous environment under varying conditions, e.g. mass concentration (50, 200 and 500 mg L^{-1}), *pH* (7, 5, 3) and UV irradiation (254 and 366 nm). The studied metals (manganese and chromium) in their anionic forms (MnO_4^-, CrO_4^{2-} and $Cr_2O_7^{2-}$) were selected due to their distinct colour in solution, which can be detected by UV/VIS spectroscopy. Applied methods of characterization were infrared spectroscopy, powder X-ray diffraction and ultraviolet and visible light spectrophotometry.

The infrared spectroscopy measured using the ATR technique, revealed characteristic bands of a primary amine at 3473 (ν_{as}(NH)) and 3376 (ν_s(NH)) cm^{-1}, the carboxylate was displayed at 1565 ($\nu_{as}(COO^-)$) and 1381 ($\nu_s(COO^-)$) cm^{-1}, in comparison with the starting material of 2-aminoterephthalic acid new signal was observed at 654 (ν(ZrO)) cm^{-1} which corresponds to the zirconium oxygen bond. Observed absorption bands are consistent with the literature describing UiO-66-NH_2 structure. The measured PXRD pattern aligned with the previously described record [2] with peaks at 7.40°, 8.55° and 25.70°, which correspond to (111), (200) and (600) crystal planes, respectively. The characterization was complete through the techniques mentioned above.

UiO-66-NH_2 has semiconductive properties due to its favourable band gap energy. The energy was determined from UV/VIS spectra by Tauc plot analysis. Both direct and indirect transitions were calculated with values being 2.82 eV and 2.52 eV, respectively. Arising from this fact, photocatalytic degradation of MnO_4^- was investigated. Adsorption capacity increased under 254 nm UV irradiation compared to no UV irradiation (see Table 1).

The pseudo-first and pseudo-second order models were applied to the obtained data with the aim of a better understanding of the adsorption kinetics. Determined values of the maximum adsorption capacity, i.e. capacity in equilibrium and corresponding rate constants, are shown in Table 1.

Table 1 Kinetic models.

	Pseudo-first order			Pseudo-second order		
	Q_{max} [%g^{-1}]	k_1 [min^{-1}]	R^2	Q_{max} [%g^{-1}]	k_2 [$g\,\%^{-1}\,min^{-1}$]	R^2
$pH = 3, t = 30\,°C, C_0 = 50\,mg\,L^{-1}$						
MnO_4^-	96.73	0.758	0.9991	97.05	0.0839	0.9991
CrO_4^{2-}	83.21	0.646	0.9784	84.08	0.0398	0.9795
$Cr_2O_7^{2-}$	89.09	0.463	0.9916	90.14	0.0215	0.9884
$pH = 5, t = 30\,°C, C_0 = 50\,mg\,L^{-1}$						
MnO_4^-	93.51	0.779	0.9996	93.85	0.0883	0.9996
CrO_4^{2-}	72.06	0.143	0.9813	79.46	0.00251	0.9531
$Cr_2O_7^{2-}$	56.58	0.321	0.9991	58.59	0.0125	0.9968
$pH = 7, t = 30\,°C, C_0 = 50\,mg\,L^{-1}$						
MnO_4^-	95.80	0.965	0.9996	95.78	0.430	0.9995
CrO_4^{2-}	58.57	0.332	0.9905	60.35	0.0137	0.9849
$Cr_2O_7^{2-}$	39.26	0.351	0.9639	39.91	0.0291	0.9493
without UV irradation, $pH = 7, t = 30\,°C, C_0 = 100\,mg\,L^{-1}$						
MnO_4^-	76.36	0.207	0.9965	82.62	0.00398	0.9847
$\lambda = 366\,nm, pH = 7, t = 30\,°C, C_0 = 100\,mg\,L^{-1}$						
MnO_4^-	89.94	0.440	0.9976	92.18	0.0145	0.9982
$\lambda = 254\,nm, pH = 7, t = 30\,°C, C_0 = 100\,mg\,L^{-1}$						
MnO_4^-	94.68	0.676	0.9996	95.15	0.0591	0.9992

After successful synthesis, characterization, and adsorption studies of anionic heavy metals MnO_4^-, CrO_4^{2-} and $Cr_2O_7^{2-}$, findings indicated that in acidic conditions, the adsorption was more efficient compared to neutral *pH* conditions. There was an evident correlation between decreasing *pH* and increasing adsorption capacity. Similarly, UV irradiation had an influence on the amount of adsorbate (MnO_4^-) left in solution. Decreasing the UV wavelength led to a reduction in the amount of anionic metal left in the aqueous phase.

Acknowledgements

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H_4MTA-Based MOF Material as Efficient Heterogeneous Catalysts for the Knoevenagel Condensation

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Advancing heterogeneous catalysis represents one of the central challenges in contemporary organic chemistry, with emphasis placed on sustainability, reusability, and high catalytic efficiency. The Knoevenagel condensation, as a fundamental carbon–carbon bond-forming reaction, finds broad application in the synthesis of pharmaceuticals, bioactive molecules, fine chemicals, and functional materials. Metal–organic frameworks (MOFs) have emerged as highly promising heterogeneous catalytic platforms. Their tunable structures, high porosity, and the ability to rationally design active sites make them ideal candidates for efficient and selective catalysis under relatively mild conditions [1].

In this work, a new gadolinium-based coordination polymer, **GdMTA**, was prepared utilizing the tetracarboxylate ligand **H_4MTA** as a structural building block. The compound was synthesized via a solvothermal procedure in a sealed glass vessel. The reaction mixture contained 0.045 mmol of $Gd(NO_3)_3 \cdot 6H_3O$, 0.09 mmol of H_4MTA, 6 mL of *N,N′*-dimethylformamide (DMF), and 2 mL of deionized water. The sealed 23 mL vial was heating to 80 °C, maintained at this temperature for six days, and cooled to room temperature. The process yielded orange, needle-shaped crystals of **$\{[Gd_4(MTA)_3] \cdot 6H_2O \cdot 3DMF\}_n$**. The product was isolated by filtration, thoroughly washed with DMF and acetone, and dried in an air stream. Comprehensive characterization was carried out using infrared spectroscopy (IR), thermogravimetric analysis (TGA), elemental analysis (CHN), and powder X-ray diffraction (PXRD).

The activated form of the catalyst, **GdMTA**, was subsequently employed in the Knoevenagel condensation between benzaldehyde and malononitrile, performed in toluene under varying temperatures. Reaction progress and product distribution were monitored by gas chromatography. The optimal catalytic performance was observed with a dosage of 100 mg of **GdMTA** at 100 °C, affording a maximum conversion of 95% with complete (100%) selectivity towards the desired product. Reducing the catalyst amount by half resulted in a decrease of conversion to 60%. Regeneration experiments demonstrated that **GdMTA** retains its catalytic performance upon reuse, with only a 22% drop in conversion after five consecutive reaction cycles. These findings highlight the remarkable combination of high efficiency, complete selectivity, and recyclability of **GdMTA**, underscoring its potential as a sustainable heterogeneous catalyst. The successful utilization of the **H_4MTA** tetracarboxylate linker in conjunction with gadolinium provides new opportunities for the rational design of lanthanide-based MOFs for environmentally friendly and efficient organic transformations.

Acknowledgements

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Schiff Base Stabilization of Ce(IV): Structure and Properties of *o*-vanillin-based Complexes

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The lanthanide elements most commonly exhibit the +3 oxidation state. In contrast, cerium readily interconverts between the +3 and +4 oxidation states, a feature widely utilized in redox chemistry and catalysis [1-3]. The stability of the Ce(IV) oxidation state arises from the noble gas configuration [Xe]4f^0 [4]. Cerium(IV) ammonium nitrate, a well-known compound with high redox potential, serves as a powerful one-electron oxidant in numerous inorganic and organic transformations [5].

A new neutral mononuclear Ce(IV) complex, [Ce(*o-van-pn*)$_2$] (**1**), has been successfully synthesized through aerial oxidation of a Ce(III) precursor, $CeCl_3 \cdot 7H_2O$, in the presence of the Schiff base ligand derived from *o*-vanillin and propane-1,3-diamine. The ligand, H_2(*o-van-pn*) = bis(2-hydroxy-3-ethoxybenzylidene)propane-1,3-diamine, was prepared by a simple condensation reaction and subsequently employed to stabilize the higher oxidation state of cerium. Complex **1** was comprehensively characterized by elemental and NMR analyses, infrared and UV-Vis spectroscopy, and single-crystal X-ray diffraction. Structural analysis confirmed the molecular nature of the compound, consisting of discrete [Ce(*o-van-pn*)$_2$] units in which the Ce(IV) central atom is octacoordinated by two deprotonated tetradentate Schiff base ligands, forming an O_4N_4 donor set.

The thermal stability of the complex was investigated by thermogravimetric analysis under both air and inert (N_2) atmospheres. The results showed that complex **1** remains stable up to approximately 260 °C, and the final decomposition product in air was identified as CeO_2. In contrast, thermal treatment under nitrogen led to a carbonization process, indicating a pronounced dependence of the decomposition pathway on the surrounding atmosphere. Electrochemical measurements using cyclic voltammetry revealed an irreversible Ce(IV)/Ce(III) redox process, consistent with the high stability of the Ce(IV) oxidation state in this coordination environment.

In addition to complex **1**, four structurally related Ce(IV) complexes with Schiff bases of analogous H_2L types: H_2(*o-van-en*), H_2(*o-van-dap*), H_2(*o-van-dmdap*) and H_2(*o-van-pen*) (*en* = ethylenediamine; *dap* = 1,2-diaminopropane; *dmdap* = 2,2-dimethyl-1,3-propanediamine; *pen* = 1,2- phenylenediamine) were synthesized and characterized by spectroscopic and analytical techniques. The results suggest formation of [Ce(L_2)] complexes analogous to complex **1**.

The present study thus contributes to the understanding of Schiff base stabilization of Ce(IV) centers and provides insight into the thermal and redox properties of these systems, which may be relevant for the development of redox-active coordination materials and hybrid inorganic-organic frameworks.

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A New Generation of Anticoagulants carriers: Nanosilica-Based Targeted Delivery of Apixaban

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Despite extensive research on stable and controlled-release drug systems, most new compounds show limited clinical success due to low bioavailability. Silica nanomaterials provide a biocompatible, porous platform ideal for efficient drug delivery. Porous SiO_2 nanoparticles possess large surface area, tunable pores and functional groups (–OH, $–NH_2$, –SH, –Cl) which significantly enhance its applicability and performance in various applications. Their chemical stability and compatibility render them suitable for biomedical applications [1]. Apixaban (APX) is an oral anticoagulant functioning as a selective and reversible inhibitor of coagulation factor Xa. It is commonly used to prevent and treat thromboembolic disorders such as atrial fibrillation, pulmonary embolism, and deep vein thrombosis. APX shows about 50% bioavailability, reaches peak plasma levels within 4 hours and has a 12-hour half-life, supporting twice-daily dosing [2].

The experimental design encompassed three synthesis stages, each with distinct aims and reaction conditions, focusing on improving drug encapsulation and release performance of SiO_2 nanocarriers. In the first synthesis, the primary objective was to establish optimal experimental conditions. Samples of SMS-APX containing 5, 25, and 50 mg of APX (with 250 mg of carrier) were prepared and compressed into tablets. The tablets were tested in 50 mL of physiological saline solution pH= 2 to simulate gastric conditions and pH= 7 to stimulate blood. Fraction samples were collected at defined time intervals (0–120 h) to monitor the release kinetics of the active pharmaceutical ingredient.
The second synthesis focused on optimizing key parameters, particularly the volume of the release medium and the form of drug administration. Selected impregnated samples (SMS-APX, SMS-SH-APX, SMS-NH_2-APX, SMS-Cl-APX; 50 mg each) were directly dispersed into the solution without tablet formation. The release studies were performed in two series using 400 mL of physiological saline solutions at pH= 2 and pH= 7.
In the third synthesis, once the optimal parameters had been determined, the focus shifted to evaluating potential toxicity and release dynamics. This stage aimed to estimate safe and effective dosage levels and assess the risk of possible overdosing under simulated physiological conditions. Precisely 50 mg of SMS-APX was dispersed into 400 mL of distilled water adjusted to pH= 2 and pH= 7. Fraction samples were collected at fixed time intervals, following the same procedure as in previous syntheses. Unlike the earlier experiments, an additional 50 mg of SMS-APX was introduced after 72 hours, and the sampling procedure was repeated. After another 72 hours (approximately 145 hours from the start of the experiment), a third portion of 50 mg SMS-APX was added, followed by continued sampling to observe the cumulative release profile over time.

Acknowledgements

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Study of interactions between MIL-101(Cr) and MIL-101(Cr)-NH_2 with drug metabolites: Potential for environmental applications

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The global lack of access to drinking water affects approximately one-third of the world's population.. Water pollution from toxic inorganic, organic, and biological contaminants, such as heavy metals, dyes, detergents, pesticides, antibiotics, pharmaceuticals, and their metabolites poses serious risks to humans, fauna, and flora. Although purification techniques such as filtration, precipitation, coagulation, electrochemical treatment, membrane separation, oxidation, photocatalysis, and ozonation exist, adsorption using nanomaterials has recently proven highly effective. Among them, metal-organic frameworks (MOFs), porous crystalline materials composed of metal nodes and organic linkers show great potential for pollutant removal, as well as for energy storage, drug delivery, photocatalysis, and greenhouse gas capture [1].
Our research focuses on MIL-type of MOFs, specifically MIL-101(Cr) and its amino-functionalized form MIL-101(Cr)-NH_2, synthesized solvothermally using 2-aminoterephthalic acid as the organic ligand. The materials were characterized by FTIR, PXRD, TGA, and nitrogen adsorption/desorption analyses, determining BET surface areas of 2655.99 m^2/g for MIL-101(Cr) and 1928.88 m^2/g for MIL-101(Cr)-NH_2. Adsorption experiments were performed with model solutions of drug metabolites-resorcinol, salicylaldehyde, and 3-hydroxybenzoic acid at concentrations of 31,25;62,5;125;250;500 mg/L, using 10 mg of adsorbent in 50 mL of solution stirred for 24 h at laboratory temperature. Adsorbed amounts were determined by UV-VIS spectrophotometry, and adsorption isotherms were fitted to the Langmuir, Freundlich, Temkin, Redlich–Peterson, and Henry models. For MIL-101(Cr), adsorption of 3-hydroxybenzoic acid and salicylaldehyde followed the Redlich–Peterson model, describing systems between homogeneous and heterogeneous adsorption, with maximum adsorption capacities (Q_{max}) of 183,3 mg/g and 232,2 mg/g, respectively. MIL-101(Cr)-NH_2 exhibited a multilayer chemisorption mechanism best described by the Freundlich model, with Q_{max} values of 203,4 mg/g for 3-hydroxybenzoic acid and 179,8 mg/g for salicylaldehyde, indicating surface heterogeneity. Resorcinol adsorption on MIL-101(Cr) fitted the Temkin model, where adsorption heat decreases linearly with surface coverage, reflecting adsorbate interactions and a transition between physisorption and chemisorption, with a Q_{max} of 310,3 mg/g. For MIL-101(Cr)-NH_2, resorcinol adsorption followed the Henry model, corresponding to linear adsorption at low concentrations and low surface coverage.

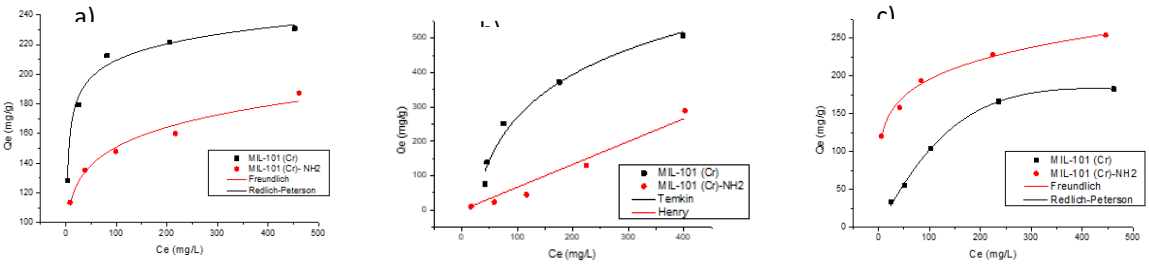

Figure 1 Adsorption isotherms of solutions: a) salicylaldehyde b) resorcinol c) 3-hydroxybenzoic acid.

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Amino-Functionalized MIL-101(Al)-NH_2 as a Multifunctional Carrier for Light-Activated Antibacterial and Immune Therapy

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The emergence of multidrug-resistant bacteria necessitates alternative strategies that combine antimicrobial and immunostimulatory actions. This study explores the amino-functionalized metal–organic framework MIL-101(Al)-NH_2 as a nanocarrier for penicillin G (PEN) and hypericin (Hyp), evaluating its physicochemical properties, drug release, immunomodulatory activity, and antibacterial efficiency under photodynamic therapy (PDT).

Comprehensive characterization confirmed the successful encapsulation of PEN and Hyp while preserving the MIL-101 topology. FT-IR spectra revealed PEN-specific carbonyl vibrations at 1684 cm^{-1} and minor Hyp contributions, whereas PXRD patterns verified structural integrity after loading. Nitrogen adsorption indicated a reduction in surface area from 1570 to 1140 $m^2\ g^{-1}$ and pore volume from 0.92 to 0.68 $cm^3\ g^{-1}$, confirming pore occupation by both drugs. Thermal analysis demonstrated high stability up to 120 °C and loadings of 10 wt% PEN and 0.02 wt% Hyp.

Release experiments in physiological saline supplemented with fetal bovine serum (FBS) revealed distinct mechanisms for both drugs. Hypericin exhibited rapid FBS-triggered liberation, reaching ~80% within 6 h and nearly complete release after 24 h, following a super case-II kinetic model driven by protein interactions. In contrast, PEN displayed a biphasic, diffusion-controlled release reaching 60% after 24 h, consistent with hydrogen bonding between the carboxyl and amino groups of PEN and the framework.

The in vivo immunomodulatory effects were examined using a quail chorioallantoic membrane (CAM) model. MIL-101(Al)-NH_2 and its composites showed high biocompatibility, with no embryo mortality and visible fluorescence confirming tissue internalization. Gene expression analyses revealed increased interferon-α (IFN-α) levels, confirming an intrinsic immunostimulatory response, while Hyp-containing systems upregulated VEGF-A and Quek1, suggesting pro-angiogenic and tissue-regenerative activity.

Under bacterial infection, Hyp- and Hyp/PEN-loaded MIL-101(Al)-NH_2 induced strong immune activation and antibacterial effects upon light exposure. Although Gram-negative *E. coli* remained resistant, Gram-positive *Staphylococcus epidermidis* showed pronounced susceptibility. Upon irradiation (590 nm), PDT with Hyp or Hyp/PEN significantly reduced bacterial colonies, outperforming free PEN and chloramphenicol controls. Co-delivery of Hyp and PEN effectively overcame bacterial resistance to PEN, confirming synergistic enhancement via ROS-mediated damage and antibiotic activity.

In summary, MIL-101(Al)-NH_2 serves as a multifunctional nanoplatform with high stability, biocompatibility, immunostimulatory potential, and photodynamically enhanced antibacterial action. The synergistic Hyp/PEN system offers an efficient route to combat antibiotic resistance and infections associated with medical implants. These findings demonstrate the promise of MOF-based therapeutics that integrate immune activation, controlled drug release, and light-triggered antibacterial mechanisms.

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Design and Characterization of Cysteine-Modified UiO-66(Zr)-NH_2 for Enhanced Bioconjugation and Targeted Delivery

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Infectious diseases are on the rise every year and challenge the readiness of scientists. It is therefore important to be prepared for these problems right from the start of an outbreak. For example, the last coronavirus disease pandemic in 2019 affected more than one hundred million individuals and had dramatic consequences for society, public health and the economy [1]. Prevention, early detection and targeted treatment are three important principles that take centre stage in emergency intervention.

Among the promising approaches are modular nanoparticles, which combine versatility, multifunctionality and the ability to enable real-time monitoring of therapeutic efficacy. This group of nanoparticles also includes a metal–organic framework (MOF) material, specifically UiO-66(Zr)-NH_2 — a highly stable and biocompatible porous material composed of zirconium clusters linked by 2-aminoterephthalate linkers. The advantages of UiO-66(Zr)-NH_2 are small size, chemical stability, catalytic properties and high drug loading capacity. Its key benefits include a high surface area and amine functional group for surface modification, suitable for targeted drug delivery and subcellular transport [2]. Previous studies had confirmed its potential in anti-inflammatory treatments and wound healing. Recently, it was demonstrated that MIL-101(Al) can be used for antiviral drug delivery, immobilisation of spike protein and applied in bioimaging and antibacterial photodynamic treatment [3].

This work focuses on the synthesis and characterization of material UiO-66(Zr)-NH_2 modified with cysteine molecules to enable subsequent functionalization with proteins via disulfide interactions. This approach aims to improve the material's ability to interact with biological molecules and cells, which may ultimately improve targeting efficiency as well as biocompatibility.

The basic material UiO-66(Zr)-NH_2 was carried out by the solvothermal method, where precursors were zirconium chloride and 2-aminoterephthalic acid. The subsequent surface modification with cysteine molecules was achieved through the formation of an amide bond between amine group of MOF and carboxyl group from cysteine. The prepared compounds were analysed by available physicochemical methods, specifically by using infrared spectroscopy, powder X-ray diffraction analysis, argon adsorption/desorption and thermogravimetric analysis. Infrared spectra and argon adsorption/desorption measurements confirmed successful cysteine bonding to the framework, while PXRD data showed that the crystallinity and structural integrity of MOF remained intact after modification. The results from thermogravimetric analysis showed that materials are stable up to 400 °C, corresponding to the decomposition of the organic linker and quantified the bound cysteine at 22.6 mg g^{-1}.

Acknowledgement

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Copper(II) Complexes Based on 1,2,4-Triazoles: Design and Characterization

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Schiff bases, characterized by the presence of an imine group, are attractive due to their simple preparation and remarkable ability to coordinate with various transition metal ions, exhibiting outstanding chelating properties. In terms of stability, aromatic Schiff bases are more stable than their aliphatic counterparts and exhibit a wide range of biological and industrial applications, including anticancer, antioxidant, antibacterial, antiviral, and anti-corrosion activities [1]. Their versatile chemical properties make them important ligands in coordination chemistry and material science [2].

Complex formation involves the binding of a *d*-block metal ion to electron-donating atoms within the ligand, which changes the metal's steric and electronic environment. This interaction enhances the stability of the metal ion and helps control its reactivity, especially for ions that are less stable in higher oxidation states. Common donor atoms in such coordination include nitrogen, oxygen, or sulfur [3]. 1,2,4-Triazole and its derivatives are versatile multi-nitrogen donor ligands that coordinate first-row transition metals in mononuclear or polymeric complexes [4].

Newly synthesized Schiff base ligands, formed via the condensation of 4-amino-3,5-di-2-pyridyl-4*H*-1,2,4-triazole (abpt) and methoxy derivatives of salicylaldehyde, specifically 2-hydroxy-3-methoxybenzaldehyde (*L1*), 2-hydroxy-4-methoxybenzaldehyde (*L2*), and 2-hydroxy-5-methoxybenzaldehyde (*L3*), were subsequently used for the synthesis of complexes with a central Cu(II) atom. The prepared complexes $[Cu(L1)_2](NO_3)\cdot H_2O$ (**1**) (Figure 1), $[Cu(L2)_2]\cdot 2MeOH$ (**2**) and $[Cu(L3)_2]$ (**3**), were characterized by IR spectroscopy, elemental analysis, and mass spectrometry. In all cases, the products were crystalline, which made it possible to study their structures by X-ray structural analysis. All complexes were studied in terms of their stability using UV-Vis spectroscopy.

Such types of ligands also represent potential candidates for use as metalloligands in the preparation of complexes containing not only 3*d* but also 4*f* metals, which opens up further possibilities for their application.

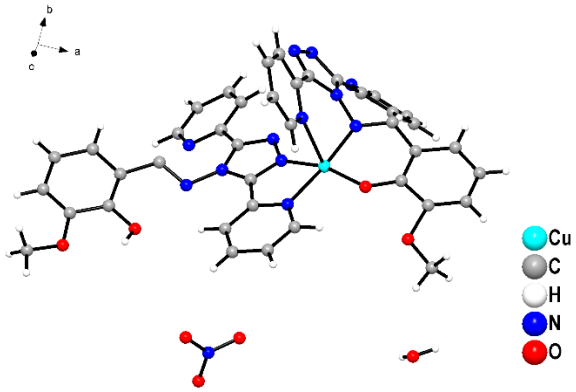

Figure 1 Crystal structure of (**1**).

Acknowledgement

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Design, synthesis, characterision and photovoltaic application of CdTBDTA

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Metal–organic frameworks (MOFs) have emerged as versatile crystalline materials with tunable pore architectures, high surface areas, and a broad spectrum of functional properties, making them attractive for applications ranging from gas storage and separation to catalysis and optoelectronics. Within this family, azo-containing ligands hold particular interest due to their ability to undergo reversible trans–cis photoisomerization, enabling dynamic modulation of the framework's geometry and electronic structure in response to external light stimul. Moreover, multidentate azo-ligands can promote the formation of extended coordination networks with enhanced stability and distinct optoelectronic features. Such characteristics position azo-based MOFs as promising candidates for next-generation photovoltaic materials, where controlled light–matter interactions can be directly translated into improved energy conversion performance [1]. Herein, we report the hydrothermal synthesis of a novel cadmium-based MOF, **CdTBDTA**, along with its structural characterization, stability evaluation, and investigation of photovoltaic properties, highlighting its potential for solar energy applications.

The newly obtained porous coordination polymer $\{[Cd_3(TBDTA)_2]\cdot 6DMF\cdot H_2O\}_n$ (**CdTBDTA**), incorporating the tritopic carboxylate linker **H_3TBDTA**, was synthesized via a solvothermal reaction by dissolving 20 mg (0.029 mmol) of **H_3TBDTA** and 8.95 mg (0.029 mmol) of $Cd(NO_3)_2\cdot 4H_2O$ in 8 mL of *N,N′*-dimethylformamide (DMF). To this solution, 0.5 mL of distilled water was added, and the mixture was sonicated for 5 minutes to ensure complete dissolution of the reactants. The resulting homogeneous solution was sealed in a glass vial and heated at 80 °C for 4 days. After cooling to ambient temperature, the orange crystalline product was isolated by filtration, washed several times with DMF and acetone, and dried in an air stream. The yield of **CdTBDTA** was 86 % based on the initial molar amounts of the reactants. The obtained material was characterized by IR spectroscopy, thermogravimetric analysis (TGA), and powder X-ray diffraction (PXRD) measurements. PXRD analysis showed that **CdTBDTA** is highly crystalline in its fresh state (**CdTBDTA-AS**), but exposure to moisture causes gradual lattice degradation. Despite this sensitivity, the material demonstrates full structural regeneration upon re-exposure to the mother liquor, effectively restoring its original framework properties.

Acknowledgements

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Series of lanthanide-based MOFs as efficient sorbents for carbon dioxide capture

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Greenhouse gases represent one of the main causes of global climate change, with carbon dioxide being one of the most prevalent components. The development of efficient technologies for capturing and removing CO_2 from the atmosphere and industrial emissions is therefore essential to mitigate environmental damage. Metal-organic frameworks (MOFs), owing to their exceptional porosity, tunable modular structures, and versatile chemical functionalities, have emerged as promising materials for selective sorption of greenhouse gases. Particularly significant are MOFs that incorporate polydentate carboxylate ligands in their structure, forming stable and permeable networks with suitable active sites for gas capture [1]. Among these are lanthanide-based MOFs synthesized using azo-carboxylate tetratopic ligands such as **H_4MTA**, which, due to their unique properties and structures, find broad application in the sorption of gases like carbon dioxide.

In this study, we present the synthesis and detailed characterization of fourteen lanthanide-based metal-organic frameworks (**LnMOFs**) developed as efficient sorbents for carbon dioxide capture. The novel coordination polymers were prepared via solvothermal reaction between the tetratopic organic linker **H_4MTA** [2] (0.09 mmol) and lanthanide nitrates $Ln(NO_3)_3 \cdot xH_2O$ (0.045 mmol) in a mixed solvent system of *N,N´*-dimethylformamide and water (6:1 ratio) at 80 °C over seven days. This synthetic strategy yielded a complete series of stable $\{[Ln_4(MTA)_3] \cdot 7H_2O \cdot 9DMF\}_n$ **LnMTA** (Ln^{3+} = La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu) frameworks encompassing all stable lanthanide elements.

The sorption properties of **LnMTA** complexes were studied using CO_2 adsorption experiments. From the measured values, it follows that all lanthanoid MOFs exhibit a pronounced affinity for CO_2 adsorption at a pressure of 1 bar, with the highest capacity at 0 °C achieved by **TbMTA** (3.7 mmol/g), followed by **TmMTA** (3.2 mmol/g) and **EuMTA** (3.1 mmol/g). At an elevated temperature of 20 °C, the adsorption values decreased as expected; however, materials such as **GdMTA** and **TmMTA** still demonstrated relatively high capacity (2.3 mmol/g). The adsorption properties of **PrMTA** and **GdMTA** were further investigated at high pressures and temperatures of 0 °C, 10 °C, and 25 °C (see Figure 1). These results confirm the high potential of **LnMTA** for efficient CO_2 capture.

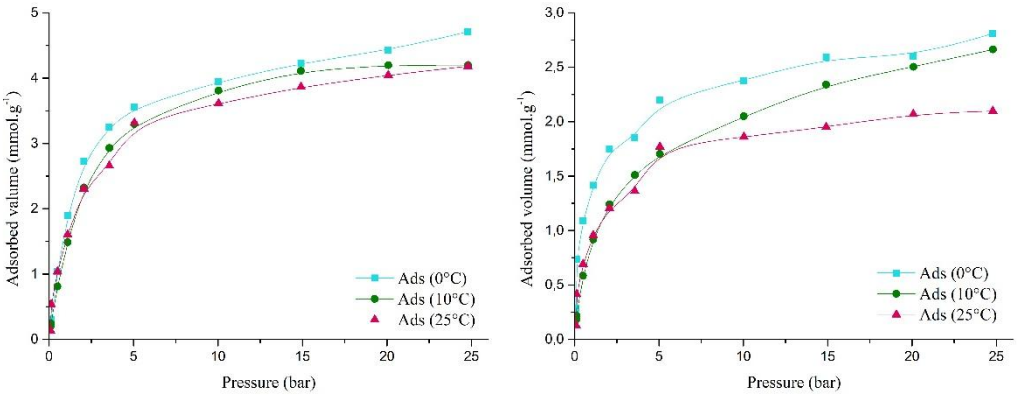

Figure 1 a) GdMTA - adsorbed valume of CO_2, b) PrMTA - adsorbed valume of CO_2.

Acknowledgements

This work was supported by VEGA 1/0058/25, 1/0442/25 and Funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V05-00008 (VVGS-2023-2923).

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New Azo-Based Multitopic Ligands for MOFs Construction

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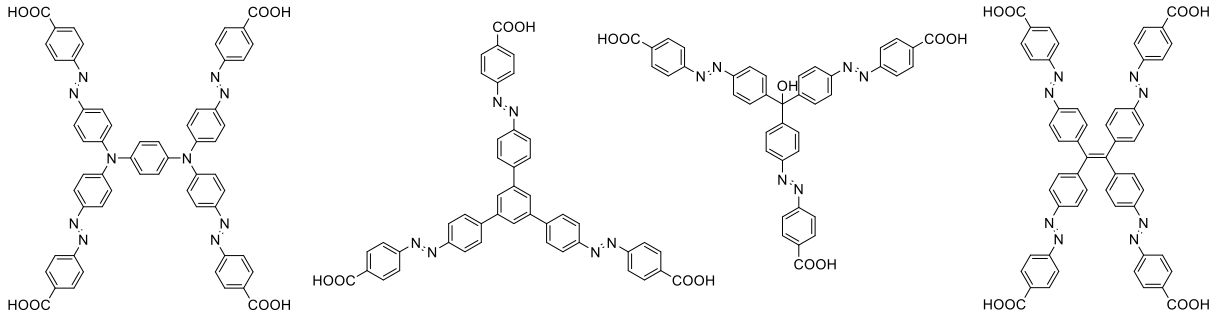
Metal–organic frameworks (MOFs) are among the most promising modern materials due to their high porosity, structural versatility, and broad application potential. Particular attention is given to systems based on multitopic azo-organic ligands, whose reversible photo- and thermo-induced isomerization enables modulation of the properties of the resulting structures. These ligands facilitate the formation of complex networks with unique functional characteristics and offer potential for the development of intelligent materials with adaptive behavior. The synthesis of such ligands represents a key step toward new generations of MOFs with expanded application scope [1].

In this work, we focused for synthesis of four new organic ligands (**H_4TAPPDA**, **H_3APTD**, **H_3MTATB-OH** and **H_4ETAN**) incorporating an azo linkage within their structure. All ligands were obtained through azo coupling via Mills condensation between the corresponding amine and ethyl 4-nitrobenzoate. The reactions were carried out under laboratory conditions in an inert dinitrogen atmosphere, employing methanol, acetic acid, or dichloromethane as solvents. The resulting ligands were successfully isolated and fully characterized by NMR and IR spectroscopy. These organic acids are currently being explored as building blocks for the design of novel MOF materials, with further results of this ongoing research to be presented.



H_4TAPPDA **H_3APTD** **H_3MTATB-OH** **H_4ETAN**

Figure 1 New Azo-Based Multitopic Ligands for MOF synthesis.

Acknowledgements

This work was supported by VEGA 1/0058/25, 1/0442/25 and Funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V05-00008 (VVGS-2023-2923).

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Silver(I) complexes with basic amino acids – their solution behaviour, solid state study and biological activity

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Until the discovery and invention of antibiotics, silver was one of the few medicines capable of treating infections, burns, wounds, as well as preventing contagious diseases. The introduction of antibiotics in the 20th century drastically reduced the use of silver in medicine, however nowadays, with the increasing resistance of bacteria to antibiotics, it is necessary to use other effective antimicrobial agents for treatment. Currently, there are many ways to treat infectious diseases and one of the advancing solutions is the production of silver-based materials, such as complexes. It has been confirmed that the selection of a suitable ligand is very important in silver(I) complexes. A properly selected ligand can ensure more stable structures and more effective biological properties of compounds. The amino acids, we used, have a high affinity for silver(I), occur naturally in the human body and are non-toxic [1]. Furthermore, silver(I) complexes of amino acids have attracted considerable interest because of their wide-ranging antimicrobial properties and a variety of binding modes [2].
In the present study we focused on the formation of silver(I) complex species in solution by potentiometric titrations in order to design the synthesis conditions. Our work was also focused on the synthesis of silver(I) complexes with basic amino acids *L*-lysine (Lys) and *L*-Arginine (Arg) and its derivatives. Prepared complexes were characterized by various physico-chemical methods, e.g. elemental analysis, infrared spectroscopy, structural analysis, thermal analysis and ^{1}H NMR spectroscopy. The crystal structure of complex $[Ag(H_2Lys)(NO_3)]NO_3$ (AgLys) is depicted in Figure 1. Moreover, the antimicrobial and anticancer activity of several complexes were also evaluated.

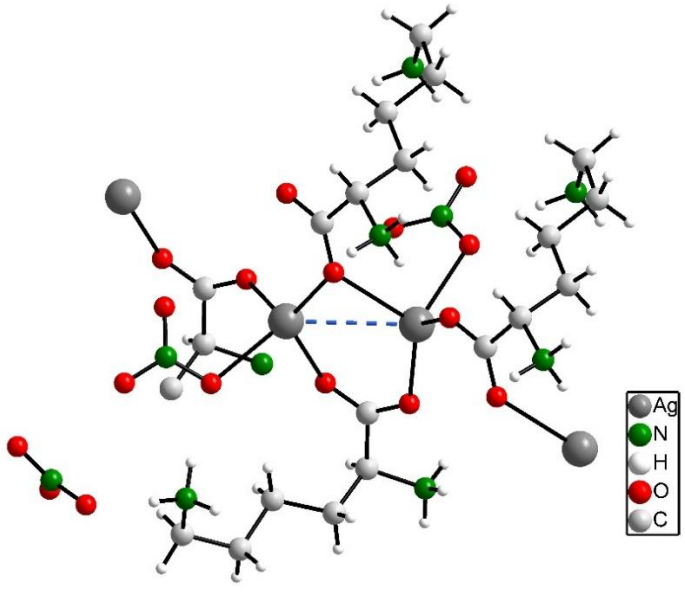

Figure 1 Crystal structure of complex $[Ag(H_2Lys)(NO_3)]NO_3$ (AgLys).

Acknowledgements
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Influence of Pore Hierarchy on the Catalytic Efficiency of Metal–Organic Frameworks HKUST-1 in Knoevenagel Condensation

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Metal–organic frameworks (MOFs) are hybrid crystalline materials composed of metal ions or metal clusters interconnected by organic linkers. Their exceptionally high specific surface areas, structural versatility, and tunable pore dimensions have made them prominent candidates for applications in heterogeneous catalysis [1].

In this study, two hierarchical porous materials, HKUST-1(A) and HKUST-1(B), were synthesized via a solvothermal approach employing different surfactant concentrations. Infrared spectroscopy confirmed the successful formation and activation of the frameworks as well as the efficient removal of the surfactant species. Nitrogen and argon adsorption/desorption analyses provided detailed insight into the porosity and textural properties of the materials. The templated synthesis route resulted in a significant enlargement of the pore dimensions compared to the parent HKUST-1, with pore diameters increasing from 0.9 nm to 8.5 nm. The isotherm profiles revealed that both HKUST-1(A) and HKUST-1(B) possess a combination of micro- and mesopores, with BET surface areas of 1687 $m^2 \cdot g^{-1}$ and 1554 $m^2 \cdot g^{-1}$, respectively.

The catalytic performance of the synthesized frameworks was evaluated using the Knoevenagel condensation of benzaldehyde with malononitrile as a model reaction. Systematic optimization of reaction parameters, including solvent, temperature, and catalyst loading, demonstrated that both materials exhibit pronounced catalytic activity. Furthermore, the influence of electron-withdrawing (Figure 1) and alkyl substituents in various positions relative to the carbonyl group was investigated, providing deeper insight into substrate–catalyst interactions. Notably, HKUST-1(B) consistently exhibited superior catalytic performance compared to HKUST-1(A), which can be attributed to its higher mesopore content, facilitating more efficient transport of reactants and products as well as improved accessibility of the active sites.

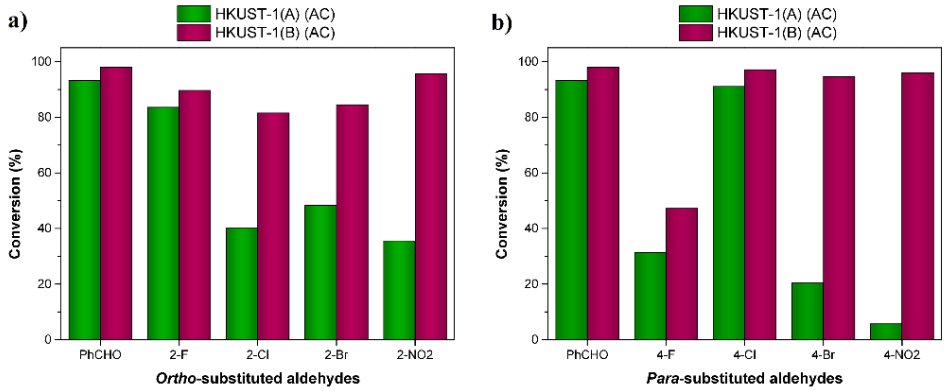

Figure 1 Comparison of conversion for reaction of benzaldehyde, a) *ortho*- and b) *para*-substitueted benzaldehydes with malononitrile using HKUST-1(A) (AC) and HKUST-1(B) (AC) as catalysts.

Acknowledgement

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Heterogeneous Catalysis of the A³-Coupling Reaction over HKUST-1: A Green Synthetic Approach to Propargylamines

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The A^3-coupling reaction represents a three-component condensation of an aldehyde, an amine, and a terminal alkyne to afford propargylamines (Figure 1). One of the major advantages of this transformation lies in its excellent atom economy, as all atoms of the substrates are incorporated into the final product except for a single water molecule released during imine formation. This characteristic minimizes the formation of by-products, making the reaction an environmentally friendly synthetic approach that is well aligned with the principles of green chemistry. Moreover, A^3-coupling reactions can often be performed under solvent-free conditions, at moderate temperatures (frequently even at ambient temperature), and in the presence of recyclable heterogeneous catalysts. Such reaction conditions not only reduce environmental impact but also facilitate product separation and catalyst recovery. Among the most promising catalytic systems for this transformation are metal–organic frameworks (MOFs) [1].
Metal–organic frameworks (MOFs) are crystalline materials composed of metal ions or clusters coordinated to organic ligands, forming porous three-dimensional networks characterized by high surface areas, tunable pore dimensions, and remarkable structural stability. Owing to their exceptional versatility, MOFs have found wide-ranging applications in gas storage and separation, catalysis, drug delivery, and sensing. Their unique structural features have attracted significant attention in the field of heterogeneous catalysis, primarily due to their highly customizable architectures, large surface areas, and well-defined pore networks [2].
This study focused on the A^3-coupling reaction catalyzed by the porous metal–organic framework HKUST-1. The reaction involved the coupling of paraformaldehyde, phenylacetylene, and either diethylamine or piperidine. In a typical experiment, 10 cm^3 of toluene, an internal standard (200 µl), paraformaldehyde (1.8 mmol), phenylacetylene (1.8 mmol), amine (1.8 mmol), and 50 mg of the catalyst were introduced into a reaction flask and heated to 120 °C. Upon completion, the catalyst was separated by centrifugation, and the resulting products were analyzed by gas chromatography.

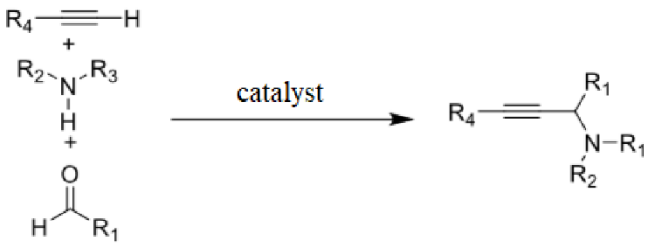

Figure 1 General scheme of the A^3-coupling reaction.

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Kinetic Adsorption Pathways of Co(II) and Congo Red on Pristine and Schiff Base–Modified MIL-101(Fe)-NH_2 Frameworks

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The study [1] explores the adsorption kinetics and mechanisms of heavy metal ions (Co(II)) and azo dye (Congo red) using pristine and surface-modified MIL-101(Fe)-NH_2 metal–organic frameworks. The modification was achieved through Schiff base formation with 2-pyridinecarboxaldehyde, yielding MIL-101(Fe)-Pyr, designed to enhance the material's adsorption properties via the introduction of pyridine functionalities and additional coordination sites. Comprehensive characterization by FTIR, TG/DTA, ss-NMR, XPS, PXRD, and N_2 adsorption–desorption analyses confirmed the successful functionalization, high surface area, and preservation of the MIL-101(Fe) framework after modification.

Kinetic investigations demonstrated that MIL-101(Fe)-Pyr exhibited superior adsorption capacity and faster uptake rates for Co(II) compared to unmodified MIL-101(Fe)-NH_2, achieving a maximum adsorption capacity of 5.67 mmol g^{-1} for Co(II) and 0.608 mmol g^{-1} for Congo red. The pseudo-second-order kinetic model best described the adsorption behavior for both pollutants, indicating a chemisorption-dominated process. Boyd's diffusion analysis suggested that external diffusion significantly influences the rate-controlling step, particularly during the initial adsorption phase.

Isothermal modeling using Langmuir and Freundlich equations confirmed monolayer adsorption predominance for Co(II) ions and heterogeneous multilayer adsorption for Congo red molecules. Thermodynamic evaluations revealed spontaneous and endothermic adsorption processes for both contaminants, with stronger and more stable coordination between Co(II) ions and pyridine nitrogen sites on MIL-101(Fe)-Pyr. The adsorption mechanism involves chelation and electrostatic interactions for Co(II) and a combination of electrostatic and π–π stacking interactions for Congo red, demonstrating the material's multifunctional adsorptive nature.

While MIL-101(Fe)-Pyr showed excellent initial adsorption performance, structural instability and partial amorphization after repeated adsorption–desorption cycles were observed, posing challenges for reusability. Nevertheless, the modified framework remains a promising candidate for single-use or short-cycle applications in wastewater treatment targeting heavy metal removal, while both pristine and modified MIL-101(Fe)-based materials perform effectively for dye adsorption.

These findings highlight the potential of Schiff base-modified MIL-101(Fe)-NH_2 frameworks as adaptable adsorbents for environmental remediation. Future research will focus on enhancing the structural robustness and recyclability of these materials to facilitate their transition toward practical, large-scale water purification systems.

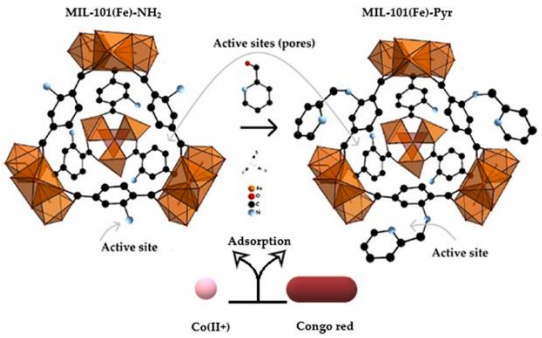

Figure 1 Schematic representation of the adsorption mechanism of Co(II) ions and Congo red dye on pristine MIL-101(Fe)-NH_2 and Schiff base-modified MIL-101(Fe)-Pyr.

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This work was supported by the project VEGA 1/0058/25 and SK-CZ-RD-21-0068.

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Simulated Two-Decade Ageing of Functionalized SBA-15: Insights into Structural Stability, Surface Chemistry, and Application Resilience

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The long-term environmental stability of mesoporous silica remains a critical yet often overlooked factor in its safe use as a drug delivery carrier. In this study [1], pristine and surface-functionalized SBA-15 materials bearing polar (amine (–NH_2), thiol (–SH), polyethylenimine (–PEI)) and non-polar (methyl (–CH_3), phenyl (–Ph)) groups were subjected to accelerated aqueous and soil ageing designed to simulate multi-year environmental exposure. Pristine SBA-15 exhibited a partial but significant porosity loss (S_{BET} decreased from 729 → 514 $m^2\ g^{-1}$), confirming gradual hydrolysis of the silica framework. Among functionalized samples, hydrophilic modifications were least stable: SBA-15-NH_2 lost over 60 % of its surface area after aqueous ageing, while SBA-15-PEI displayed an apparent 16 % increase due to polymer leaching. In contrast, non-polar modifications improved resilience, with SBA-15-CH_3 and SBA-15-Ph retaining 82 % and 76 % of their initial surface areas, respectively. Soil ageing introduced a more complex deterioration pathway involving ion exchange, mineral deposition, and adsorption of organic matter—processes that most strongly affected polar groups. Nevertheless, the amorphous silica matrix remained structurally intact, demonstrating intrinsic stability even under harsh exposure. These results confirm that surface functionalization critically dictates the long-term fate of mesoporous silica and that hydrophobic modifications markedly enhance environmental resilience. The findings highlight key design principles for sustainable mesoporous silica carriers: (1) Hydrophobic surface groups (–CH_3, –Ph) improve long-term stability and minimize degradation; (2) Polar functionalities (–NH_2, –PEI, –SH) should be incorporated selectively or shielded via hybrid coatings to maintain drug–carrier affinity; (3) Structural reinforcement, such as thicker pore walls or hierarchical porosity, may mitigate hydrolytic and ion-exchange degradation. This accelerated ageing study represents a "worst-case" scenario, with conditions intentionally intensified to simulate decades of environmental stress (25–30 °C; acid rain pH ≈ 5.0–5.6; variable soil composition). Despite these challenges, the silica framework preserved its integrity, confirming SBA-15 as a robust and environmentally compatible carrier platform. Future work will focus on correlating structural degradation with functional performance through molecular-scale studies using solid-state NMR, in situ FTIR/UV-Vis, and TEM–EDS mapping of aged, drug-loaded SBA-15 samples.

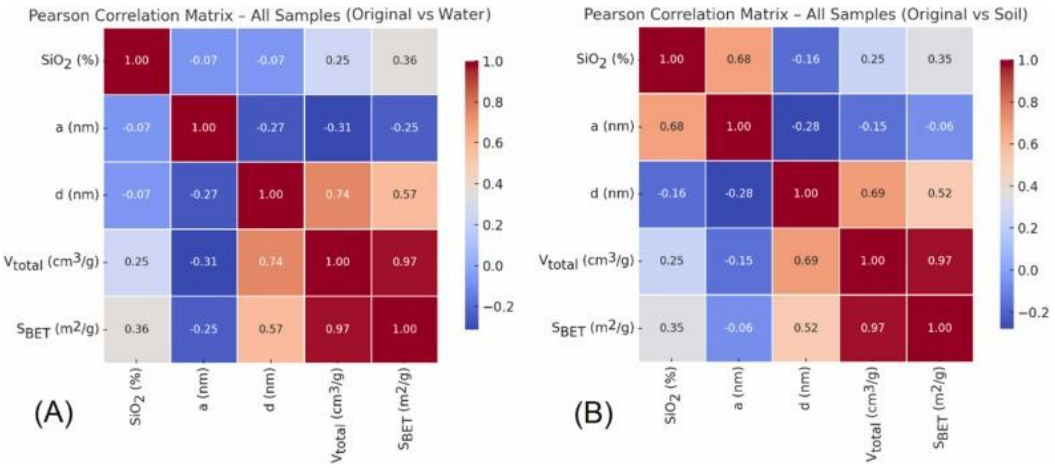

Figure 1 Pearson correlation matrixes showing the linear relationships between SiO_2 content (XRF), structural ordering (SAXS-derived lattice parameter), and nitrogen sorption-derived textural properties (modal pore diameter, total pore volume, and BET area) for SBA-15 materials exposed to A) water and B) soil (typical experimental uncertainties are ±3 % for textural parameters (S_{BET}, V_{total}, d, a) and ±4 % for elemental composition (SiO_2, XRF).

Acknowledgements

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Advanced MIL-101-Cr/Carbon Composite Systems for Targeted Delivery of 5-Fluorouracil and Pemetrexed

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In recent years, the development of advanced drug delivery systems has gained increasing attention as an effective strategy to enhance the therapeutic efficacy of anticancer agents while simultaneously reducing their systemic toxicity. A key aspect of these systems is the selection of an appropriate carrier that ensures high drug-loading capacity, stabilization of the active substance during transport, and controlled release at the target site of action. Metal–organic frameworks (MOFs) are considered promising drug carriers, as their tunable porosity, large surface area and flexible structure enable effective drug storage and subsequent controlled release [1]. In combination with hierarchically porous carbon materials, their stability, loading capacity, and biocompatibility can be further enhanced, resulting in composite systems with expanded functional properties [2].

In this study, a novel composite material was synthesized by integrating the chromium-based MIL-101-Cr framework into a hierarchically porous carbon monolith (MMM) using an in situ approach, which enabled the direct growth of the framework within the carbon structure [3]. The prepared composites were characterized using X-ray diffraction (XRD) (Figure1A), nitrogen adsorption–desorption measurements (Figure 1B) and scanning electron microscopy (SEM) (Figure 1C), confirming the successful formation and uniform distribution of the MOF phase while preserving the hierarchical porosity of the carbon support.

These composite materials were designed as potential carriers for anticancer drugs, specifically 5-fluorouracil and pemetrexed, with the aim of achieving high loading capacity and controlled, potentially pH-responsive release at the site of therapeutic action. Future work will focus on drug encapsulation studies and evaluation of release profiles under physiologically relevant conditions.

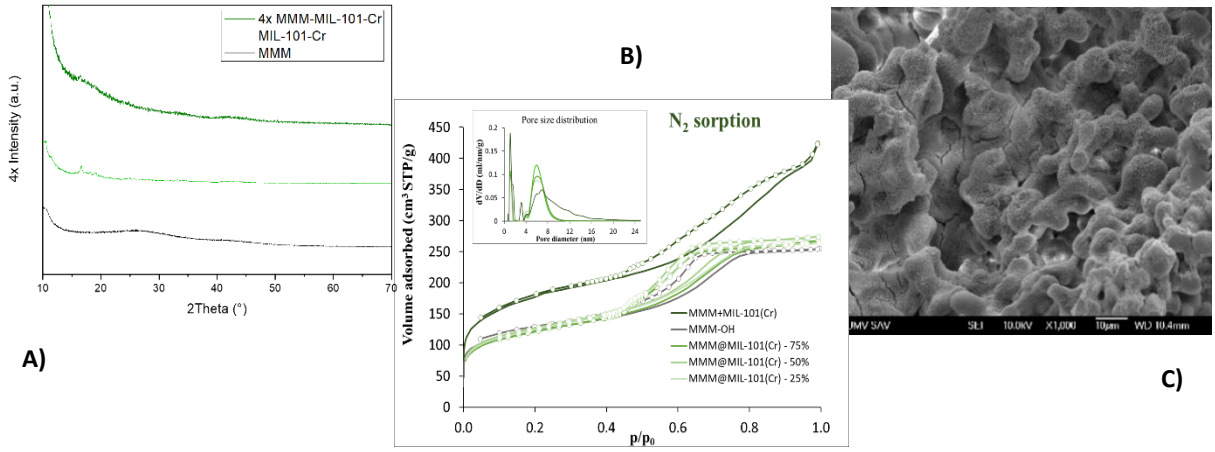

Figure 1 A) XRD results, B) N_2 (77K) sorption results and C) SEM analysis of composite MMM@MIL-101-Cr.

Acknowledgement

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Metal–organic framework composites for adsorption of volatile organic compounds

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Volatile organic compounds (VOCs) are a diverse group of organic chemicals with high vapor pressures (≥ 0.01 kPa at 20 °C) and low water solubility that easily evaporate under ambient conditions. They originate from both natural and anthropogenic sources such as industrial processes, vehicle emissions, solvents, paints, and household products. The presence of VOCs in the atmosphere represents a major environmental and health concern due to their toxicity, carcinogenicity, and role in the formation of tropospheric ozone and secondary organic aerosols. Chronic exposure to VOCs can lead to respiratory disorders, neurological damage, and increased cancer risk. Therefore, the effective removal of VOCs from air streams is a global challenge requiring efficient, selective, and regenerable adsorbent materials.[1,2]

Among various technologies developed for VOC abatement−such as catalytic oxidation, membrane separation, and absorption−adsorption is regarded as the most efficient and energy-saving approach. Conventional adsorbents, including activated carbon and zeolites, often suffer from drawbacks such as limited regeneration ability, structural instability, or poor performance under humid conditions.[3] In this context, metal–organic frameworks (MOFs) and their derived or composite materials have emerged as promising alternatives due to their exceptional surface area, tunable pore size, functionalizable surfaces, and high chemical and thermal stability.[4] Their hybrid organic–inorganic nature allows fine control over adsorption sites and the strength of host–guest interactions, enabling selective capture of VOCs with different chemical functionalities.

The aim of this work is to synthesize, characterize, and study MOFs (MIL-101(Cr), UiO-66) and MOF-based composite materials for the adsorptive removal of volatile organic compounds. The research will focus on designing hierarchically porous MOF–carbon composites combining the structural tunability of MOFs with the robustness of carbon matrices. Comprehensive physicochemical characterization (PXRD, SEM, BET, TGA, FTIR) will be performed to evaluate the structure properties and establish the relationship between structural features and adsorption behavior. Adsorption experiments using various representative VOCs (polar, nonpolar, aromatic, aliphatic, aldehydes) will be carried out to determine adsorption capacities, selectivity, kinetics, and regeneration efficiency under different conditions.

By systematically comparing the adsorption performance of different MOFs and their composites, this study aims to identify the most efficient and stable materials for practical VOC capture. The expected outcomes will contribute to understanding the adsorption mechanisms at the molecular level and provide a foundation for developing advanced adsorbents for air purification and environmental protection.

Acknowledgements

This work was supported by the Ministry of Education, Science, Research and Sport of the Slovak RepublicVEGA project no. 1/0058/25.

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Antibacterial Delivery of Cinnamic Acid and Cinnamaldehyde from SBA-15 and Coumarin-Modified Silica: Loading, Release and Efficacy

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Cinnamic acid and its derivative cinnamaldehyde are naturally occurring phenylpropanoids broadly distributed in plant sources such as cinnamon and balsam species. Both compounds display a wide spectrum of biological and pharmacological effects, including antioxidant, antimicrobial, anti-inflammatory, and anticancer activities. Their low cytotoxicity and biocompatibility make them promising candidates for applications in targeted and stimuli-responsive therapeutic systems [1,2]. Cinnamaldehyde and cinnamic acid have reported activity against implant-relevant bacteria (e.g., Staphylococcus aureus, Staphylococcus epidermidis, Pseudomonas aeruginosa), which motivates their evaluation as antibacterial payloads. To effectively utilize these bioactive molecules in controlled-release formulations, a suitable carrier matrix is required to ensure their stability and sustained delivery. Mesoporous silica SBA-15 represents an excellent platform for this purpose owing to its highly ordered pore structure, large surface area, and tunable pore volume, which enable efficient encapsulation and gradual release of small molecules [3].

Building upon this concept, our study focuses on the impregnation of cinnamic acid and cinnamaldehyde within a modified silica framework. The aim is to investigate their distribution, mutual interactions, the release behaviour and the resulting antibacterial performance against planktonic cells and surface-associated biofilms. In this work, the surface of SBA-15 was post-synthetically functionalized with coumaric acid following a procedure analogous to previously reported photo-responsive silica systems [4]. The modification introduces photoactive moieties capable of reversible [2+2] cycloaddition under UV irradiation. This light-induced transformation enables modulation of pore accessibility via dimerization and cleavage of cinnamic groups, thereby allowing reversible "open–close" control of molecular transport. Here, we leverage this platform primarily to modulate release profiles that govern antibacterial efficacy.

Subsequently, the pores were loaded with different molar ratios of cinnamic acid and cinnamaldehyde to investigate the effect of their composition on diffusion behaviour and release kinetics. Antibacterial activity will be assessed by broth microdilution MIC and implant-relevant biofilm assays on standard strains (e.g. S. aureus, S. epidermidis, P. aeruginosa), using both particle suspensions and released fractions to link chemistry to biological outcomes. The resulting hybrid materials will be characterized by different methods (FTIR, PXRD, SEM, TGA, adsorption/desorption measurements of N_2) to confirm the preservation of mesostructural order, successful surface grafting of cinnamic species, and the presence of organic functionalities within the silica framework. Release experiments (PBS, 37 °C) coupled to UV quantification of each payload will be correlated with MIC/MBIC values to identify compositions that maximize antibacterial potency.

The anticipated outcomes of this study are expected to contribute to the design of sustainable and biocompatible mesoporous carriers integrating natural therapeutic agents with external photo-control, offering a versatile platform for precision drug delivery and smart biomedical applications. We expect cinnamaldehyde-rich or mixed formulations to outperform single-agent systems, providing tunable and sustained antibacterial effects suitable for implant-associated infection mitigation.

Acknowledgements

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Synthetic approach to novel cyanoacetohydrazone derivatives of atranorin

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Lichens present pioneer organisms, which can live in extreme habitats. These symbiotic organisms can deal with very specific conditions of environment because they produce secondary metabolites, which provide them good protection against various negative physical and biological influences [1]. One of the most common lichen secondary metabolites is atranorin, which is characteristic of numerous lichen families. It belongs to the depsides group, consisting of two monocyclic aromatic units linked by ester bond. Atranorin exhibits number of biological activities including antioxidant, anti-inflammatory, analgesic, antiviral, antibacterial, antifungal, cytotoxic and immunomodulatory activities [2].

N-acylhydrazone pattern can be recognized in many bioactive molecules and stability of these compounds can be increased with aromatic substituents. A number of acylhydrazones show antimicrobial, antibacterial, haemostatic, anti-HIV, anti-inflammatory and cytotoxic activities [3,4].

We report synthetic approach to a novel aromatic cyanoacetohydrazones **3** derived from atranorin **1** (Figure 1). Using catalytic amount of acetic acid and ethanol as solvent, products of transesterification with ethanol **4** and **5** were isolated. However, aromatic cyanoacetohydrazones derived from compound **4** are also of interest. Atranorin used in these experiments was isolated from lichen *Stereocaulon grande* collected during a field trip in certain regions of Finland in September 2024.

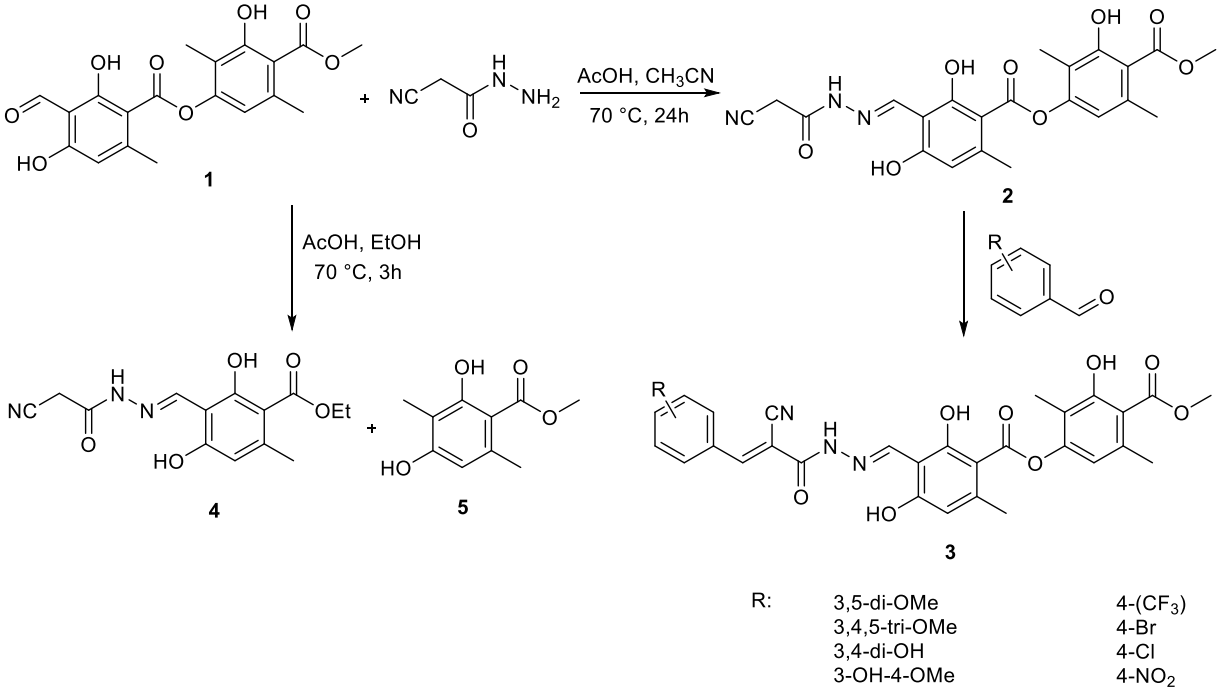

Figure 1 Synthetic approach to novel cyanoacetohydrazone derivatives of atranorin.

Acknowledgements

This work was supported by the KEGA 008UPJŠ-4/2023.

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Electrosynthetic Hydrolysis of Dihyhydropyrimidinones

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A central goal of modern chemistry is the development of novel, cost-effective biologically active compounds that enhance therapeutic efficacy while reducing or ideally eliminating adverse side effects. Notably, statistical analyses indicate that over 85% of known bioactive molecules contain heterocyclic frameworks [1]. Among the most versatile synthetic strategies for accessing such structures are multicomponent reactions (MCRs) [2]. Using the Biginelli MCR, we synthesized a dihydropyrimidinone (DHPM), which was subsequently modified electrochemically (Figure 1A). In particular, we accomplished the electrochemical hydrolysis of an ester group that has been reported to exhibit exceptional resistance toward hydrolytic attack [3]. Consistent with this literature precedent, our control experiment demonstrated that compound **1** remains remarkably stable under harsh basic conditions (pH > 14, 100°C, 48 h), with only approximately 1% ester cleavage observed.
To further understand this reactivity, the kinetics of the electrochemical hydrolysis of compound **1** (Figure 1A) were investigated by cyclic voltammetry across scan rates ranging from 25 to 150 $mV \cdot s^{-1}$.This analysis was performed in a three-electrode setup with a Pt working electrode, Pt counter electrode, and an Ag/AgCl (3 M KCl) reference electrode. At each scan rate, the oxidation peak current (I_p) was extracted for further analysis. The slope of the logarithm of the maximum current response (I_p) versus the logarithm of the scan rate (v) (Figure 1B, 0.566) close to 0.5 indicates that the studied process is controlled by diffusion [4].

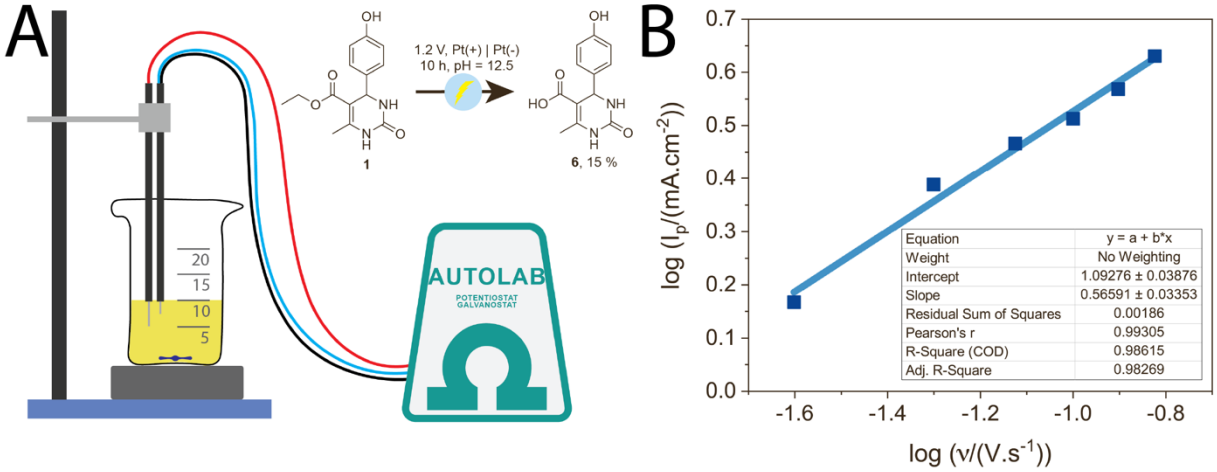

Figure 1 A) Setup and scheme of the electrochemical hydrolysis and B) the log of peak current (I_p) versus the log of the scan rate (v).

Acknowledgements

Part of the research results was obtained using the computational resources procured in the national project National competence centre for high performance computing (project code: 311070AKF2) funded by European Regional Development Fund, EU Structural Funds Informatization of society, Operational Program Integrated Infrastructure, and by the Grant Agency of the Ministry of Education, Science, Research and Sport of the Slovak Republic: KEGA Grant No. 008UPJS-4/2023.

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Synthetic Approach to 6-Bromo Derivatives of Indole Phytoalexins and Their Anticancer Profile

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1-Methoxybrassinin (**1**), 1-methoxyspirobrassinol methyl ether (**2**) and cyclobrassinin (**3**, Figure 1) belong to the class of indole phytoalexins produced by plants of the *Brassicaceae* family and are characterized by remarkable cytotoxic activity against various human cancer cell lines with IC_{50} values at the micromolar level [1]. A wide range of derivatives of these indole phytoalexins has been synthesized, and some structural modifications **4-7** (Figure 1) resulted in a significant increase in antiproliferative activity compared to parent molecule [2].
To expand the structure–activity relationship of this natural products class towards human cancer cells, we carried out another structural variation, and we have prepared a library of 6-bromoderivative of these indole indole phytoalexins (Figure 1). Novel 6-bromo-1-Boc-brassinin and its amino analogues **8** were synthesized from 6-bromo-1*H*-indole-3-carboxaldehyde using a four- or five-step procedure. The bromospirocyclization of derivatives **8** in the presence of various nucleophiles (methanol or a suitable aniline) has been applied to the synthesis of spirocycles **9**. Cascade reactions of the spirocyclic products **9** promoted by TFA led to the formation of 7-bromocyclobrassinin and its 2-amino analogues **10**. Several newly synthesized 6-bromoderivatives have shown potential as cancer treatments by inhibiting cancer cell growth [3].

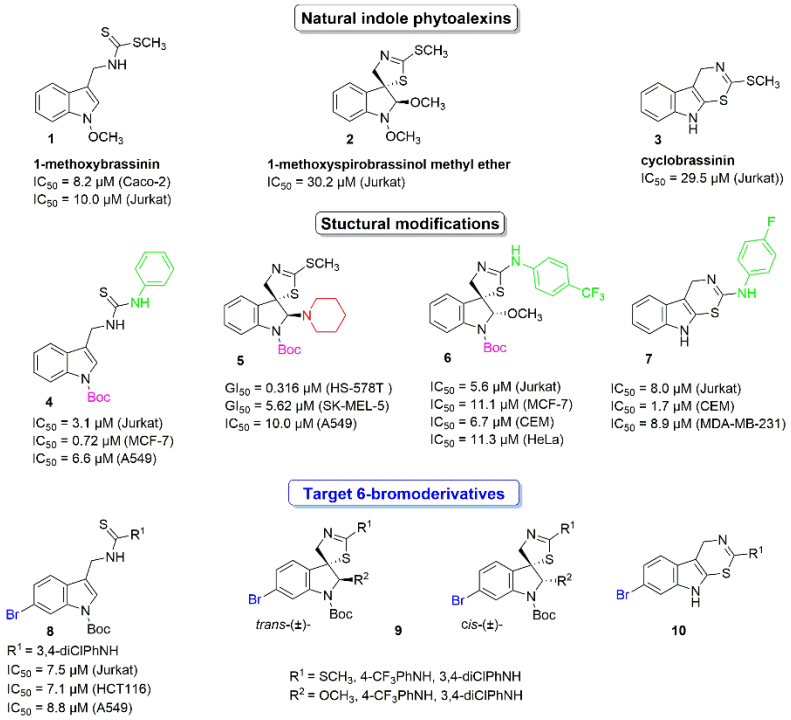

Figure 1 Natural indole phytoalexins and their structural modifications.

Acknowledgements

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Total synthesis of (–)-deoxoprosopinine and its analogues

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Nature has afforded a wide variety of piperidine alkaloids as secondary metabolites, which have been identified primarily in terrestrial plants. A remarkable subclass within this group, also referred as "alkaloid lipids" (AL), has been isolated from the stems, leaves, and roots of *Prosopis* and *Cassia* species. These molecules are characterised by a variably substituted long alkyl chain at C-6 and a polar C-2 hydroxymethyl substituted 3-hydroxypiperidine unit (Figure 1). In addition to their distinctive architecture, both natural AL and their synthetic analogues exhibit a broader spectrum of biological activities, including cytotoxic, antifungal, antibiotic, anesthetic, and stimulant effects. These interesting pharmacological findings have stimulated a number synthetic efforts, and several strategies and aproaches have been reported. [1,2,3]

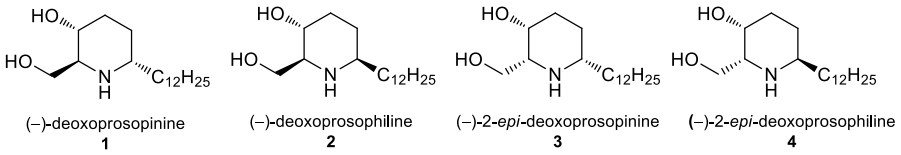

Figure 1 Structures of selected alkaloid lipids **1**–**4**.

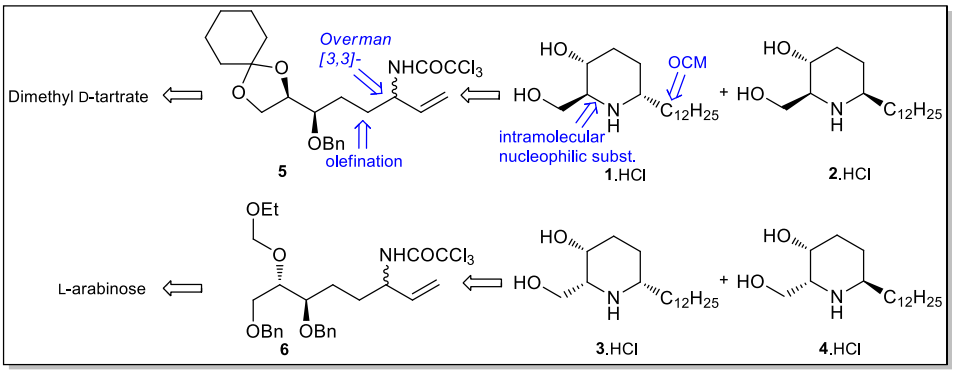

Figure 2 Retrosynthetic analysis of our target *C*-alkyl piperidines **1**.HCl–**4**.HCl.

A straightforward route to a small library of the stereoisomeric alkaloid lipids **1**.HCl–**4**.HCl starting from the advanced synthons **5** and **6**, was deveoleped. The core scaffolds were constructed *via* olefination steps, followed by an Overman rearrangement to introduce the novel stereochemistry. Formation of the piperidine ring was achieved through an intramolecular nucleophilic substitution, while the hydrophobic alkyl branche was installed at a later stage in the synthesis using olefin cross-metathesis. The prepared final compounds **1**.HCl–**4**.HCl are currently being evaluated for their *in vitro* antiproliferative activity on a panel of cancer cell lines.

Acknowledgements

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Molecular docking study of novel pyrrolidine derivatives as multi-target modulators

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Nowadays, the research about the biological potential of long-chain pyrrolidine derivatives has been attracted the scientists. In this work, we investigated a series of newly synthesized pyrrolidines. Specifically, MF-101, MF-HOV104, SR14, SS14, MA-201, TP3, TP5 and MA-20 were tested *in silico* using molecular docking and interaction energy analyses toward key protein targets involved in tumor growth, and lipid signaling: HER2 receptor [1], LDL receptor, sphingosine-1-phosphate phosphatase, LC3BI, cathepsin B, M6PR and protein kinase C (PKC) δ and α. All the docking calculations were conducted via Autodock software.

Docking simulations revealed favorable binding energies for several derivatives. Among these, MFHOV104 and TP5 showed the strongest and most consistent binding affinities. MFHOV104 exhibited favorable interactions with HER2 (-6.51 kcal/mol) and PKCα (-6.23 kcal/mol), while TP5 bound effectively to cathepsin B (-5.96 kcal/mol) PKCδ (–6.00 kcal/mol), and the LDL receptor (–5.68 kcal/mol). Overall, PKC isoforms, Cathepsin B, and HER2 emerged as key potential targets, whereas LC3B I displayed weak interactions across all compounds. These findings suggest that MFHOV104 and TP5 are the most promising candidates for further investigation. Initial *in vitro* studies should focus on confirming HER2 and PKCα inhibition by MFHOV104, and Cathepsin B and PKCδ inhibition by TP5, to validate their predicted biological activities.

Overall, these computational findings support the hypothesis that the tested pyrrolidine derivatives could act as multi-target modulators influencing key pathways in cancer [2]. The results provide a valuable framework for further *in vitro* validation and optimization of these compounds as potential anticancer agents.

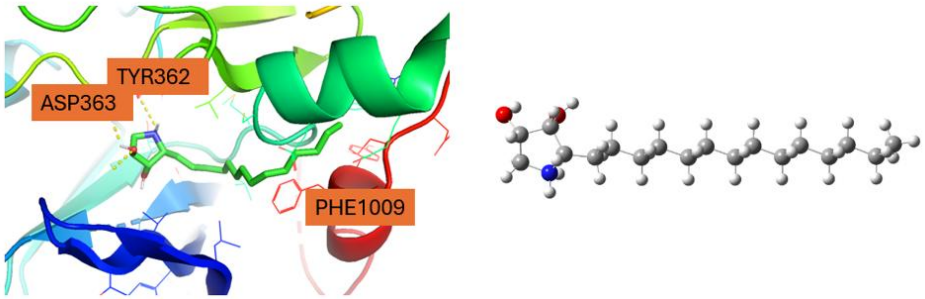

Figure 1 (left) Docking pose of MFHOV104 in HER2 receptor and (right) structure of MFHOV104.

Acknowledgements

The work has been supported by the project "Consortium for Advanced Protein Biotechnology: A Model to Support Economic Growth and Migrate Brain Drain from Eastern Slovakia" (APBC) funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09-I02-03-V01-00021 and the project BCOrgFluorIDA No. 09I03-03-V04-00007.

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Bis-Indole Analogues Derived from Indole Phytoalexins: Synthesis and Antiproliferative Profile

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Indole phytoalexins include a group of secondary metabolites biosynthesized de novo by plants of the family *Brassicaceae* in response to biotic or abiotic stress. These phytoalexins exhibit antimicrobial, antiobesity, anti-inflammatory, antidiabetic, antiatherosclerotic, and anticancer properties [1,2].
In this work, we prepared a small library of bis-indole compounds inspired by indole phytoalexins (Figure 1), which have the SCH_3 group replaced by another indole ring. We designed and synthesized novel bis-indole thioureas **I** with various combinations of substituents on the *N*-1 and *N´*-1 indole nitrogens as brassinin analogues. The cyclization protocol of thioureas **I** using methyl bromoacetate provided bis-indole thiazolidin-4-one derivatives **II**. The formation of the spiro center at carbon C-3 in bis-indole derivatives of spirobrassinin **III** was ensured by oxidative spirocyclization of thioureas **I** using chromium trioxide. A two-step process involving bromospirocyclization of thiourea **I** with methanol and TFA-induced rearrangement led to the formation of the bis-indole analogue of cyclobrassinin **IV**. Some novel bis-indole compounds have shown significant potential in reducing the growth of human cancer cells (HCT-116, MCF7, and A2780) to a greater extent than cisplatin.

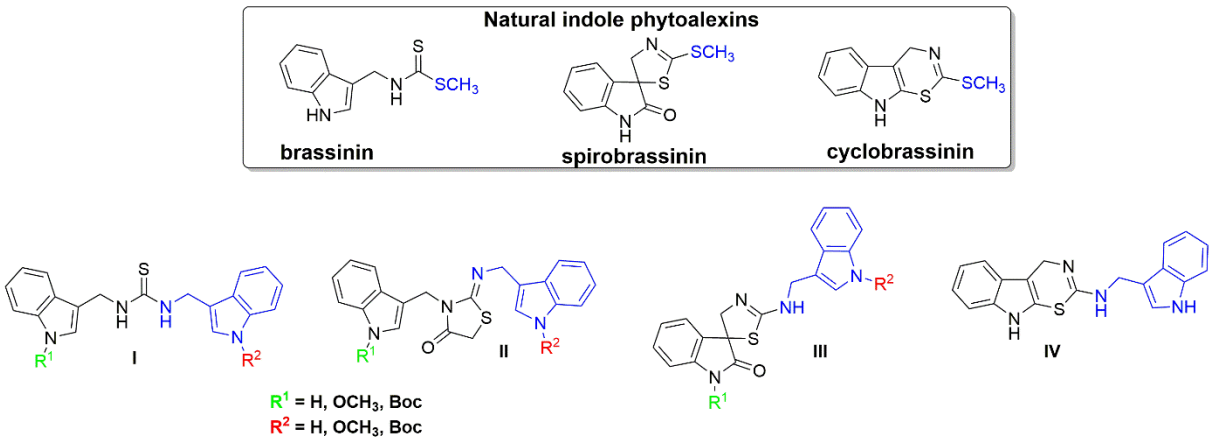

Figure 1 Bis-indole analogues derived from indole phytoalexins.

Acknowledgements

This research was funded in part by the Grant Agency of Ministry of the Education, Science, Research and Sport of the Slovak Republic (VEGA 1/0347/23 a VEGA 1/0037/22).

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Development of 2,9-disubstituted acridines as topoisomerase IIα inhibitors

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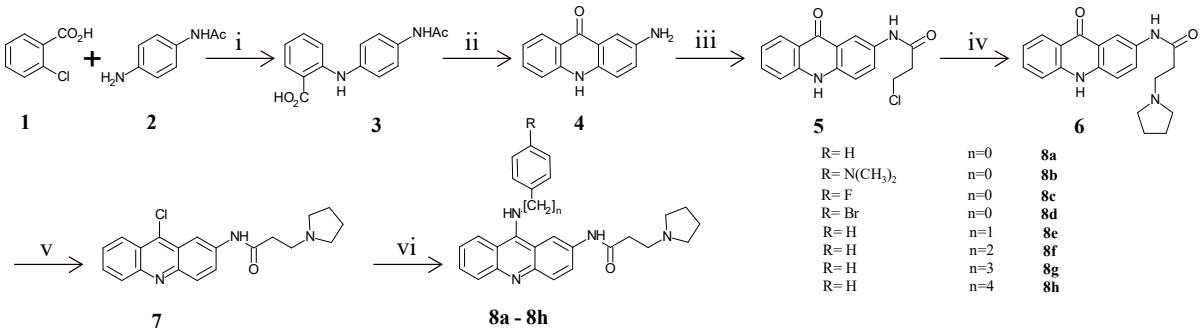
A series of 2,9-disubstituted acridines (8a–8h) was synthetized and assessed for their biological activities [1]. The acridines featured various 9-anilino or 9-phenylalkyl substituents and were prepared via a linear sequence of six steps using commercially available starting materials. The relationship between the physico-chemical properties of the 2,9-disubstituted acridines and their biological activity was studied, and the DNA binding capacities of the synthetized acridines were determined using spectroscopic (Kb 0.5–10.4 × 104 M-1) and thermal denaturation (Tm 4.2–9.8°C) methods. The inhibitory potential of acridines 8a–8h toward human topoisomerase I/IIα was evaluated, and 9-phenylbutyl acridine 8h was found to inhibit human topoisomerase IIα at concentrations as low as 5 μM. Acridines 8a–8h were also subjected to in vitro screening against selected cancer cell lines; the most potent anticancer activity was observed against melanoma A2058 cell lines at IC50 values ranging from 3 to 6 μM.



Reagents and reaction conditions. i: 2-ethoxyethanol, Cu(s), CuO, K_2CO_3, 130°C, 4h., 82%; ii: a.) 98% H_2SO_4, 100°C, 1h., b.) 50% H_2SO_4, 100°C, 1.5h., 60%; iii: 2-chloropropionyl chloride, 100°C, 1h., 68%; iv: pyrrolidine, KI, etanol, reflux, 3h., 86%, v: $POCl_3$, N_2(g), 100°C, 2h., 70%; vi: 4-R-Ph-(CH_2)n-NH_2, DMF, 110°C, 5h.

Figure 1 Sythesis of 2,9-disubstituted acridines **8a - 8h**.

Acknowledgements

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A simple approach to novel pyrrolidine-containing sphingomimetics

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Nature produces a wide variety of sphingolipid molecules with both open and cyclic structures. [1] An important point in the research on this lipid family in particular was the year 2002, when pachastrissamine **1** (Figure 1) was isolated from the marine organisms. [2] The findings regarding the strong cytotoxic profile of **1** have directed the attention of organic chemists toward the construction of its analogues. [3] The design of our novel compounds was inspired by the work of Génisson and co-workers [3], who prepared a series of pyrrolidines, the structure of which is illustrated by compound **2**. Over a period of five years, we successfully synthesised a small library of *C*-alkyl pyrrolidine-diols [4], some of which have proven to be very interesting in terms of their anticancer activity (Figure 1).

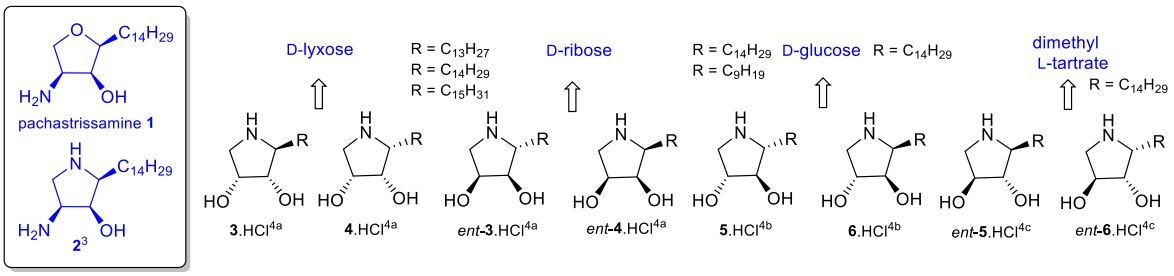

Figure 1 Pachastrissamine **1**, its analogue **2** and structures of our 2-*C*-alkyl pyrrolidine-3,4-diols.

The interesting results observed from the cytotoxic studies [4] of pyrrolidine-containing sphingomimetics (Figure 1) led us to the idea of extending the range of prepared cyclic sphingolipids by further derivatives **7**–**8** bearing the novel C-N bond in the side branch. As shown in our retrosynthetic analysis (Figure 2), the target pyrrolidines **7** and **8** were constructed by the alkylative cyclisation of open-chain intermediates **9** and **10**, respectively. These compounds were synthesised from amides **11** and **12** via a cross-metathesis reaction. We envision that diastereoisomers **11** and **12** could be obtained by the Overman rearrangement of an allylic template derived from ester **13**. The corresponding unsaturated system **13** is accessible from the known derivative **14**. [4a]

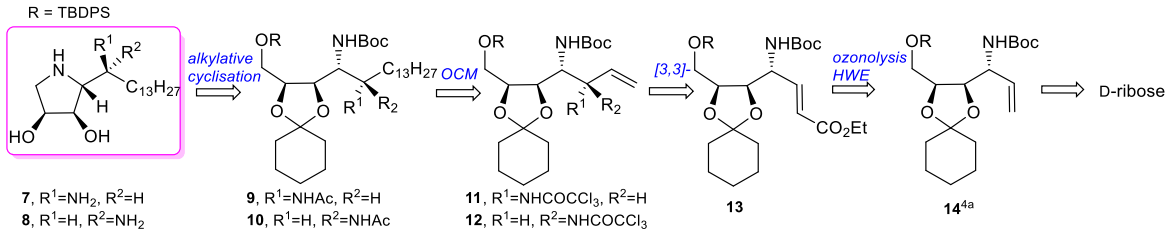

Figure 2 Retrosynthetic analysis of the final sphingomimetics **7** and **8**.

Acknowledgement

This work was funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V04-00751.

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Stereoselective synthesis of sphingofungin-based mimetics

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Sphingofungins **1**–**8** (Figure 1) are produced by several fungi, and members of this family have been identified as disruptors of SLs biosynthesis (based on SPT inhibition) with primarily antifungal properties. [1] Serine palmitoyltransferase (SPT) is a PLP-dependent enzyme that catalyses the first step of *de novo* biosynthesis of sphingolipids. These fungal products (Figure 1) represent SPT active substrates, which can react with the SPT cofactor due to their free amino group, providing a form of intermediate related to that for the normal enzymatic process (**9**, Figure 1). [2] Sphingofungins A–F (**1**–**6**, Figure 1) were isolated successively from two natural sources; sphingofungins A–D from the strain of *Aspergillus fumigatus* by Merck and Glaxo in 1992 and sphingofungins E and F from the fermentation broth of *Paecilomyces variotii* by Merck in the same year. The last two sphingofungin molecules – G (**7**) and H (**8**) – were discovered in the solid-state fermentation of *Aspergillus penicilliodes* by Zhang and coworkers in 2019. A survey of strategies leading to target sphingofungins A–F shows that 16 fully original total syntheses have so far been developed. [3]

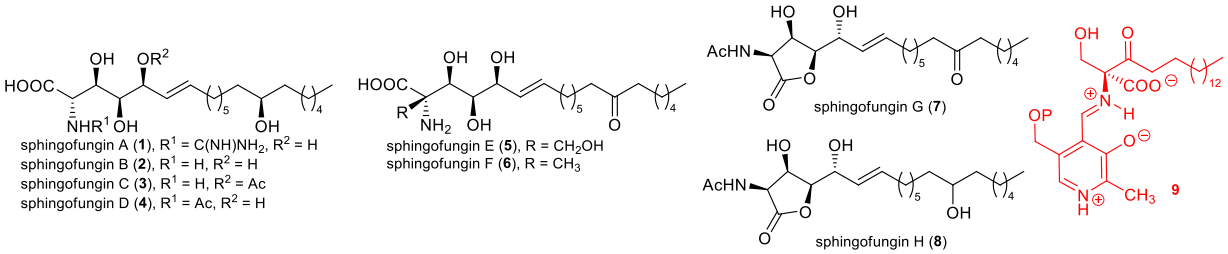

Figure 1 The structures of sphingofungins **1**–**8**, including the intermediate **9** of the normal SPT enzymatic process.

The retrosynthetic approach to this sphingofungin-based mimetics is illustrated by the construction of compounds **10** and **11** (Figure 2), which were obtained from amides **12** and **13**, respectively, via ozonolysis (Ph_3P work up), followed by Pinnick oxidation. The advanced diastereoisomeric synthons **12** and **13** were achieved via Overman rearrangement of an allylic substrate derived from the unsaturated system **14**. The corresponding ester **14** was generated from alkene **15** through an olefin cross metathesis and HWE olefination. Both target compounds will be evaluated for their antiproliferative/cytotoxic activity on various human cancer cell lines, with the aim of the revealing promising lead molecules for the development of novel anticancer-oriented drugs.

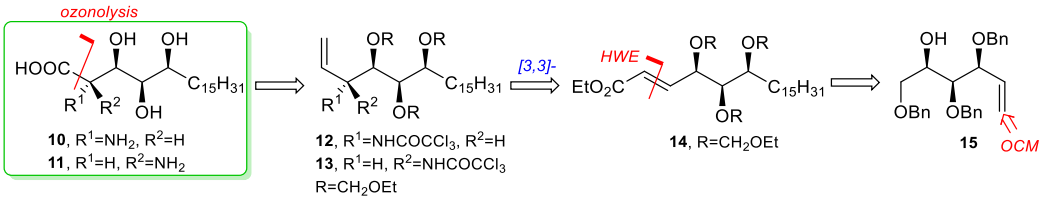

Figure 2 Retrosynthetic approach towards sphingofungin-based mimetics **10** and **11**.

Acknowledgements

The present work was supported by the Grant Agency (no. 1/0278/23) of the Ministry of Education, Slovak Republic. This work is also the result of the project implementation: Open scientific community for modern interdisciplinary research in medicine (OPENMED), ITMS2014+: 313011V455 supported by the Operational Programme Integrated Infrastructure, funded by the ERDF.

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Synthesis and anticancer profile of 6-hydroxysphingosine-based analogues

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Sphingoid bases represent an interesting class of compounds, which in addition to their structural roles in sphingolipid construction are also included in various cell signalling pathways. [1,2] It was found that D-*erythro*-sphingosine **1**, D-*ribo*-phytosphingosine **2** and (6*R*)-hydroxysphingosine **3** (Figure 1) create the key backbone of mammalian ceramides. [3] These compounds have been identified in the extracellular spaces of the *stratum corneum* (SC). The SC is the uppermost epidermal layer; it makes the human skin impermeable to water, thereby preventing lethal dehydration [2,3]. But unlike **1** and **2**, little is known about structure-activity relationships in **3** and its analogues, in particular, on the role of the stereochemistry of the vicinal amino alcohol motif on the biological profile. Based on these findings, we undertook the synthesis and cell viability experiments of the novel (6*R*)-hydroxysphingosine-based analogues.

Figure 1 illustrates our retrosynthetic approach to target derivatives **4** and **5**. The construction of their carbon backbone was achieved via a Wittig olefination of advanced intermediates **6** and **7**, respectively. We anticipated that **6** and **7** would be accesible through a [3,3]-sigmatropic rearrangement on allylic substrate **8**. Alcohol **8** was obtained from the known synthon **9** [4] using HWE reaction as the key step. Crystallographic analysis of the oxazolidinone **10** derived from **7** permitted to us to confirm the C-2 stereochemistry of **4** and **5**. The preliminary cytotoxic screening indicates that the designed sphingomimetic **5** has a promising capacity to alter the viability of the Jurkat and HeLa cancer cell lines.

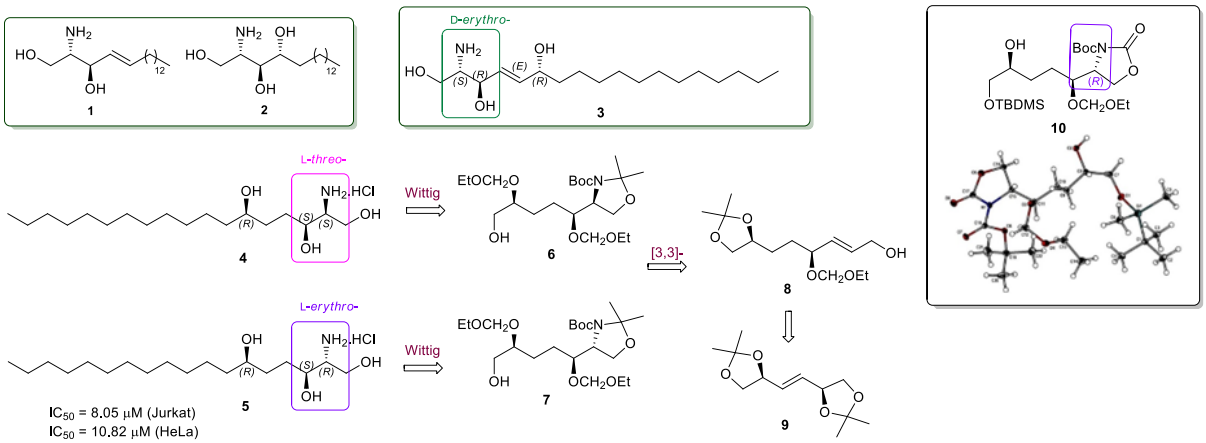

Figure 1 Retrosynthetic analysis of novel sphingoid bases **4** and **5**.

Acknowledgements

The present work was supported by the Grant Agency (no. 1/0278/23) of the Ministry of Education, Slovak Republic. Financial support from the Internal Scientific Grant System (no. vvgs-2025-3492) at Faculty of Science of P.J. Šafárik University in Košice is also gratefully acknowledged. This work was also funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09-I02-03-V01-00021.

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Novel 2,3-diaminopropanols for the construction of bioactive L- and D-Dap-containing molecules

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The discovery of nonproteinogenic 2,3-diamino acids in a range of natural products has stimulated considerable interest in this unique family of molecules. [1,2] L-2,3-Diaminopropanoic acid (L-Dap, **1**), and to a lesser extent its enantiomer D-Dap (*ent*-**1**) (Figure 1), have been identified in various natural sources, including plants, insects, and bacteria. [1,3] L-Dap (**1**) serves as a key structural motif in the biosynthesis of several natural antibiotics (e.g., viomycin and capreomycin) [3] as well as other bioactive peptides. [1] In the context of drug discovery and structure-activity relationship studies, α,β-diamino acids have been widely employed as versatile building blocks for the synthesis of a variety of analogues. [1,2,4]. Our retrosynthetic strategy (Figure 1) for the target 2,3-diaminopropanols (**12**, *ent*-**12**) started with a Wittig olefination of the protected D-erythrofuranoses **9** and *ent*-**9**, followed by a sequential Overman rearrangement, and concluded with ozonolysis and reductive workup of the corresponding derivatives **11** and *ent*-**11**. [5]

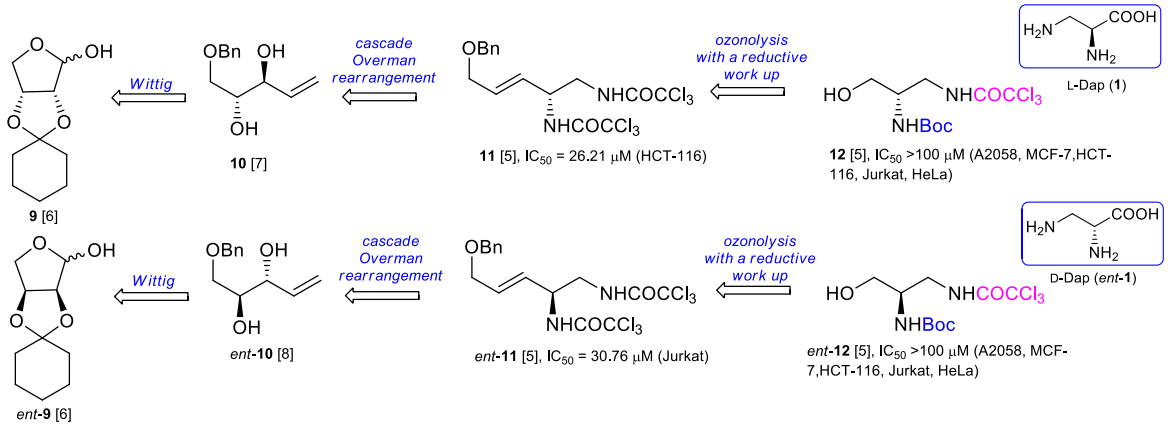

Figure 1 Retrosynthetic analysis of protected 2,3-diaminopropanols **12** and *ent*-**12**.

Acknowledgement

The present work was funded by the Grant Agency (no. 1/0278/23) of the Ministry of Education, Slovak Republic. Financial support from the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09-I02-03-V01-00021 and Internal Grant System (no. vvgs-2025-3492) at the Faculty of Science of P.J. Šafárik University in Košice are also gratefully acknowledged.

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Stereoselective synthesis of jaspine B-based mimetics

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Cancer is the second leading cause of death worldwide. Modulation of sphingolipid biosynthesis and metabolism is expected to be one of the promising approaches for therapy of the aforementioned disease.[1] Jaspines, represented by jaspine B (1) (Figure 1) [1] belong to the class of anhydrophytosphinosine-type compounds produced by marine organisms. The remarkable cytotoxicity of 1 was demonstrated on at least 30 human cancer cell lines, with IC50 values ranking at micromolar levels. [2] Due to the impressive biological properties and challenging structural motif based on the presence of substituted THF core, a great deal of effort has been expended for the construction of 1 and its various analogues (Figure 1). [2,3]

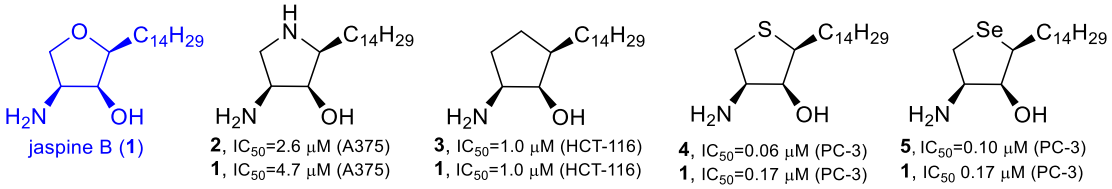

Figure 1 Jaspine B and its several cytotoxic mimetics **2**–**5**. [2,3]

The retrosynthetic approach to novel isomeric jaspine B mimetics **6** and **7** is depicted in the Figure 2. The prepared analogues have an interesting vicinal amino alcohol motif bearing a tetrasubstituted stereocentre, with the resulting arrangement of the amino and hydroxyl functionalities being in the opposite mode compared to the parent molecule **1**. Moreover, the novel C-N bond was also installed in the side chain. We envision that the designed compounds **6** and **7** could be accessible from derivatives **8** and **9**, respectively, via OCM reaction, followed by a deoxygenation protocol. The requisite trichloroacetamides might, in turn, arise from an allylic substrate derived from **10** using Overman reaction. The corresponding ester **10** was easily obtained from the known alcohol **11** [4] through [3,3]-sigmatropic rearrangement and HWE olefination.

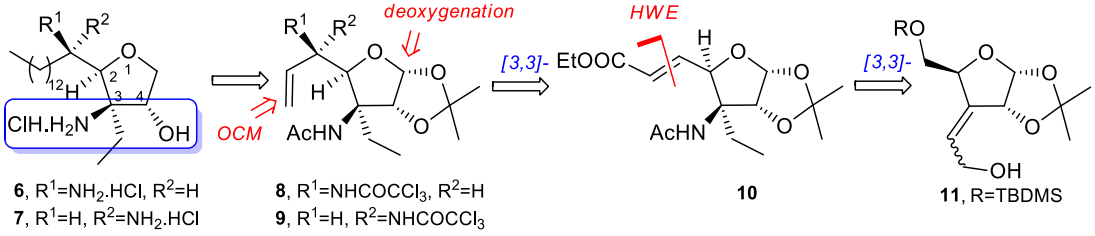

Figure 2 Retrosynthetic strategy toward mimetics **6** and **7**.

Acknowledgements

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DIX-like azasugars – synthesis and antiproliferative profile

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Iminosugars and related azasugars have attracted considerable attention over the past three decades owing to their broad spectrum of biological activities. [1] 1,5-Dideoxy-1,5-iminoxylitol 1 (DIX, Figure. 1) belongs to the group of the natural unmodified hydrophilic 1-N-iminosugars. [2] This compound was isolated from the plant Eupatorium fortunei Turz which is used in traditional Chinese medicine as well as in Japanese folk medicine for its diuretic, antipyretic and antidiabetic properties. DIX was one of the first candidates, which were identified as pharmacological chaperones (PCs) for the treatment of lysosomal storage disorders such as Gaucher disease. [3] In view of the impressive biological profile of 1, several interesting approaches leading to this natural 3,4,5-trihydroxypiperidine as well as to its synthetic analogues, including O- and C-alkylated derivatives 2 and 3, respectively, and the C-branched compound 4 (Figure 1) have been elaborated. [2] Among DIX-based analogues illustrated in Figure 1, the 2-C-nonyl iminosugar 3 displayed a remarkable inhibitory capacity toward the human acid β-glucosidase with the IC50 value in a nanomolar range. [4]

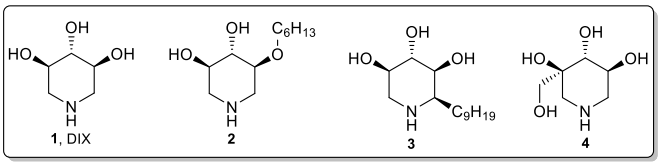

Figure 1 DIX **1** and its analogues **2**–**4**.

Recently, our group developed a simple stereodivergent route to DIX-like 1-*N*-iminosugars **5**.HCl and **6**.HCl from D-xylofuranose chiron **10** (Figure 2). The advanced scaffolds **7** and **8** were assembled by Wittig olefination, followed by the heterosigmatriopic rearrangement to establish the novel stereochemistry. Subsequent OCM reaction introduced a hydrophobic alkyl branch and finally, the 6-*exo-tet* type cyclisation led to a piperidine core. Crystallographic analysis of the oxazolidinone **9** confirmed the stereochemistry established by the rearrangement reaction. Cell viability experiments showed that the prepared *C*-alkyl piperidine-3,4,5-triols **5**.HCl and **6**.HCl have a capacity to inhibit the proliferation of cancer cell lines *in vitro*.

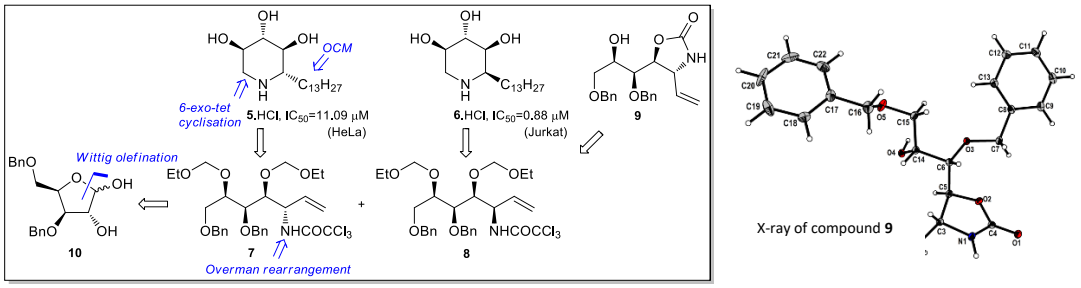

Figure 2 Retrosynthetic analysis of our target DIX analogues **5**.HCl and **6**.HCl.

Acknowledgements

The present work was supported by the Grant Agency (No. 1/0278/23) of the Ministry of Education, Slovak Republic. This work was also funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09-I02-03-V01-00021.

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2-*C*-Tridecyl piperidine-3,4,5-triols: Synthesis and Preliminary Biological Evaluation

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Piperidine-type iminosugars have shown a rich variety of relevant pharmacological activities against glycosidase enzymes, and many of them have been highlighted as lead candidates for the treatment of various diseases, including cancer, diabetes, viral infections, and lysosomal storage disorders, e.g. Gaucher and Fabry disease. [1, 2] Iminosugars with *N*- and *O*- linked alkyl chains of varying lengths also exhibit a broad spectrum of biological properties, including antiviral, antibacterial, immunosuppressant, and anti-inflammatory activities. [3]
Our main goal herein was the design of new azasugar mimetics and their cytotoxic screening. We used independent pathways for the synthesis of four stereoisomeric 2-*C*-tridecyl piperidine-3,4,5-triols **1**.HCl–**2**.HCl and *ent*-**1**.HCl–*ent*-**2**.HCl from two different chirons: L-arabinose and D-lyxose, respectively. (Figure 1) The key step in both synthetic strategies was the [3,3]-heterosigmatropic rearrangement to install nitrogen-bearing stereocentres. Incorporation of a C-2 alkyl chain *via* olefin cross-metathesis was performed in different stages of synthetic strategies, once before and a second time after the cyclization step. The antiproliferative activity of the final compounds was tested and revealed that all of them have promising cytotoxicity against leukemia cells. Furthermore, compounds **1**.HCl and **2**.HCl exhibited to be more potent against the HeLa cell line than their corresponding antipodes *ent*-**1**.HCl–*ent*-**2**.HCl. Exploration of further alkylated piperidine analogues will expand the library of existing sugar mimetics and provide a more comprehensive view of their biological activity.

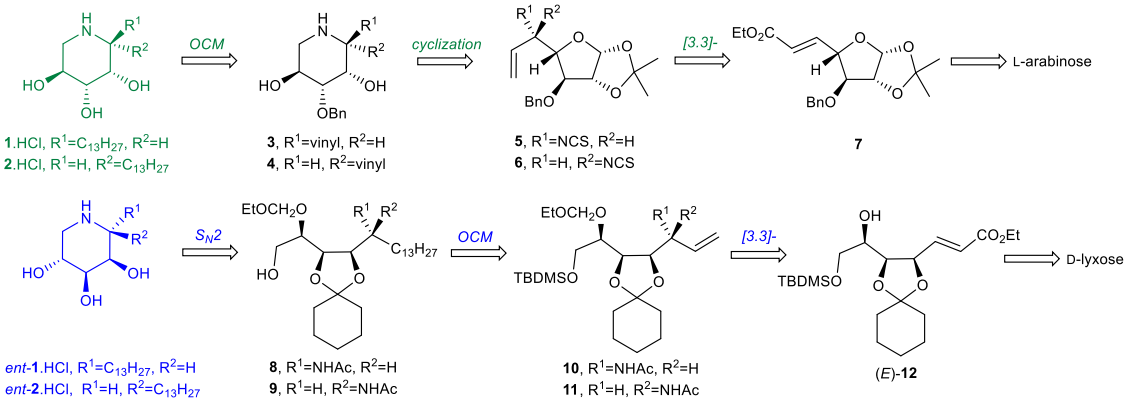

Figure 1 Retrosynthetic strategy toward piperidine trioles **1**.HCl, **2**.HCl, *ent*-**1**.HCl, and *ent*-**2**.HCl.

Acknowledgement

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Synthesis and biological profile of a novel *C*-branched pyrrolidine-based iminosugar

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Polyhydroxylated pyrrolidines are a relatively large and extensively studied subclass of the iminosugar family, covering both naturally occurring and synthetic molecules. Most of them have been shown to be promising and selective inhibitors of glycosidases, the enzymes that cleave glycosidic bonds and participate in a wide range of key biological processes. [1] It is worth noting that many of these sugar mimetics share a skeleton based on 1,4-dideoxy-1,4-imino-D-arabinitol **1** (DAB), or its enantiomeric counterpart *ent*-**1** (LAB), as the parent molecules. [1] Since the isolation of DAB in 1985, a significant number of unnatural pyrrolidine-containing sugar mimetics have been prepared in order to find novel bioactive agents as potent but still selective glycosidase inhibitors. [2,3] Among them, *C*-branched analogues have shown their capacity to specifically block various glycosidases. [4] Based on the above-mentioned findings, we decided to develop the synthesis of a novel branched iminosugar decorated with the long alkyl chain.

The retrosynthetic strategy for the target pyrrolidine-based iminosugar **2**.HCl is illustrated in Figure 1. We envisioned that **2**.HCl could arise via oxidative cleavage of the vicinal diol moiety in **3** followed by reductive work. It was anticipated that the bicyclic system in **3** would be accessible by an alkylative cyclisation from the aminofuranose **4**. The 3-*C*-alkylated derivative **4** can be derived from the vinyl scaffold **5** [5] through a pivotal OCM reaction. Cell viability experiments revealed a cytotoxic effect of the target compound **2**.HCl against Jurkat and HeLa cells (IC_{50} = 20.58 μM and 22.7 μM, respectively). In addition, docking studies [6] identified the binding modes of this novel pyrrolidine-based iminosugar to human β-glucocerebrosidase.

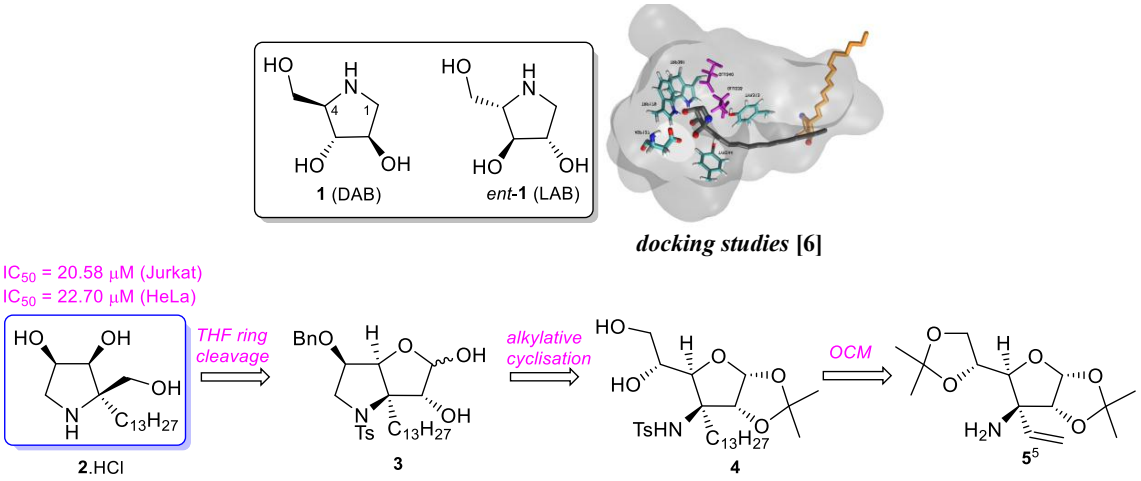

Figure 1 Retrosynthetic analysis of the branched iminosugar **2**.HCl.

Acknowledgements

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Preparation and Surface Characterization of PLA-Coated Zinc

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Internal fixators are specifically engineered to support bone repair and regeneration by stabilizing fracture sites, thereby promoting faster healing. These medical devices are manufactured in various forms, such as screws, pins, plates, and other fixation systems[1]. Among biodegradable metals, magnesium, zinc, and iron are the most commonly used [2]. Zinc exhibits a moderate degradation rate and good biocompatibility. However, its relatively low mechanical strength and the uncontrolled release of Zn^{2+} ions limit its effectiveness as a base material for biomedical applications. Therefore, surface modification is often required to effectively regulate the biodegradation behaviour of Zn-based materials [3]. Several surface modification strategies have been developed to tune the corrosion rate of Zn-based materials, such as inorganic coatings, ceramic coatings, polymer coatings, composite coatings, and sol-gel coatings. Among these strategies, polymer coatings are effective and straightforward, as they provide corrosion control, enhanced biocompatibility, and drug delivery potential. In particular, poly(lactic acid) (PLA) is attractive due to its long history of safe use in resorbable medical devices, including stents, sutures, and bone-fixation devices [4].

In this study, zinc specimens were fabricated via powder metallurgy technique and subsequently coated with a 5 wt.% PLA solution using spin-coating and needleless electrospinning techniques to compare the resulting surface morphology. The surface morphology of uncoated and coated Zn samples was studied using scanning electron microscopy (SEM) coupled with energy-dispersive X-ray analysis (EDS). Figure 1a shows SEM image of the surface of an uncoated Zn sample, at 100 – times magnification, exhibiting characteristic parallel grinding marks. The corresponding EDS analysis confirms the presence of Zn along with O caused by surface oxidation. Figure 1b and c show SEM images of PLA spin – coated on the surface of Zn sample at 100 – and 5000 – times magnification, respectively. The PLA coating forms a porous layer composed of interconnected pores of different sizes. EDS analysis confirms the presence of C and O, supporting the presence of the PLA polymer layer. Figure 1d and e show SEM images of the surface of Zn coated with PLA nanofibers, prepared by needleless electrospinning, at 100 – and 5000 – times magnification, respectively. The surface is homogenously covered with randomly oriented, smooth PLA nanofibers with thickness ranging from approximately 0.15 µm to 1 µm. Compared with spin-coated film, the electrospun layer exhibits a more open, three – dimensional fibrous structure that allows partial exposure of the underlying Zn surface. The corresponding EDS analysis confirms the presence of Zn, O, and C.

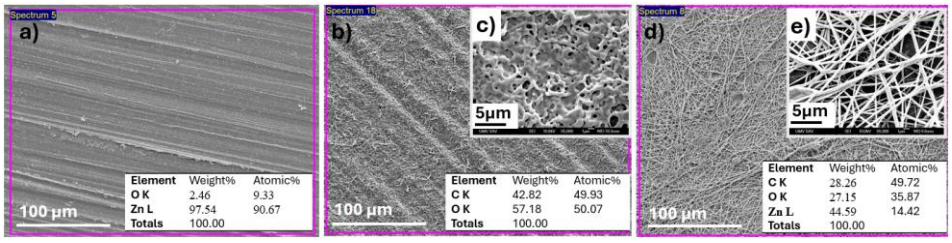

Figure 1 SEM images of the Zn sample before coating at 100 x magnification (a), after spin coating at 100 x (b) and 5000 x (c), and PLA electrospun nanofibers at 100 x (d) and 5000 x magnification.

Acknowledgements

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Carbon Nanotube–Silver Nanoparticle Composite for Electrochemical Determination of Gentamicin

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Gentamicin is a broad-spectrum aminoglycoside antibiotic widely used in human and veterinary medicine to treat infections caused by Gram-negative and some Gram-positive bacteria. Despite its clinical relevance, the excessive and uncontrolled use of gentamicin has led to environmental contamination. When used beyond therapeutic limits, gentamicin can cause severe side effects, emphasizing the need for rapid and reliable analytical methods for its monitoring [1].

Electrochemical platforms based on multi-walled carbon nanotubes (MWCNTs) combined with silver nanoparticles (AgNPs) integrate the high conductivity of carbon nanotubes with the electrocatalytic activity of silver. Therefore, the MWCNT/AgNPs modified screen-printed carbon electrode (SPCE) represents an attractive, low-cost, and portable sensing system for the rapid and reliable detection of gentamicin in pharmaceutical and biological samples.

The MWCNT/AgNPs nanocomposite was prepared by dispersing 0.5 g of MWCNTs in 200 mL of deionized water and ultrasonically homogenizing the suspension for 1 h. Then, 200 mL of 0.1 M $AgNO_3$ solution was added and the mixture was stirred for 30 min. The dispersion was heated to 85 °C, and 25 mL of NaOH was added dropwise over 10 min. The formed product was filtered, washed several times with deionized water, and dried on filter paper in a laboratory oven. The obtained powder was dispersed by mixing 0.250 g of the composite with 5 mL of ethanol and ultrasonicated for 40 min. The resulting suspension was drop-cast (1 µL) onto the surface of the working electrode and dried at room temperature before use.

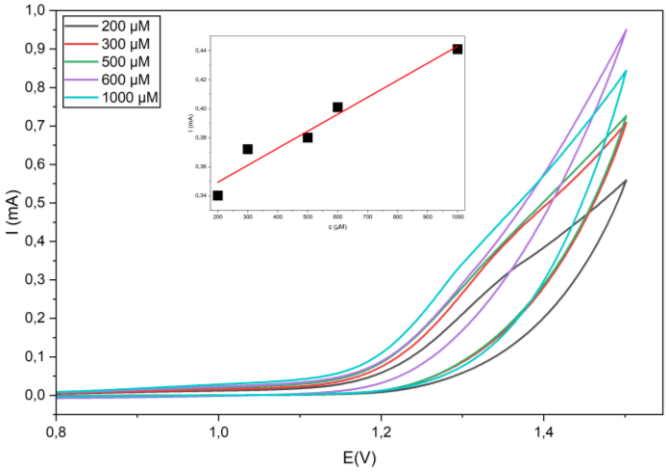

Figure 1 Cyclic voltammetry (CV) curves in PBS for gentamicin in the concentration range 200 –1000 µM with corresponding calibration plot (inset).

Based on cyclic voltammetry measurements, a linear response to gentamicin was observed in the 200–1000 µM range, which demonstrates that the MWCNT/AgNPs/SPCE is a promising platform for gentamicin determination in real samples.

Acknowledgement

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Development of Modified Screen-Printed Electrodes for Cholesterol Determination

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Cholesterol plays an essential role in the human body, serving as a precursor for the synthesis of various biologically important molecules, including hormones, vitamins, and bile acids. However, maintaining appropriate cholesterol levels in the bloodstream is crucial, as elevated concentrations are associated with serious health problems. For healthy adults, the normal cholesterol level is typically 5.2 mM exceeding this threshold are indicative of hypercholesterolemia. [1,2]. Therefore, rapid and accurate determination of cholesterol levels is crucial for early diagnosis and management of cardiovascular diseases and other related health conditions. Consequently, there is a growing demand for the development of alternative cholesterol-sensing platforms that are rapid, cost-effective, and suitable for point-of-care diagnostics [3].
In this work screen-printed carbon electrodes (SPCE) were modified by polypyrrole membrane and copper nanoparticles (CuNPs) to prepare fast, stable, selective, and sensitive electrochemical sensor for cholesterol determination. Cyclic voltammetry at potential window from -0.3V to 1.2V, v = 10 mV/s was used for pyrolle polymerization on the working electrode surface. In the next step polymer membrane was decorated with copper nanoparticles using chronoamperometry method at a constant potential (E = -0.37 V) for 160 s. As shown in Figure 1, Bare SPCE (red line) exceed no oxidation peak for cholesterol oxidation (8 mM cholesterol in PBS and 0.1 M NaOH). However, SPCE modified with polypyrrole and CuNPs (SPCE_PPy_KCl_Cu) increased the current response and the oxidation peak for direct cholesterol oxidation was observed at E = +0.1 V with Ip_A = 0.5 mA (black line). This enhancement in electrochemical response highlights the catalytic efficacy of the CuNPs within the polypyrrole matrix for cholesterol oxidation. The obtained results show a potential for developing novel electrochemical sensor for rapid and direct cholesterol determination.

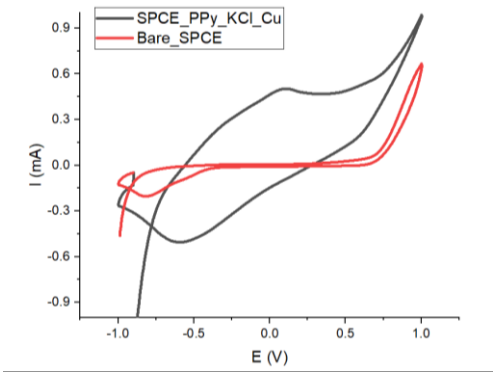

Figure 1 Cyclic voltammogram for 8mM cholesterol oxidation in PBS and 0.1M NaOH at Bare_SPCE (red line) and SPCE_PPy_KCl_Cu (black line) at potential window from -1V to 1V at scan rate 50mV/s.

Acknowledgements

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Electrochemical Quantification of Vancomycin on SPCE Carbon Surface for Multisensor Development

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Introduction

Vancomycin, a glycopeptide antibiotic, has been widely used as a first-line treatment for methicillin-resistant *S. aureus* (MRSA) and other serious bacterial infections since the 1980s. Its extensive use has contributed to the emergence of resistant strains, highlighting the need for a reliable, selective, and sensitive sensor to monitor vancomycin in blood. Such a platform could support therapeutic drug monitoring and help prevent the spread of antibiotic resistance [1, 2].

Results and Discussion

The screen-printed carbon electrode (SPCE 11L, DropSens) was modified from solution (0,03g $AuCl_3$, 0.03 mL HCl, and 25 mL KCl) during the 15 cycles by electrochemical deposition. The measurements were realized of concentration from 1 µM to 500 µM vancomycin solution in PBS with 0.1 M NaOH (Figure 1).

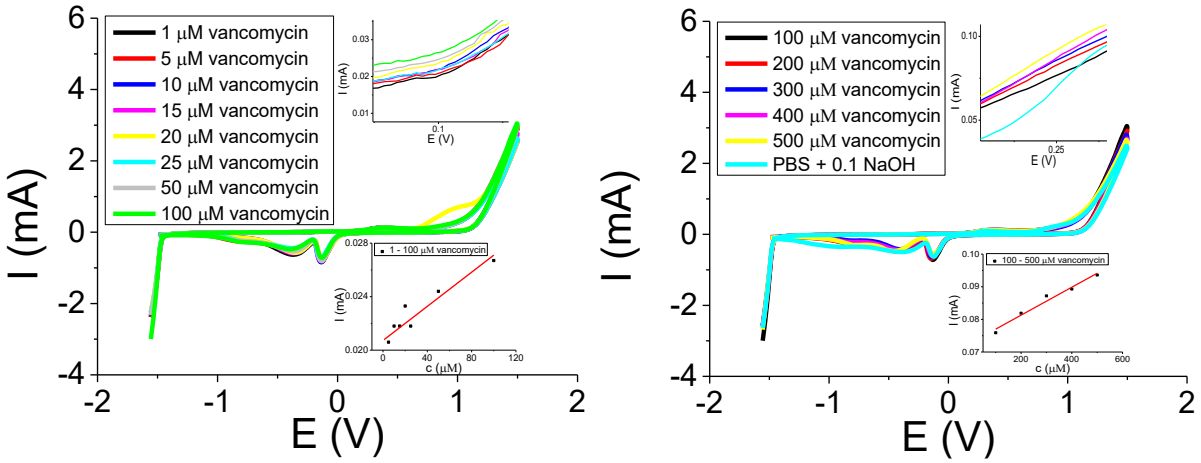

Figure 1 Calibration curves of vancomycin obtained by CV in concentration range of 1 - 100 µM and 100 – 500 µM.

Two concentration ranges were examined to encompass both the sub-therapeutic vancomycin levels typically present in human blood and the higher concentrations relevant for intraoperative antibiotic administration, with the obtained data presented in a Table 1.

Table 1 Sensitivity and limit of detection evaluated across different concentration ranges.

Concentration range	1 – 100 µM	100 – 500 µM
Sensitivity	$6{,}38*10^{-5}$ mA/µM	$4{,}28*10^{-5}$ mA/µM
Limit of detection (LOD)	17,85 µM	93,22 µM

It holds promise for clinical validation and preventing antibiotic resistance. In the future we want to develop the mutisensor for detection various antibiotics.

Acknowledgements

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Aggregation induced infrared spectral changes in π-π stacking systems on example of Anthracene using the Electronic Structure Theory

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Vander Waals interactions are often overlooked compared with various bonding types. They are considered weak compared to a Hydrogen bond, needless to say covalent or ionic ones. However, aggregation processes based on that phenomenon, like van de Waals and π-π dispersion interactions, is useful in chemical analysis, it is integral to Nucleic acids, data preservation etc [1].

There is plenty of articles focused on electronic spectra shifts caused by aggregation including those with Electronic Structure Theory use, but vibrational spectra are rarely considered. Various changes in IR spectra can, in theory, occur as a result of aggregation processes. Simplest aggregates could be dimers. There different interactions may play their role such as Hydrogen bonding, π-π stacking and charge redistribution. Carbonyl shifts due to conjugation or hydrogen bonding are well-known in organic molecules, including xanthene dyes. N-H and O-H stretching bands shift due to hydrogen bonding or solvation effects. Dimerization leads to π-π stacking interactions, reducing electron density in certain bonds, thereby shifting IR peaks. Charge delocalization affects bond strengths, especially in the C=O and aromatic regions [2]. If the dimer forms through hydrogen bonding, the stretching vibrations of functional groups involved (such as O-H or N-H) can shift to lower wavenumbers due to hydrogen bond formation. This typically broadens and shifts the O-H and N-H stretching bands.

We chose anthracene as it resembles Rhodamine 6G as well as R6B, useful analytical dyes prone to self-aggregation, and we can win up to 20x timewise on scaling with system being more than twice smaller. It should, however, retain strong enough of a pivotal π – π dispersion interactions. It also doesn't have any hetero atoms which eliminates shifts potentially caused by Intermolecular Hydrogen Bonding, which in turn could help assess whether those, caused by the interaction, occur.

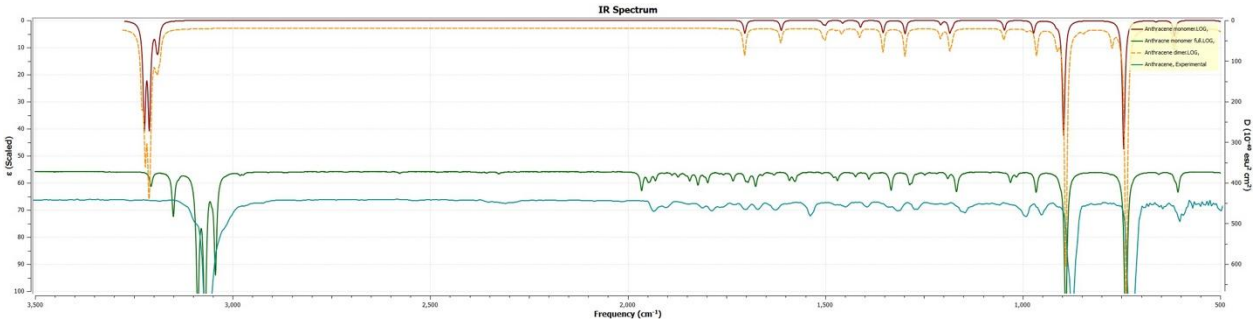

Figure 1 IR spectra of anthracene: Calculated harmonic spectrum of monomer (red solid line), dimer (yellow dashed line) and monomer with anharmonic corrections (green solid line) at APFD 6-31G (d, p) level of theory in gas phase, unscaled. The latter is contrasted with the experimental spectrum (turquoise solid line) in gas phase source: NIST [3].

We can see from Figure 1 that anharmonic corrections can play a crucial role in completeness of spectra and band positions: calculated at reasonable, 6-31G (d, p), level of theory spectrum matches the experiment well enough, minor scaling would align bands much better, however. It is worth noting that the harmonic one has the most intense bands and, in some sense, all of them if one considers them unsplit from anharmonic vibrations

The intensities in dimers increased as predicted, yet no new bands have appeared, nor did the wavenumbers shift in any considerable way in a certain direction at the harmonic approximation level. That said, anharmonic spectra may still embed some changes that may be revealing into a combined one. If so, it would be even more tangible to compute for the primary dye monomer and dimer.

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Comparative Analysis of Separator Materials and Their Influence on the Electrochemical Performance of Lithium–Sulfur Cells under Low-Electrolyte Conditions

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The ongoing effort to develop lightweight and miniaturized lithium–sulfur (Li–S) batteries has intensified the need to optimize internal cell components for improved energy density and stable operation. Among these, the separator structure plays a key role in controlling ion transport, electrolyte distribution, and suppression of the polysulfide shuttle effect [1]. In systems with a low electrolyte volume, where wetting and ionic conductivity are limited, the separator design becomes particularly crucial for ensuring efficient electrochemical utilization of sulfur and long-term cycling stability [2].

This work presents a comparative study of Li–S cells assembled with two different separators—glass fiber GF/A and polymeric Celgard® 2325—under reduced electrolyte conditions, representing a step toward miniaturized and electrolyte-lean Li–S systems. Electrochemical characterization using cyclic voltammetry (CV) and galvanostatic cycling (GCPL) shown in Figure 1 revealed distinct performance differences between the two configurations.

The cell with the GF/A separator achieved an initial discharge capacity of only 200,7 mAh g^{-1}, accompanied by rapid capacity fading and unstable cycling behavior, attributed to the limited ion transport through its thick fibrous structure and insufficient wetting under low-electrolyte conditions. In contrast, the Celgard® 2325-based cell exhibited a markedly higher initial capacity of 768,2 mAh g^{-1} at 0,1 C, with 85,4 % capacity retention after 35 cycles, demonstrating improved electrolyte utilization, better ionic conductivity, and more homogeneous activation of the cathode material.

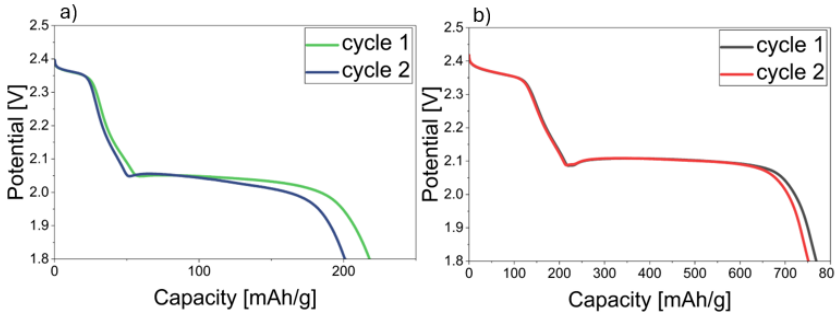

Figure 1 Comparison of Discharge Profiles for Li–S Cells with a) GF/A and b) Celgard® 2325 separators at 0,1 C.

The comparison clearly indicates that the separator type critically affects the electrochemical response of Li–S cells operating with limited electrolyte. While **GF/A** shows favorable polysulfide adsorption and stability in high-electrolyte configurations, **Celgard® 2325** offers superior compatibility with **electrolyte-lean and miniaturized cell designs**, enabling more efficient energy storage per unit mass and volume—an essential factor for the next generation of high-energy, lightweight Li–S batteries.

Acknowledgements

This work was funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project SUNFLOWERS No. 09I02-03-V01-00022 and KEGA 002UPJS-4/2024.

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Modification of screen-printed electrodes for electrochemical gentamicin detection

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Orthopaedic implants have played a crucial role in modern medicine, offering solutions for bone repair and joint replacement. Despite their clinical benefits, implant-associated infections remain a persistent and serious complication that can threaten the success of surgical procedures. To mitigate these risks, the development of antibacterial coatings capable of localised drug delivery has gained increasing attention. Gradual release of antibiotics at the implant site can reduce systemic toxicity and enhance therapeutic efficacy [1]. However, the quantitative evaluation of antibiotic release during the degradation of these coatings remains technically challenging due to the very low concentrations involved.

The aim of this study was to develop an electrochemical sensor for gentamicin detection through the modification of a screen-printed carbon electrode (SPCE) with Cr-containing metal-organic frameworks (Cr-MOF), multiwalled carbon nanotubes (MWCNTs), and Nafion. The surface of the working electrode was modified by the drop-casting method in three different ways. In the first case, the electrode was modified with a Cr-MOF complex, which was fixed onto the surface using a Nafion layer. In the second case, MWCNTs were applied to the electrode surface, followed by a Nafion layer after drying. The third modification represented a combination of the previous approaches, where the working electrode surface was modified with a suspension prepared by mixing MWCNTs and Cr-MOF in a Nafion solution. In this work the effective surface area of unmodified and modified SPCEs was investigated using cyclic voltammetry (CV) in a 5 mM $K_3[Fe(CN)_6]/K_4[Fe(CN)_6]$ solution within a potential range of 0–1.6 V at a scan rate of 0.1 V/s. Subsequently, CV measurements were also performed in a 300 µM gentamicin solution prepared in PBS in order to monitor the anodic current response associated with gentamicin oxidation on the studied electrodes.

The active surface area was highest for the unmodified SPCE electrode. Surface modification led to the occupation of active sites by the less conductive MOF material, resulting in a decrease in the electroactive area (Figure 1c). The oxidation of gentamicin is represented by a peak in the potential range of 0.2–0.5 V. The highest anodic current response for gentamicin oxidation was observed for the electrode modified with the combination of Cr-MOF and MWCNTs bound with Nafion (Figure 1). This synergistic effect can be attributed to the binding capability of Cr-MOF, which enables efficient adsorption of gentamicin, while the MWCNTs facilitate effective electron transfer. This modification showed as the most effective modification for the electrochemical determination of gentamicin.

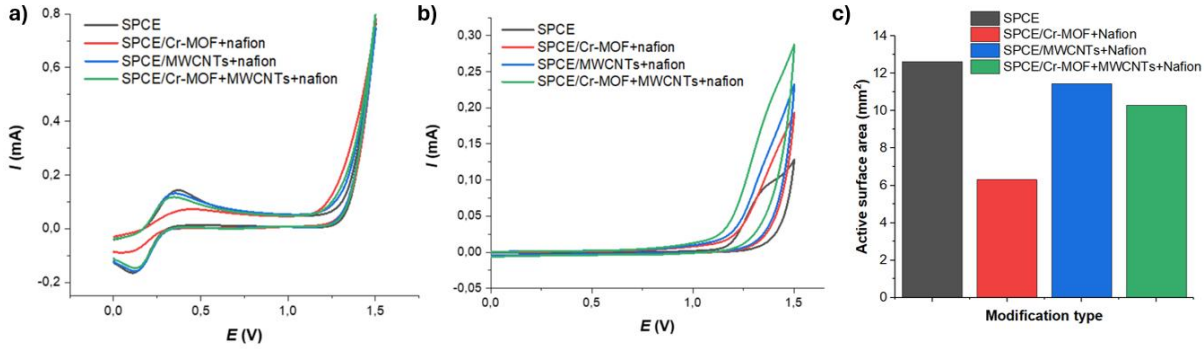

Figure 1 Cyclic voltammogram of a) 5 mM $K_3[Fe(CN)_6]/K_4[Fe(CN)_6]$ solution and b) 300 µm gentamicin sulphate solution in PBS c) comparison of the active surface area.

Acknowledgements

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Bimetallic phosphides sulfur cathode for Li-S battery

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Sulfur, a naturally abundant, low-cost, and environmentally friendly material, presents a compelling alternative to conventional Li-ion cathode materials [1]. However, significant challenges persist that impede the practical implementation of lithium-sulfur batteries (LSBs) like insulating nature of sulfur, volume changes, and performance degradation caused by the shuttle effect. Using carbon material would effectively improve conductivity of sufur electrode. However, a potential drawback of employing porous carbon materials is an increase in battery volume. Therefore, it is very important to design suitable support materials for sulphur fixation [2]. Metal phosphides have emerged as promising materials for addressing the challenges associated with lithium-sulfur batteries. The superior electronic and ionic conductivity of metal phosphides, coupled with their ample polar sites, facilitates efficient charge transfer and catalytic activity, improving the overall performance of lithium-sulfur batteries [3]. The presence of highly electronegative phosphorus atoms within the metal phosphide lattice results in electron withdrawal from the metal centers, leading to the formation of electron-rich surfaces and multi-electron orbitals. This electronic environment facilitates the adsorption of electropositive species, such as Li^+ ions, and enhances electronic conductivity, making metal phosphides promising candidates for high-performance catalytic applications [4].

In this study, composite sulfur cathodes with the addition of bimetallic phosphide (MoFeP) were prepared for application in lithium-sulfur batteries. A simple sol-gel method followed by sintering in two sintering steps (in air and reduction in hydrogen atmosphere) was used to prepare this bimetallic phosphide. The fabricated sulfur electrodes were subjected to detailed electrochemical analysis using cyclic voltammetry and galvanostatic cycling. Test cells were assembled utilizing pre-fabricated electrodes as working electrodes (WE), while lithium metal served as both the counter (CE) and reference electrode (RE). The electrode was charged and discharged between 1.8 and 2.8 V at different C-rates. Also the cyclic voltammetry was done between 1.8 and 2.8 V at 0.1 $mV.s^{-1}$. The initial capacity of the electrode with the addition of MoFeP at 0.1 C was 530 mAh g^{-1}.

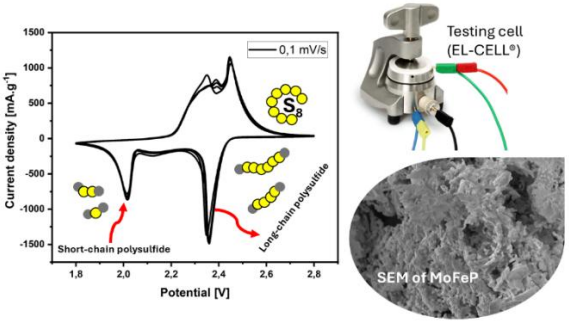

Figure 1 Polysulfide redox transitions and SEM image of the MoFeP.

Acknowledgements

Funded by the Slovak Research and Development Agency under the Contract no. DS-FR-24-0004, by the project KEGA 002UPJŠ-4/2024 and EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project SUNFLOWERS No. 09I02-03-V01-00022.

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Investigation of the Hydrogen Evolution Reaction Kinetics on a High-Entropy Catalyst

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Hydrogen is integral to numerous industrial processes, including oil refining, ammonia and methanol synthesis, and the Fischer-Tropsch process. Its annual demand has tripled over the past 50 years and is projected to increase fivefold, surpassing 500 million tons by 2050. Today, most hydrogen is produced via coal gasification and steam methane reforming, which are cost-effective but emit substantial CO2. Water electrolysis powered by renewable energy offers a more sustainable route but is currently more expensive. Reducing its cost will require the development of cheaper catalysts [1–3]. The aim of this work was to examine the effect of temperature on the kinetics of the hydrogen evolution reaction (HER) on a non-critical-feedstock-based high-entropy material in an alkaline media. This material was prepared from Cu, Fe, Ni, Mo, and Zn precursors via sol-gel autocombustion. HER kinetics on this material was investigated over 298.15 – 333.15 K by electrochemical impedance spectroscopy at -300 mV vs RHE in 1 M KOH, using a three-electrode setup with a rotating glassy carbon disk electrode modified with catalytic ink as the working electrode. The working-electrode catalyst loading was 1 mg·cm-2. The obtained data were well fitted by the equivalent circuit presented in Figure 1B, with chi-square values below 0.0056 for all fits. As shown in Figure 1A, HER kinetics is controlled by charge transfer across the entire temperature range studied. The polarization resistance decreases markedly at lower temperatures (298.15–323.15 K), from 155 Ω to 28.3 Ω, whereas at higher temperatures (323.15–333.15 K) the change is minimal (1.1 Ω), indicating that improved performance can be achieved with a slight increase in electrolyte temperature.

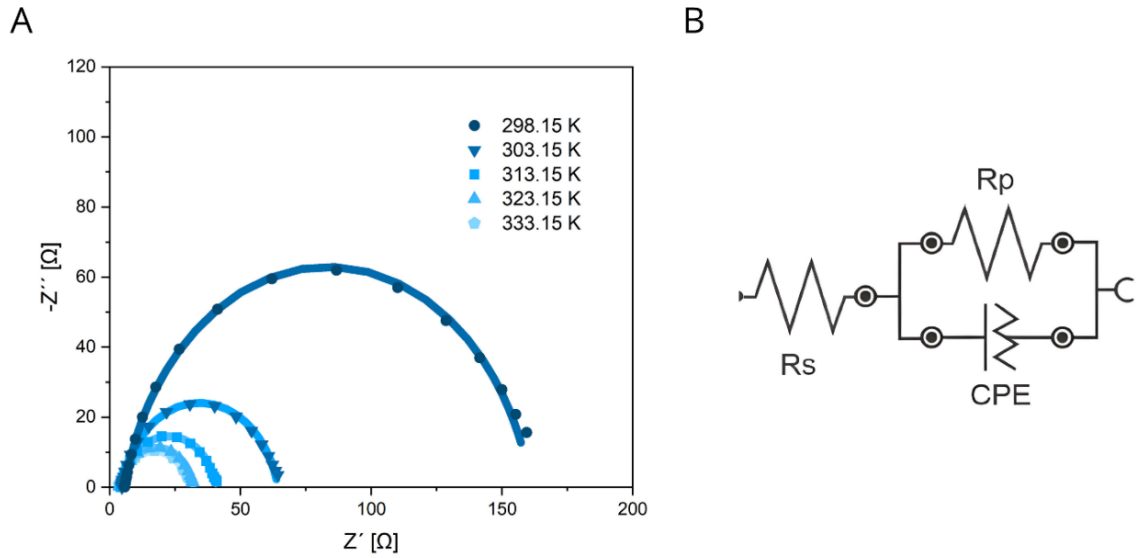

Figure 1 A) Nyquist diagrams for the prepared material 1 M KOH at −300 mV vs RHE over 298.15–333.15 K; B) equivalent circuit consisting of the solution resistance (Rs), a constant phase element (CPE), and the polarization resistance (Rp) used to fit Nyquist diagrams.

Acknowledgements

This research was supported by Internal Scientific Grant System - ESGD Program of Pavol Jozef Šafárik University in Košice (vvgs-2023-2957) funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V05-00008 and the Scientific Grant Agency of Ministry of Education, Science, Research and Sport of the Slovak Republic and the Slovak Academy of Sciences (VEGA) under project No. 1/0057/25.

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Defect-Driven Metal Doping in Graphite : A First-Principles Perspective for Vanadium Redox Flow Battery Systems

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The electrochemical performance of all-vanadium redox flow batteries (VRFBs) is closely linked to the physicochemical characteristics of their electrode materials [1]. Graphite-based electrodes are widely employed due to their high electrical conductivity, chemical stability and cost-effectiveness [2]. However, their inert basal planes limit their electrochemical activity towards vanadium redox reactions. To overcome this limitation, recent advances suggest that metal doping and defect engineering can substantially improve the catalytic performance by modifying the surface and introducing active sites for charge transfer [3, 4]. However, the atomic-scale mechanisms underlying these improvements remain largely underexplored.

To address this gap, this study aims to elucidate the atomic-scale mechanisms underlying metal incorporation and stabilization in graphite electrodes using density functional theory (DFT) simulations, specifically employing the Quantum Espresso package. Pristine and defect-containing surfaces were modelled to evaluate the influence of vacancy defects on dopant incorporation energetics and electronic structure. Focus will be placed on post-transition metal dopants, bismuth (Bi), tin (Sn), lead (Pb), and indium (In), due to their experimentally demonstrated ability to influence vanadium redox kinetics. These elements can also mitigate parasitic side reactions, such as hydrogen evolution, by selectively altering the reaction pathways by tuning the surface energetics.

Through a systematic analysis of defect formation energies, dopant-defect interactions, and electronic structure characteristics, this study establishes a theoretical framework connecting defect-assisted metal doping with improved VRFB functionality, offering insights crucial for designing more efficient, durable, and selective carbon-based electrodes for next-generation systems.

Acknowledgements

This work was supported by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V04-00109.

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Electrospun high-entropy oxide ceramic nanofibers

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This research details the synthesis and comprehensive structural analysis of oxide ceramic nanofibers with a complex composition. These materials integrate transition metals from Group IV (Ti, Zr, Hf) and Group V (Ta, Nb), with the core objective being the achievement of a pure, single-phase ceramic structure with a composition of $TiZrHfNbTaO_{11}$, thus resulting in a high entropy oxide. The foundational step involved preparation of composite PAN/MeOx precursor fibers (where Me represents the transition metal) in a rapid, one-step reactive needleless electrospinning. The subsequent transformation into porous MeOx ceramic nanofibers was achieved through controlled calcination.

To define the required thermal profile, Thermogravimetric Analysis (TGA) was used to evaluate the thermal stability of the precursor fibers. The critical finding was that pure ceramic fibers, without carbon residues, resulted from calcination performed at 600 °C. Elevated heat treatment temperatures were observed to accelerate the crystallization of the ceramic component, leading to the gradual emergence of multiple distinct phases.

Morphological changes and mean diameter variation were quantified using Electron Microscopy across the different calcination temperatures. Energy-dispersive X-ray spectroscopy (EDX) was used in conjunction with microscopy to verify elemental composition. Furthermore, nitrogen adsorption measurements established the surface area, while X-ray Diffraction (XRD) was crucial for confirming both the phase composition and the degree of crystallinity in the heat-treated fibers. Based on the obtained results, the range of potential applications for the prepared HEO fibers was evaluated.

Acknowledgements

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Electrochemical Insulin Detection Using CuO 550 and CuO 550/CNTs Fiber-Based Sensors

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Insulin, a hormone that regulates the concentration of glucose in the blood [1], is an essential marker for the diagnosis of diabetes mellitus and various metabolic disorders. Its detection often employs carbon electrodes modified with metal or oxide nanoparticles. Cu(II) and Mn(II) ions are capable of forming interactions with insulin´s amino acid residues, altering the electrochemical response and enhancing signal detection [2].

For all experiments in this study, carbon electrodes fabricated by screen printing (SPCE 11L, DropSens, Metrohm) were used, with their surfaces modified by drop casting with CuO 550 and CuO 550/CNTs. CuO 550 was prepared using a multi-stage hydrometallurgical recycling process in collaboration with colleagues from SAS. Modified electrodes were used to study the electrochemical mechanism of insulin oxidation via cyclic voltammetry (CV).

Electrochemical responses of the prepared electrodes were obtained using CV at a scan rate of 100 $mV.s^{-1}$. The results (Figure 1) indicate that in both cases, the voltammogram obtained in the presence of insulin shows an oxidation peak around 0.45 V, corresponding to insulin oxidation. However, for the CuO 550/CNTs electrode, the electrochemical response was significantly stronger.

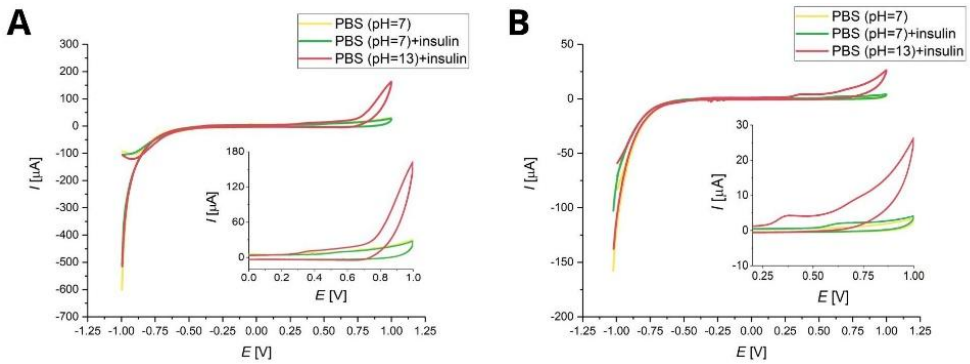

Figure 1 Cyclic voltammogram of PBS and PBS with 10 µM insulin on CuO-modified electrodes at a scan rate of 100 $mV.s^{-1}$ (A – CuO 550 without CNTs, B – CuO 550 with CNTs).

Screen-printed carbon electrodes were effectively modified with CuO 550 and CuO 550/CNTs. Electrochemical analysis demonstrated that incorporating CNTs into the CuO modification markedly enhanced the electrodes' responsiveness toward insulin.

Acknowledgements

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LIST OF POSTERS

ÚSTAV CHEMICKÝCH VIED

21.11.2025
HISTORICKÁ AULA, 9:00 HOD.

NOVEL TRENDS
IN CHEMISTRY, RESEARCH
AND EDUCATION

POSTER SESSION

1. **Andersen Herman** - Photodynamic Therapy Using UiO-66-based Metal-organic Frameworks (MOF) as Photosensitizer Carriers for Breast Cancer and Antibacterial Applications

2. **Nikitas Georgiou** - Molecular Docking Study of Novel Pyrrolidine Derivatives as Multi-target Modulators

3. **Kristína Felčíková** - Development of LOV2 Domain as Genetically Encoded Photosensitizer

4. **Barbora Borovská** - Decoding the Structural Signatures Driving Amyloid Modulation

5. **Martin Fábian** - Total Synthesis of (−)-deoxoprosopinine and its Analogues

6. **Ivana Mojžišová** - Modification of Screen-printed Electrodes for Electrochemical Gentamicin Detection

7. **Adriana Varha** - Topologically Constrained DNA, Embedding and Visualizing Non-Canonical Structures in Minicircles

8. **Oľga Parmar** - Destruction of Insulin Amyloid Fibrils by Phytoalexins with Added Antioxidant Benefit

9. **Tomáš Ján Liška** - Electrosynthetic Hydrolysis of Dihyhydropyrimidinones

10. **Monika Tvrdoňová** - 2-C-Tridecyl Piperidine-3,4,5-triols: Synthesis and Preliminary Biological Evaluation

11. **Ivan Shepa** - Electrospun High-entropy Oxide Ceramic Nanofibers

12. **Lenka Kollárová** - BSA Binding Properties of Hybrid Indole Derivatives

13. **Nikola Vargová** - Influence of Pore Hierarchy on the Catalytic Efficiency of Metal–Organic Frameworks HKUST-1 in Knoevenagel Condensation

14. **Alexandra Poliaková** - Functional Targeted Delivery of Flavin Mononucleotide by DARPin and AsLOV2 C450A Protein to Breast Cancer Cells

15. **Elena Kupcová** - Analytical Evaluation of PAH Degradation During the Cultivation of Hydrocarbon-utilizing Bacteria with Bioremediation Potential

16. **Katarína Spačeková** - Synthesis and Anticancer Profile of 6-hydroxysphingosine-based Analogues

17. **Jana Špaková Raschmanová** - DIX-like Azasugars − Synthesis and Antiproliferative Profile

18. **Dominika Snopeková** - Silver(I) Complexes With Basic Amino Acids – Their Solution Behaviour, Solid State Study and Biological Activity

LIST OF AUTHORS

Novel Trends in Chemistry, Research and Education 2025
Book of Abstracts

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