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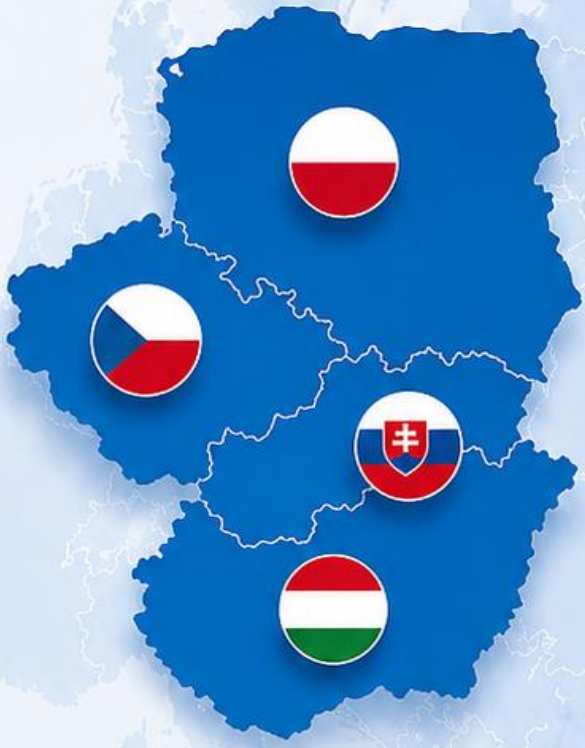

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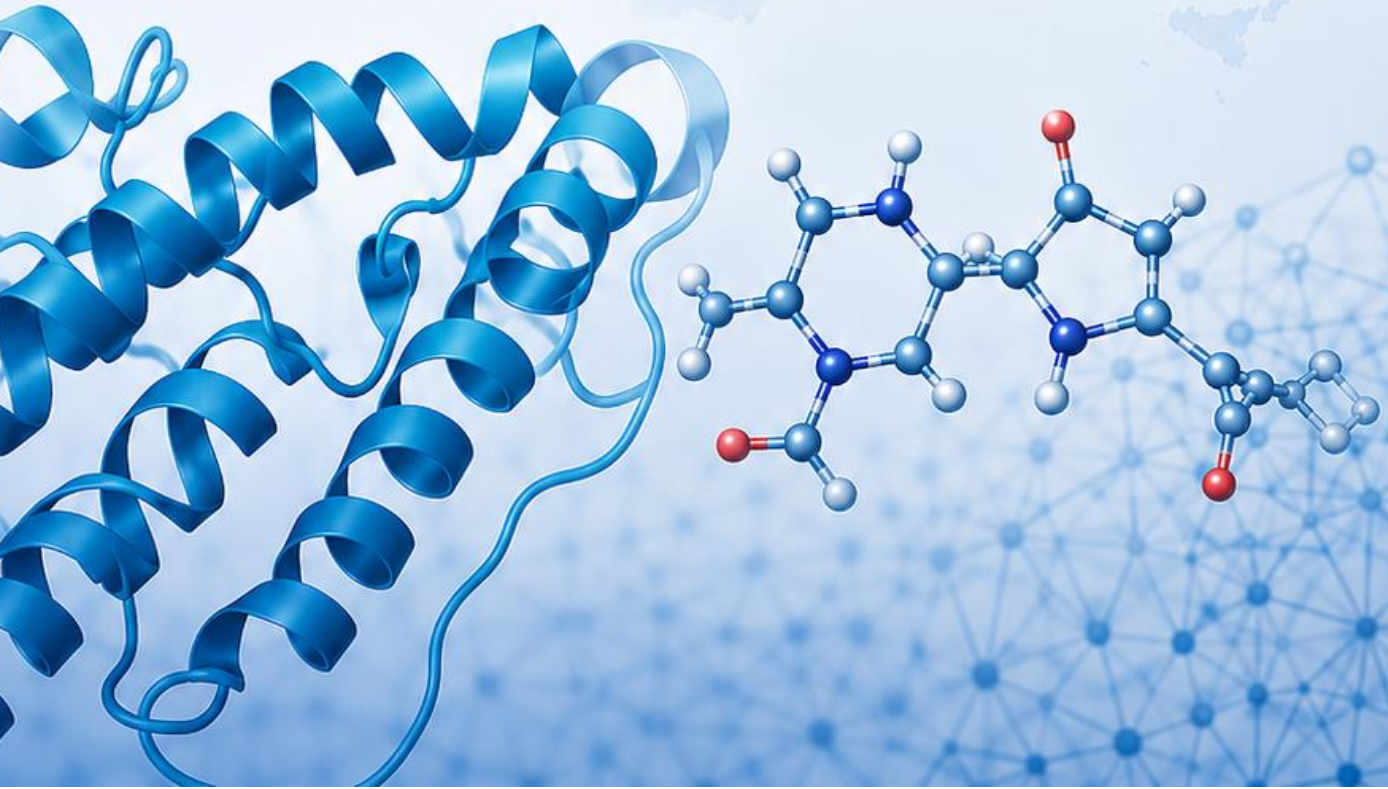

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Schedule

Wednesday 27.05.2026		
10.00-13.00	*The conference office is open*	
13.00-14.00	*Lunch*	
14.00-15.00	*Check-in to the hotel room*	
15.00-15.20	***Conference opening***	
afternoon session		
chairman:	**Marcin Palusiak**	
15.20-15.40	Michael Ries	*"Scaling up the manufacture of all-cellulose composites"*
15.40-16.00	Béla Viskolcz	*"Synthesis and targeted biotechnological applications of magnetic ferrite nanoparticles"*
16.00-16.10	Urszula Sudomir	*"Magnetic nanoparticles as an extraction tool in modern analytical chemistry"*
16.10-16.20	Timea Fóris	*"Magnetic nanoparticle based recovery of cobalt adsorbed Chlorella vulgaris biomass"*
16.20-16.30	Omid Daliri Shamsabadi	*"Electronic structure and nonlinear optical properties of functionalized cubane derivatives"*
16.30-17.00	*Coffee break*	
chairman:	**Teobald Kupka**	
17.00-17.20	Bartłomiej Kost	*"Tuning the size of nanoparticles by the composition of copolymers"*
17.20-17.40	Patryk Czapnik	*"Inclusion complexes of cyclodextrins with potential biological active compounds. Consideration on intermolecular interactions"*
17.40-17.50	Adam Buczkowski	*"pH and temperature impact on gemcitabine complexation with cucurbit[7]uril in aqueous solutions"*
17.50-18.00	Karina Kecskés	*"From adsorption to regeneration: investigation of the adsorption capacity, regenrability, and stability of zirconium-pillared montmorillonite"*
18.00-19.00	*Free time*	
19.00-21.30	*Dinner*	
Thursday 28.05.2026		
7.00-10.00	*Breakfast*	
morning session		
chairman:	**David Řeha**	
10.00-10.20	Jaroslav Burda	*"Electron pathway in Thioredoxin Reductase: from NADP to Sec-Cys redox center and how to block it"*
10.20-10.40	Nuša Matjašec	*"An enhanced molecular dynamics model of lipopolysaccharide membranes for predicting mycotoxin penetration"*
10.40-10.50	Michael Owen	*"Molecular dynamics simulations reveal the structure and stability of four apoliporotein E (ApoE) variants"*
10.50-11.00	Marek Štekláč	*"Modeling OR5A2 interactions: machine learning and docking approaches to musky odor prediction"*
11.00-11.30	*Coffee break*	
chairman:	**Jaroslav Burda**	
11.30-11.50	Teobald Kupka	*"Theoretical characteristic of selected fluorine compounds used in medicine"*
11.50-12.10	Justyna Dominikowska	*"Halide anions as halogen bond acceptors"*
12.10-12.30	Julie Mallouhi	*"Effects of deep eutectic solvents on Sinapis alba germination"*

12.30-12.40	Ioana Papa	*"Energy-entropy analysis of protein-ligand interactions"*
12.40-12.50	Khalida Khalil	*"Hemicryptophane macrocycles for water purification: targeting chloro- and fluorocarbon contaminants"*
12.50-13.00	Paulina Staniec	*"Synthesis and characterization of intermolecular interactions in a multicomponent system comprising an antidiabetic drug and a coformer designed to enhance its aqueous solubility"*
13.00-14.00	*Lunch*	
14.00-15.00	*Free time*	
afternoon session		
chairman:	**Béla Fiser**	
15.00-15.30	Mariusz Makowski	*"Recent advances from molecular design to biological activity of selected coordination compounds"*
15.30-15.50	Iwona Kuźniewska-Biernacka	*"Illuminating biomass: photocatalysis for a circular chemical economy"*
15.50-16.00	Natalia Kulik	*"Machine learning–guided prediction of rutinosidase activity toward the design of glycosylated flavonoids with antibacterial potential"*
16.00-16.10	Adrian Olszewski	*"Development of a method for the determination of citrinin in food supplements"*
16.10-16.20	Ewa Muzal	*"Large-scale physicochemical analysis of defect formation mechanisms in paraffinic organic systems using DSC"*
16.30-18.00	*Coffee break*	
16.30-18.00	**Poster session**	
18.00-19.00	*Free time*	
19.00-23.30	*BBQ Party*	
Friday 29.05.2026		
7.00-10.00	*Breakfast*	
morning session		
chairman:	**Béla Viskolcz**	
10.00-10.20	Zdenek Futera	*"Simulation techniques for electron transport in biomolecular junction"*
10.20-10.40	Babak Minofar	*"Applications of molecular modelling to address environmental challenges"*
10.40-10.50	Natalina Makieieva	*"In search of the structure-activity correlation for selected thiosulfonates – spectroscopic studies combined with molecular modelling"*
10.50-11.00	Adnan Maqbool Khan	*"$AgNO_3$ loaded polyurethane foams as light responsive materials: mechanical properties, optical response and algal toxicity"*
11.00-11.10	Wendimagegn Tagesse Dinbore	*"Optimization of glycolysis parameters for recycling polyurethane waste into repolyol and its application in flexible polyurethane foam production"*
11.10-11.20	Jonathan Netsch	*"Drude-polarizable water for protex: the impact of drude charges on collective properties"*
11.20-11.30	Valeryia Hushcha	*"Nimorazole vs isonimorazole"*
11.30-12.00	*Coffee break*	
chairman:	**Zdenek Futera**	
12.00-12.20	Ondrej Kučera	*"From biomolecular interactions to symmetry breaking in cytoskeletal networks"*
12.20-12.40	David Řeha	*"Computational study of modified lincosamide with adaptive binding to resistant ribosomes"*
12.40-12.50	György Tokaji	*"Computational study of the degradation of urethane-type molecules"*
12.50-13.00	Nesreen Alkanakri	*"Computational and experimental study of PVA-biopolymer blends"*

13.00-14.00	*Lunch*	
14.00-15.00	*Free time*	
afternoon session		
chairman:	**Babak Minofar**	
15.00-15.20	Abdenacer Idrissi	*"Interfacial plasticization of curcumin polymorphs by supercritical CO_2: insights for polymorph control in CO^{2-} based processing"*
15.20-15.40	Marion Sappl	*"Simulated spectra of metal-organic frameworks from transferable force fields"*
15.40-15.50	Tamás Horváth	*"Classical and ab initio dynamics of the Ca^{2+} and Sr^{2+} chelation by EDTA and Decorporol"*
15.50-16.00	Gergő Máté Hatvani-Nagy	*"Computational study of siderophore pyoverdine and metal interaction"*
16.00-16.30	*Coffee break*	
chairman:	**Abdenacer Idrissi**	
16.30-16.50	Béla Fiser	*"From reactants to urethanes: computational insights into amine catalysis"*
16.50-17.10	Rehana Bano	*"Rational materials engineering of single-atom catalysts for sustainable NH_3 production"*
17.10-17.20	Anikó Csábrádiné Jordán	*"Effects of DEOA Concentration and Abiotic Degradation on the Structural Integrity and Ecotoxicity of Polyurethane Foams"*
17.20-17.30	Marcin Wlaźlak	*"Influence of radiation on the crystallization of the TTCA-pyridazine system"*
17.30-18.50	*Free time*	
18.50-19.00	*Group photo*	
19.00-1.00	*Conference Dinner*	
Saturday 30.05.2026		
8.00-11.00	*Breakfast*	
8.00-11.00	*Check-out from the hotel*	

Table of Abstracts

Online Oral Presentation

SCALING UP THE MANUFACTURE OF ALL-CELLULOSE COMPOSITES

M. E. Ries, Haitham Alrajhi.

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All-cellulose composites (ACCs) have attracted growing attention as sustainable alternatives to petroleum-based composites. In these materials, both the matrix and the reinforcing phase are derived entirely from cellulose, avoiding the need for mixed constituents. Because cellulose is abundant, renewable, and obtainable from waste biomass, it aligns well with concerns about climate impact and resource depletion. It also offers strong mechanical performance and good thermal stability while remaining biodegradable. These advantages, combined with the potential for recycling and circular-economy use, position ACCs as potential next-generation, bio-based engineering materials. Dissolving cellulose is essential before regenerating it into useful materials through antisolvent coagulation. During this step, cellulose chains reorganise into amorphous regions and cellulose II crystals.

This study examines the effect of water content on ACC production; understanding this behaviour is important because imidazolium-based ionic liquids readily absorb moisture, which weakens the anion's hydrogen-bonding ability and reduces their effectiveness as cellulose solvents. Even small amounts of water, which could not be readily avoided in an industrial setting, have been shown to hinder dissolution by disrupting solvent-cellulose interactions. As a result, moisture content plays a critical role in determining how efficiently cellulose can be regenerated and limits the manufacture of ACCs at scale.

Dimethyl sulfoxide (DMSO), originally identified in the late 1800s as a by-product of wood-pulp processing, is a colourless, water-miscible, polar aprotic solvent. Although it cannot dissolve cellulose on its own, its low viscosity, low toxicity and low cost make it an effective co-solvent. By reducing ionic-liquid viscosity, DMSO enhances mass transport and improves cellulose solvation. This work explores how DMSO, in addition, mitigates water contamination and improves the resulting mechanical performance of all-cellulose composites. This has the potential to lead to a practical way of upscaling the manufacture of all-cellulose composites.

Oral Presentation

RATIONAL MATERIALS ENGINEERING OF SINGLE-ATOM CATALYSTS FOR SUSTAINABLE NH_3 PRODUCTION

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The development of advanced nanomaterials for sustainable energy conversion has attracted significant attention, particularly for electrochemical nitrogen reduction reaction (NRR) under ambient conditions as a green alternative to the Haber-Bosch process. Single-atom catalysts supported on nanostructured materials have emerged as promising candidates due to their high atomic utilization efficiency, tunable electronic properties, and enhanced catalytic activity. Density functional theory (DFT) calculations have been employed to systematically explore transition metal-decorated oxide-based nanostructures (TM = Sc-Zn) as promising single-atom catalysts for NRR. Most transition metal systems exhibit strong chemisorption toward N_2, with interaction energies ranging from -2.49 to -1.11 eV, whereas Zn displays comparatively weak physisorption behavior [1]. Incorporation of transition metals significantly reduces the electronic energy gap of the host nanostructure, leading to enhanced electrical conductivity and improved charge transfer characteristics, which are essential for efficient catalytic performance. Comprehensive electronic structure analyses, including density of states, natural bond orbital, interaction region indicator, and quantum theory of atoms in molecules calculations, reveal that transition metal doping markedly enhances N_2 activation compared to the pristine support. Among the studied systems, the Mn-based catalyst demonstrates the highest NRR performance, delivering a low limiting potential of -0.84 V via the alternating pathway. Reaction energetics and intermediate stability were further examined to identify the most favorable ammonia formation mechanism. These findings provide theoretical insights into the rational design of nanostructured single-atom catalysts and highlight the potential of engineered nanomaterials for efficient ambient ammonia synthesis.

Acknowledgments

RB is grateful for the financial support provided by the University Research Scholarship Program of the Ministry for Culture and Innovation, funded by the National Research, Development, and Innovation Fund. We acknowledge the Digital Government Development and Project Management Ltd. for awarding us access to the Komondor HPC facility based in Hungary. Calculations have also been carried out using resources provided by Wroclaw Centre for Networking and Supercomputing (http://wcss.pl).BF was supported by the János Bolyai Research Scholarship of the Hungarian Academy of Sciences.

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ILLUMINATING BIOMASS: PHOTOCATALYSIS FOR A CIRCULAR CHEMICAL ECONOMY

I. Kuźniarska-Biernacka[1], P. Miranda, B. Valentim[2].

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The increasing reliance on fossil fuels has contributed to severe climate issues, including extreme heat, droughts, and flooding, driven by greenhouse gas emissions. Therefore, sustainable alternatives for chemical and fuel production are urgently needed. Biomass offers a promising route to reduce our dependence on fossil fuels. High amounts of lignocellulosic biomass are produced (~180 billion tons annually), which can be converted into 5-hydroxymethylfurfural (HMF), a key platform molecule for value-added chemicals (Fig. 1). [1]

Conventional HMF oxidation relies on oxidants such as hydrogen peroxide or tert-butyl hydroperoxide, often requiring hazardous solvents (e.g., toluene, DMF) and noble metal catalysts. These drawbacks highlight the need for greener approaches. [2]

Herein, coal fly ash (CFA), an abundant industrial waste, is valorized as a precursor for the preparation of innovative multicomponent photocatalytic composites. The developed materials consist of magnetic particles recovered from CFA, natural biopolymers, and photoactive sites. These act as both photocatalysts and adsorbents, enabling efficient and sustainable transformation processes under mild conditions. [3]

The synthesized TiO_2-free composite demonstrated outstanding photocatalytic performance, achieving 92.5% HMF conversion with high selectivity (90.5%) toward 2,5-diformylfuran (DFF). In contrast, conventional thermal oxidation using tert-butyl hydroperoxide at 100 °C resulted in near-complete conversion (99.7%) but significantly lower selectivity (5%) toward DFF.

These results highlight the potential of fly ash-derived photocatalysts as sustainable, efficient, and selective systems for biomass valorization, contributing to the advancement of green chemistry and circular economy strategies.

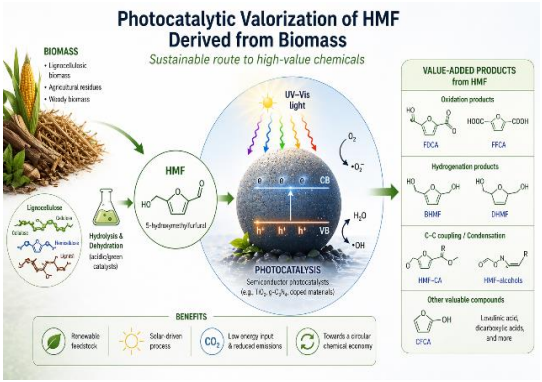

Figure 1. HMF conversion route map.

Acknowledgments

The authors thank the Foundation for Science and Technology for support of this work through the projects INSUB (DRI/India/0315/2020; https://doi.org/10.54499/DRI/India/0315/2020), and CATCH (Operação n.º 16006, Ref. 2023.16411.ICDT; COMPETE2030-FEDER-00714500; https://doi.org/10.54499/2023.16411.ICDT).

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INTERFACIAL PLASTICIZATION OF CURCUMIN POLYMORPHS BY SUPERCRITICAL CO_2: INSIGHTS FOR POLYMORPH CONTROL IN CO_2-BASED PROCESSING

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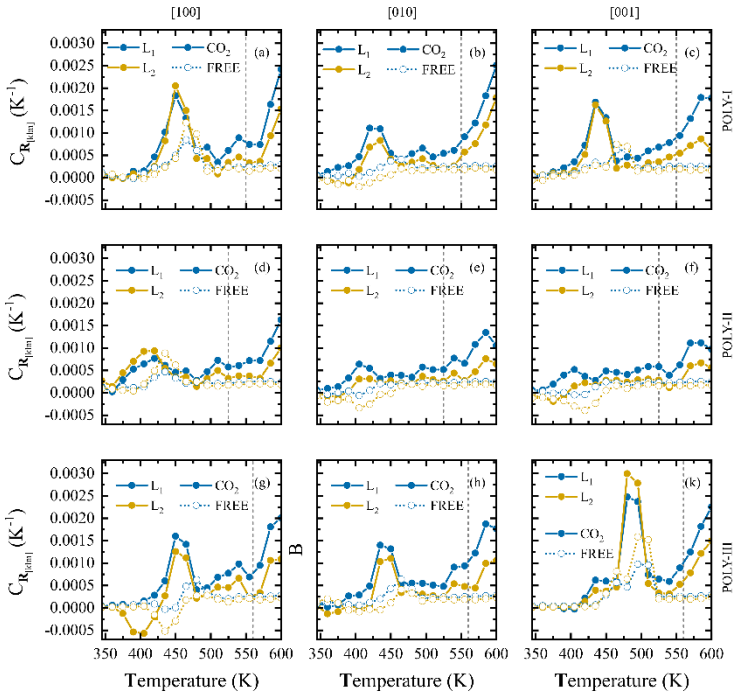
Polymorph selection in molecular active pharmaceutical ingredients (APIs) is increasingly recognized as an interfacial rather than a bulk-governed phenomenon. At crystal–air or crystal–fluid boundaries, molecules experience reduced coordination, enhanced mobility, and distinct conformational preferences that accelerate nucleation and bias polymorph outcome. Crystallization can be orders of magnitude faster at free surfaces than in the bulk, an effect demonstrated for indomethacin by Sun and co-workers, who observed upward crystal growth driven by enhanced surface mobility [1]Similar findings across diverse APIs show that interfacial packing, orientation, and functional-group exposure can stabilize specific polymorphs, enabling selective crystallization on engineered substrates. Such interfacial-driven behavior directly influences solubility, stability, wettability, and mechanical performance, and has motivated substantial efforts to control polymorphs through solution, melt, mechanochemical, microfluidic, or solid-state routes. Building on our prior characterization of the free curcumin interface and our validated CO_2 force field calibrated to reproduce the experimental critical point [2], the present study investigates how temperature and $scCO_2$ reorganize CUR surfaces at the molecular scale. Simulations were conducted along an isochore corresponding to the density $\rho = 1.1\rho_c$, where ρ_c is the CO2 critical density, spanning 350–500 K (70–750 bar), where $scCO_2$ retains high fluidity and strong sorption capacity. Under these conditions, the number of $scCO_2$ molecules far exceeds that of CUR, ensuring that $scCO_2$ behaves as a bulk reservoir whose thermodynamic state is not perturbed by the presence of the solid. The talk is organized into two complementary parts. The first examines how exposure to $scCO_2$ modifies the structure and dynamics of interfacial CUR molecules using five coupled classes of observables. The average layer position, $\langle R_{[klm]} \rangle$, and its normalized thermal sensitivity, $C_{\langle R_{[klm]} \rangle}$ (see Figure 1) quantify the outward displacement of the first two interfacial layers and identify the onset of thermally activated softening. The positional fluctuations, $\langle R_{[klm]} \rangle$, probe the roughening and dynamic broadening of the interfacial region. The site-specific distance $\langle \mathrm{d}(\mathrm{CUR}_{(O)} - \mathrm{CO_2}_{(C)}) \rangle$ reports how closely $scCO_2$ can approach chemically distinct oxygen-bearing moieties of CUR in the first interfacial layer and therefore directly measures local interfacial accessibility. The orientational descriptors P(ψ) and P(R,ψ) reveal how molecular orientation is

coupled to layer-normal position within L1 and L2, while the conformational populations quantify the intramolecular response of CUR to interfacial softening. Together, these observables disentangle the respective roles of $scCO_2$ access, layer mobility, orientational reorganization, and conformational redistribution, thereby providing a unified molecular picture of $scCO_2$ driven polymorph- and face-selective plasticization. The second part then examines the reciprocal organization of interfacial CO_2 molecules at the CUR surface through their own layer-resolved positional, fluctuation, and orientational descriptors.

Figure. Temperature dependence of the normalized distance sensitivity parameter $C_{\langle R_{[klm]}\rangle} = \frac{1}{\langle R_{[klm]}\rangle}\frac{d\langle R_{[klm]}\rangle}{dT}$ for the first (L_1) and second (L_2) molecular layers of curcumin polymorphs POLY-I (a-c), POLY-II (d-f), and POLY-III (g-i) along the [100], [010], and [001] crystallographic directions. Filled symbols correspond to $scCO_2$-exposed surfaces, while open symbols represent free surfaces



Acknowledgments

This work was performed using computational facilities of the Centre de Resources Informatiques (CRI) de l'Université de Lille

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ELECTRON PATHWAY IN THIOREDOXIN REDUCTASE: FROM NADP TO SEC-CYS REDOX CENTER AND HOW TO BLOCK IT

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Thioredoxin reductase (TrxR) belongs to the family of reduction enzymes responsible for elimination of ROS in cells. In natural state TrxR is arranged in hexamer associate where three pairs of monomeric units represent working unit. Electron flux starts from reduced form of NADP coenzyme transferring electron pair via FAD coenzyme to first Cys-Cys redox center. While these three parts are in close vicinity and proton assisted electron transfer (PAET) can be expected as a reduction mechanism, final reduction pathway to the other redox Cys-Sec center occurs through helical channel ca 10 Å long. Moreover, this second redox unit is localized in the C-terminus of second monomer unit. From literature, it is known (or better generally accepted) that this Cys-Sec is the place where enzymatic activity can be successfully blocked. Gold(I) metallodrugs were reported as effective complexes capable for such a blocking coordination.

INCLUSION COMPLEXES OF CYCLODEXTRINS WITH POTENTIAL BIOLOGICAL ACTIVE COMPOUNDS. CONSIDERATION ON INTERMOLECULAR INTERACTIONS

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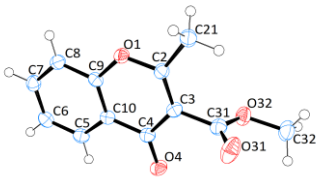
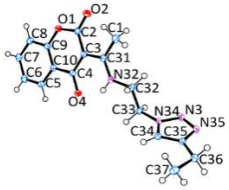
The most effective way to search for new anticancer drugs is chemical modification of known compounds with confirmed biological activity. Many medicinal substances contain a chromone or triazole skeleton in their structure (e.g. diosmin with anti-inflammatory properties [1] and tazobactam - antibacterial effect [2]). Due to the limited reports about biological activities of chromone analogues condensed with compounds *N*-containing heterocyclic ring, we decided to synthesize 2 esters of chromones and 12 chromone analogues condensed with triazoles, imidazole, and pyrazoles. Molecular structures of two representative synthesized chromone derivatives are shown in **Figure 1**. We performed fully physicochemical characterization of newly synthesized compounds and comprehensive analysis of noncovalent interactions. Biological studies of new compounds we performed by carrying out preliminary *in silico* calculations and *in vitro* studies. Another aim of our research was to attempt the crystallization and characterization of the interactions in cyclodextrin inclusion complexes with commercially available compounds [4], followed by the characterization of the interactions in cyclodextrin-chromone analogues.

a) 

b) 

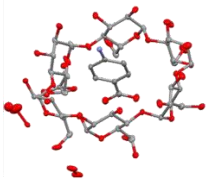
c) 

Figure 1. Molecular structures of a) ester of chromonecarboxylic acid, b) ester condensed with triazole [3], inclusion complex of cyclodextrin [4]

Acknowledgments

We gratefully acknowledge Polish high-performance computing infrastructure PLGrid (HPC Center: ACK Cyfronet AGH) for providing computer facilities and support within computational grant no. PLG/2025/018176 and the Wroclaw Centre for Networking and Supercomputing (http://www.wcss.pl) for providing access to HPC machines, as part of the calculations were performed using the Gaussian 16 software.
This work was supported by found of University of Lodz Doctoral School of Exact and Natural Sciences, grant no. B2410000000013.05 (P. Czapnik) and by Medical University of Lodz (grant No. 503/3-016-02/503-31-001).

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HALIDE ANIONS AS HALOGEN BOND ACCEPTORS

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Halide anions may serve as efficient mono- and multidentate acceptors of halogen bonds. The survey of the Cambridge Structural Database (CSD) [1] is performed to establish how common are C−X···Y^- (X, Y = F, Cl, Br or I) contacts of different types, [2] and to study the frequency of occurrence of halide anions as halogen bond acceptors in the context of their denticity. [3] The obtained results are further compared with the findings based on computational studies performed for the following model systems: F_3C−X···Y^- [2] and $(F_3C–I)_n$···Y^- (X, Y = F, Cl, Br or I; $n \leq 5$). [3] A canonical energy decomposition analysis (canonical EDA) [4] together with the quantitative Kohn−Sham molecular orbital model and the many-body expansion of the interaction energy allow to understand the properties of studied systems, especially the behaviour of fluorides being exceptional among halides as halogen bond acceptors.

Acknowledgments

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FROM REACTANTS TO URETHANES: COMPUTATIONAL INSIGHTS INTO AMINE CATALYSIS

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In this work, a diverse set of amine catalysts were examined to identify key properties relevant to selecting the most suitable species for specific applications in polyurethane synthesis. Both structural and energetic descriptors were evaluated, including steric parameters (expressed as %Vbur) and proton affinities (PA). It was found that 1-(3-aminopropyl)imidazole (APIM) has the lowest calculated proton affinity (905.8 kJ mol^{-1}) among the studied set of compounds, indicating a greater tendency of its conjugate acid to donate a proton. In contrast, steric analysis revealed that tertiary amines generally exhibit higher buried volumes than primary and secondary amines. Notably, the differences in %VBur values between 2,2'-dimorpholinodiethylether (DMDEE) (67.0%), dimethylaminoethylether (DMAEM-1N*) (66.4%), and *N*-Ethylmorpholine (NEM*) (65.8%) are relatively small; these values indicate similar steric environments, rather than a strictly greater steric effect for one catalyst over the others. However, given the small numerical differences, these catalysts can be considered to exhibit comparable steric profiles. Additionally, the catalysts were analyzed based on their impact on catalytic urethane formation as well. Overall, this work provides deeper insight into how electronic and steric factors influence urethane formation and offers a rational basis for selecting appropriate catalysts tailored to specific applications.

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SIMULATION TECHNIQUES FOR ELECTRON TRANSPORT IN BIOMOLECULAR JUNCTION

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The charge-transport properties of molecular systems are governed by structural motifs, chemical composition, redox-active sites, environmental effects, and thermal fluctuations. In metal–molecule junctions, band alignment between molecular states and the electrode Fermi level is also a key factor, so both the mechanism and efficiency of transport can change markedly with the environment. For example, redox proteins commonly transfer electrons by hopping in biological environments, but may support tunneling in metallic junctions used in molecular nanoelectronics [1,2]. Advances in this field have gone hand in hand with the development of computational methods that help interpret experiments and provide microscopic insight.

Non-equilibrium Green's function (NEGF) methods combined with electronic-structure approaches such as density functional theory (DFT) are the standard tools for calculating tunneling currents and conductance in open molecular systems. However, their computational cost limits their application to relatively small systems. Approximate but reliable methods are therefore needed for realistic biomolecular junctions involving peptides and proteins. These include semi-empirical and tight-binding models, band-alignment correction schemes, approximate treatments of electrode self-energies, and linear-response descriptions of external fields [3]. Because these systems are also subject to significant thermal fluctuations, dynamical approaches that include non-adiabatic and electron–nuclear coupling effects are essential. In this presentation, I will discuss the accuracy of these techniques using model biomolecular systems relevant to molecular nanoelectronics.

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TUNING THE SIZE OF NANOPARTICLES BY THE COMPOSITION OF COPOLYMERS

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The precise control of nanoparticle size is a critical factor influencing the efficiency of drug delivery systems, particularly in cancer therapy [1]. In this study, we investigate the relationship between copolymer composition and the resulting size of polymeric nanoparticles designed for pH-responsive drug delivery. Amphiphilic copolymers based on lactide or ethylene glycol with allyl glycidyl ether were synthesized and subsequently functionalized with various chemical groups to modulate their physicochemical properties. Nanoparticles were prepared using a self-assembly approach, and their size, distribution, and stability were systematically characterized using dynamic light scattering (DLS) and electron microscopy techniques. The results demonstrate that the ratio of hydrophobic to hydrophilic segments in the copolymer plays a decisive role in determining nanoparticle size. Increased hydrophobic content led to the formation of larger particles, while higher incorporation of functionalized hydrophilic moieties resulted in smaller, more uniform nanoparticles. Additionally, the presence of ionizable functional groups enabled pH-responsive behavior, influencing both particle stability and size under varying environmental conditions. This tunability is particularly relevant for targeting tumor microenvironments, where pH variations can be exploited for controlled drug release.

Acknowledgments

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FROM BIOMOLECULAR INTERACTIONS TO SYMMETRY BREAKING IN CYTOSKELETAL NETWORKS

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Biological systems rely on symmetry breaking at all scales: cells polarise, tissues acquire structure, and organisms develop defined axes and handedness. At the molecular level, many components are themselves polar or chiral, yet this alone does not explain how organised asymmetry arises at larger scales from molecular interactions.
The cytoskeleton provides a natural setting for addressing this problem. It is a dynamic network of protein filaments, molecular motors, and crosslinking proteins that organises the cell interior and generates forces for transport, division, and shape change. Molecular motors, which read the structural polarity of filaments, introduce microscopic directionality, yet their presence alone does not always determine the large-scale outcome. Instead, asymmetry can arise from seemingly symmetric interactions that, in filamentous systems, bias filament rearrangements through geometric constraints.
In this talk, I will focus on a small number of non-canonical examples from minimal reconstituted filament systems. These systems allow asymmetry to be examined under well-defined conditions and reveal how collective interactions among filaments, motors, and crosslinkers give rise to large-scale asymmetries. Along the way, I will touch on concepts such as multivalency, steric constraints, entropic effects, and kinetic trapping.

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THEORETICAL CHARACTERISTIC OF SELECTED FLUORINE COMPOUNDS USED IN MEDICINE

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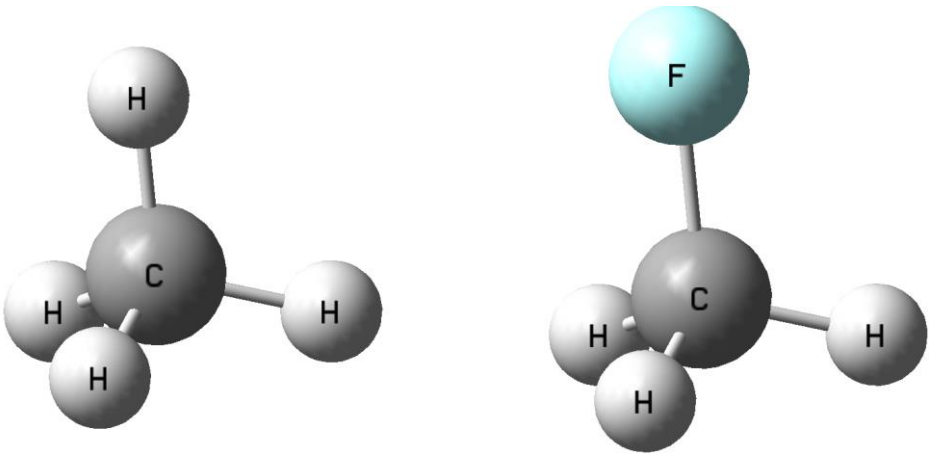
Fluorine containing compounds are very often used in medical treatment. Their application starts from simple anesthetic till antibiotics and anticancer drugs. The structure-chemical relationship, property and biological activity of compounds containing fluorine is well recognized. As continuation of our previous studies on fluorine-containing molecules, we decided to study the geometry and NMR properties of CF4, CF3H, CF2H2, CFH3 using sophisticated coupled cluster theory in the complete basis set limit. The reference molecule was methane.
The obtained reference data enabled us to assess the performance of arbitrary selected 28 density functionals. As an example of DFT performance, we compared the experimental NMR chemical shift with the theoretical prediction.



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RECENT ADVANCES FROM MOLECULAR DESIGN TO BIOLOGICAL ACTIVITY OF SELECTED COORDINATION COMPOUNDS

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The growing challenge of therapeutic resistance in both infectious diseases and cancer necessitates the continuous development of novel bioactive compounds with diverse mechanisms of action. In this context, metal–ligand systems have emerged as a versatile platform for the design of next-generation therapeutics, enabling fine-tuning of physicochemical properties and biological activity.

This presentation summarizes the most significant recent findings from our research group in the field of biologically active organic compounds and their coordination compounds with *d*-block metal ions. Particular attention will be devoted to sulfonamide derivatives and their metal complexes, which exhibit a wide spectrum of bioactivity, including antimicrobial and anticancer effects. The relationship between molecular structure and activity has been explored through combined experimental and computational approaches, highlighting the importance of parameters such as hydrogen bonding, lipophilicity, and acid–base equilibria [1]. In addition, selected transition metal complexes, including Rh(III), Ir(III), and Cd(II) systems, have been synthesized and characterized, revealing diverse coordination modes and structural features [2,3,4]. Their interactions with biomolecules, such as DNA and serum proteins, were investigated using modern analytical techniques, providing insight into their mechanisms of action [5]. Biological studies demonstrate that these compounds exhibit promising activity profiles, including selective cytotoxicity and antifungal effects, depending on both ligand design and metal center selection [6,7].

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EFFECTS OF DEEP EUTECTIC SOLVENTS ON *SINAPIS ALBA* GERMINATION

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Deep eutectic solvents (DESs) have emerged as a new class of environmentally friendly solvents with promising applications across various industrial sectors [1], [2]. Despite their growing utilization, their potential ecological effects, particularly on biological systems, remain insufficiently understood [3]. In this study, DES systems based on Choline Chloride: Urea (ChCl: Urea, 1:1 and 1:2), Glucose: Urea (Glu: Urea, 1:1 and 1:2), and Choline Chloride: Ascorbic acid (ChCl: AsA, 2:1) were prepared and characterized using FTIR, density, and viscosity measurements. FTIR analysis confirmed the formation of strong hydrogen-bonding interactions in all systems, with more pronounced spectral shifts observed at higher urea ratios. Density trends varied depending on composition, while all systems exhibited non-Newtonian shear-thinning behavior, with viscosity decreasing as urea content increased. Glu: Urea (1:1) showed the highest viscosity due to its extensive hydrogen-bonding network.

Biological activity was assessed using *Sinapis alba* seed germination at concentrations ranging from 0.1 to 10% (w/w). At low concentrations, ChCl: Urea (1:1) showed no toxicity, achieving ~100% germination, while other systems maintained moderate germination rates (77–87%). However, germination significantly decreased at ≥0.5%, indicating a concentration-dependent effect. ChCl: AsA (2:1) exhibited inhibitory behavior due to its acidic nature, while all DESs were fully toxic at higher concentrations (5–10%). These findings highlight the tunable physicochemical and biological properties of DESs, emphasizing the importance of concentration control for environmentally relevant applications.

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AN ENHANCED MOLECULAR DYNAMICS MODEL OF LIPOPOLYSACCHARIDE MEMBRANES FOR PREDICTING MYCOTOXIN PENETRATION

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Absorption is a key process in toxicology, drug development, and bioavailability studies. In biological systems, this process is strongly influenced by the presence of the microbiota, which can mask the actual number of bioavailable molecules [1]. To investigate these processes at a molecular level, molecular dynamics (MD) simulations were employed to study membrane penetration processes [2]. Starting from the lipopolysaccharide (LPS) membrane of Gram-negative bacteria, we focused on the penetration of foodborne contaminants - mycotoxins, which have been shown to accumulate inside the bacterial pellets [3]. Two MD systems were constructed using CHARMM-GUI, differing in the structural complexity of the lipopolysaccharides. One system represented a simplified membrane containing only lipid A, while the second included a more complex model including the oligosaccharide moiety. Each system was built with 10 ligands to improve the statistical reliability of penetration events, although this promoted artificial clustering. To prevent this, intermolecular interactions between ligands, as well as between ligands and water, were adjusted accordingly. Each system was simulated using openMM in five replicates with ten ligand molecules per simulation box over the timescale of 500 ns. The resulting trajectories were analyzed with a focus on ligand distribution along the membrane in the z-direction, the number of ligands penetrating the membrane and their retention times. The results highlight the critical role of oligosaccharide chains as a protective barrier that reduces membrane penetration. Among the tested compounds, alternariol monomethyl ether penetrated into the membrane, whereas tenuazonic showed no membrane penetration, which is in agreement with the available experimental data [3]. Overall, the developed MD framework provides a more realistic representation of bacterial membranes and is broadly applicable to the study of membrane permeability in complex biological systems.

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APPLICATIONS OF MOLECULAR MODELLING TO ADDRESS ENVIRONMENTAL CHALLENGES

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Environmental pollution is a major global concern, with contamination of water and soil by persistent organic pollutants, pharmaceuticals, hormones, and other emerging contaminants posing risks to ecosystems and human health. Addressing these challenges requires a deeper understanding of the molecular mechanisms governing the behavior, transport, and transformation of such compounds, which are often difficult to explore through experiments alone.

Molecular modelling provides valuable tools to complement experimental studies by offering detailed insights at the atomic level. Classical molecular dynamics (MD) simulations have been widely used to investigate contaminant behavior in complex environments, enabling understanding of processes that are otherwise inaccessible. These approaches help clarify intermolecular interactions, solvation effects, and dynamic processes influencing contaminant fate.

This contribution brings insights from molecular-level understanding to explore the influence of different media and the use of novel solvent classes to address environmental challenges. Using molecular dynamics simulations, we elucidate key phenomena observed experimentally and provide mechanistic insights that support the design of improved remediation strategies [1-3]. Integrating molecular-level understanding with laboratory and pilot-scale studies contributes to the development of scalable and sustainable environmental solutions.

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COMPUTATIONAL STUDY OF MODIFIED LINCOSAMIDE WITH ADAPTIVE BINDING TO RESISTANT RIBOSOMES

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Lincosamides, an important class of antibiotics in human medicine, inhibit translation by binding to the catalytic centre of the ribosome. However, their efficacy is impaired by the widespread acquisition of genes coding for erythromycin resistance methyltransferase (Erm), which confer resistance by dimethylating adenine A2058 in the 23S ribosomal RNA, rendering all clinical lincosamides ineffective. The clincelin, a novel chimeric lincosamide engineered by structurally combining the natural compounds celesticetin and lincomycin can partially retains its efficacy against erm-mediated resistant pathogens. The MD simulations were applied to study the binding of the clincelin to the drug-sensitive versus A2058-dimethylated *Staphylococcus aureus* ribosomes. The simulations show that the salicylate moiety adopts distinct binding modes on drug-sensitive versus dimethylated ribosomes. A comprehensive functional understanding of lincosamide structural modifications will enable the development of novel agents designed to overcome existing resistance.

SIMULATED SPECTRA OF METAL-ORGANIC FRAMEWORKS FROM TRANSFERABLE FORCE FIELDS

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Metal–organic frameworks (MOFs) are challenging materials in classical molecular dynamics (MD) simulations, because their chemical diversity, functionalizability, and periodicity make force field fitting costly. Transferable force fields offer a practical alternative, often with some loss of accuracy. We evaluate two approaches for MOFs: the universal classical force field tailored for MOFs, UFF4MOF [1], and a MOF-trained machine-learned interatomic potential (MLIP), MACE-MP-MOF [2]. To compute infrared spectra from MD without resorting to computationally demanding periodic quantum vibrational analyses, we employed a fixed-charge workflow. Periodic quantum calculations were used only to assign atomic partial charges, which are held constant during trajectory analysis. These charge calculations are cheaper and less failure-prone than full periodic frequency calculations, enabling simple spectroscopy predictions.

Across a representative set of MOFs spanning varied linkers and metal nodes, simulated spectra from the two force fields are compared with each other and, where available, with experimental spectra. The fixed-charge approximation provides spectral intensities, while band positions are dictated by the force field. Systematic deviations are force field dependent: UFF4MOF consistently blue-shifts carbonyl and aromatic stretching bands, whereas MACE-MP-MOF reproduces peak positions with higher accuracy. These results indicate that MLIPs specifically trained on MOFs can deliver computational vibrational spectra with transferability by design. We restrict periodic quantum mechanical calculations to charge assignment, which keeps the workflow straightforward for large, periodic MOFs.

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SYNTHESIS AND TARGETED BIOTECHNOLOGICAL APPLICATIONS OF MAGNETIC FERRITE NANOPARTICLES

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This work presents the synthesis of novel, functionalized ferrite-based magnetic nanoparticles (MNPs) including superparamagnetic $MnFe_2O_4$, $MgFe_2O_4$, and $CuFe_2O_4$, alongside the development of unique, high-efficiency separation and diagnostic protocols.

In the field of diagnostics, an optimized HILIC-LC-MS-based glycomic approach was employed to demonstrate that serum N-glycosylation patterns can serve as promising non-specific biomarkers for early-stage Parkinsons disease (PD). PD-specific glycan alterations were identified, with a particular focus on the significantly elevated levels of high-mannose glycans observed in male patients.

For molecular biology applications, a unique nucleic acid isolation method was developed based on amine-functionalized $MgFe_2O_4$ nanoparticles. This procedure enables the extraction of high-purity plasmid and genomic DNA from complex biological matrices without the use of toxic reagents, providing a cost-effective alternative to commercial kits.

Regarding environmental bioremediation, a combined system was established using *Chlorella vulgaris* algae to sequester heavy metals (cobalt) from aqueous phases. The magnetic separation of the biomass was achieved via pH-dependent electrostatic interactions using our synthesized functionalized particles, reaching a separation efficiency exceeding 99% within 60 seconds.

To advance MRI diagnostics, solvothermally synthesized PB-$MnFe_2O_4$-NH_2 and PVP-$CuFe_2O_4$-NH_2 contrast agents were evaluated. In vivo studies confirmed excellent biocompatibility and significant relaxivity, enabling high-resolution imaging of the liver and spleen. Our results demonstrate that these novel nanostructures and their associated protocols offer effective alternatives to conventional biotechnological methods.

The results presented herein underscore the transformative impact of specialized magnetic nanoparticles in streamlining complex biotechnological processes while offering superior performance over conventional methods.

Short Oral Presentation

COMPUTATIONAL AND EXPERIMENTAL STUDY OF PVA-BIOPOLYMER BLENDS

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The electrospinning of natural biopolymers, such as collagen and chitosan, is challenging due to their low solubility and limited chain entanglement [1]. The ways in which synthetic polymers enhance their spinnability are not yet fully understood. This study combines experimental electrospinning with molecular dynamics simulations to examine how molecular interactions influence nanofiber formation in collagen–PVA and chitosan–PVA blends at different ratios (1:1, 1:2, and 2:1). Results show that the blend composition affects solvent accessibility, hydrogen-bonding patterns, and the enthalpy of inter-chain interactions, which together determine solution cohesion and stability during electrospinning. PVA-rich (1:2) systems display an optimal balance between polymer–polymer cohesion and polymer–water interactions, forming compact yet sufficiently hydrated molecular structures that promote chain association without excessive swelling. This molecular organization enables stable jet formation and produces uniform, bead-free nanofibers with the smallest fiber diameters among the tested systems. In contrast, blends rich in biopolymers exhibit excessive hydration, greater solvent exposure, and reduced intermolecular cohesion, leading to unstable electrospinning behavior. These results provide a molecular-level explanation for PVA's role in improving solubility and spinnability, and demonstrate that combining molecular simulations with experimental validation enables predictive optimization of biopolymer electrospinning systems.

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pH AND TEMPERATURE IMPACT ON GEMCITABINE COMPLEXATION WITH CUCURBIT[7]URIL IN AQUEOUS SOLUTIONS

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Temperature and pH value of solution are important factors having impact on supramolecular complexation of ligands with cucurbiturils in aqueous solutions. One of the intense studied supramolecular host with potential biomedical application is the seven-membered cucurbituril (cucurbit[7]uril, Q7), which can be used for complexation, stabilization and transporting molecules of selected anticancer drugs, like gemcitabine (Gem). Isothermal titration calorimetry (ITC) results show that Gem in cationic form is efficiently included inside the cavity of Q7 cucurbituril, forming thermodynamically stable supramolecular complexes with 1:1 stoichiometry in aqueous solutions at room temperature (25°C) [1-3]. Acidification of the medium [4, 5] as well as lowering temperature (from 50°C to 5°C) increases binding constant *K* of the formed Gem-Q7 complex. pH of medium has impact on the equilibrium between protonated and unprotonated forms of gemcitabine in aqueous solutions. Therefore both ITC calorimetry and ^{1}H-^{1}H DOSY spectroscopy were used to assess the difference in affinity of Q7 macrocycle towards neutral and protonated Gem ligand.

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MAGNETIC NANOPARTICLE BASED RECOVERY OF COBALT ADSORBED *CHLORELLA VULGARIS* BIOMASS

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The treatment of heavy metal contaminated waters and the recovery of valuable metals have become increasingly important from both environmental protection and resource management perspectives. The presentation describes the recovery of heavy metal-adsorbed *Chlorella vulgaris* biomass using different magnetic nanoparticles, with particular emphasis on the mechanisms governing nanoparticle–biomass surface interactions.

Cobalt-adsorbed algal biomass was separated using γ-Fe_2O_3 (maghemite) nanoflowers and amine functionalized $MgFe_2O_4$ ($MgFe_2O_4$-NH_2) nanoparticles. Nanoparticle biomass interactions and material properties were characterized by TEM/HRTEM, SEM, FTIR, VSM, and zeta potential analysis. Magnetic separation of cobalt-adsorbed biomass was achieved rapidly and efficiently for both nanoparticle systems, significantly outperforming conventional sedimentation. The enhanced separation performance was attributed to electrostatic interactions between nanoparticle functional groups and the negatively charged algal surface, which were strengthened by protonation at low pH and promoted stable nanoparticle–biomass binding [1,2].

These findings demonstrate a biocompatible, rapid, and potentially scalable platform for cobalt removal and biomass recovery, highlighting the promise of microalgal–magnetic nanoparticle systems for sustainable industrial wastewater treatment.

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PHYSICOCHEMICAL PROPERTIES AND DRUG-RELEASE BEHAVIOR OF SURFACE-ENGINEERED FE–CD CORE–SHELL SYSTEMS

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Magnetic core–shell systems are increasingly investigated as multifunctional drug carriers due to their ability to integrate transport, therapeutic action, and magnetic guidance within a single platform. Such materials enable cancer treatment via magnetic hyperthermia and may additionally support bone tissue regeneration, while external magnetic fields allow for targeted drug accumulation and reduced nonspecific distribution [1,2]. In this work, iron–cadmium (Fe–Cd) magnetic core–shell systems and their surface-modified derivatives are presented as pH-responsive carriers for anticancer drug delivery.

The physicochemical properties, magnetic behavior, and functional performance of the systems were studied with particular emphasis on their interaction with the anticancer drug daunorubicin. Structural and chemical characterization was performed using transmission electron microscopy, Fourier-transform infrared spectroscopy, and Mössbauer spectroscopy over a range of temperatures, providing insight into the core–shell architecture and the influence of shell modification on the local chemical environment of the iron-containing core.

Drug adsorption and release were investigated under different pH conditions, with special attention paid to acidic environments corresponding to the tumor microenvironment. The results demonstrate that appropriately surface-engineered Fe–Cd core–shell systems exhibit high drug adsorption efficiency and enhanced drug release at lower pH values. Furthermore, surface modification was found to influence the cytotoxic properties of the materials. Overall, the findings highlight the potential of Fe–Cd core–shell systems with tailored surface properties as pH-responsive nanocarriers for targeted anticancer therapy.

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CLASSICAL AND AB INITIO DYNAMICS OF THE Ca^{2+} AND Sr^{2+} CHELATION BY EDTA AND DECORPOROL

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In this work, the interaction of calcium and strontium ions with the chelating agents EDTA, Kryptofix 22 (22, 1,7,10,16-Tetraoxa-4,13-diazacyclooctadecane) and Decorporol ((7,16-bis-malonate)- 1, 4, 10, 13- tetraoxa- 7,16-diazacyclooctadecane – bis -malonicacid)) was investigated using a combined experimental and computational approach. As the number of nuclear power plants increases, greater health risks associated with strontium-90 exposure are created, and the development of chelating agents that can selectively bind Sr^{2+} over Ca^{2+} is becoming critical. To evaluate, a multi-level modelling approach with reliable accuracy was required. For this purpose, quantum chemical calculations were performed, and it was found that the r^{2}SCAN-3c composite density functional (DFT) method, together with the SMD solvation model, reproduces ion-exchange free energies with near-chemical accuracy. Known thermodynamic data for EDTA were used as a reference, and the computational results were shown to be on par with experimental values. Molecular dynamics (MD) simulations were then carried out, and funnel-metadynamics was applied to follow the chelation process and to calculate binding free energies. To improve the model, atomic partial charges were recalculated with the MBIS method, which resulted in better sampling and more stable free-energy profiles. Parallel to the computational work, ITC experiments were performed to obtain binding enthalpies, association constants, and binding Gibbs free energies for the systems examined. The simulations for EDTA agreed with the experimental results and the results demonstrated that Decorporol exhibits a stronger affinity for Sr^{2+} than for Ca^{2+}, as indicated by an exergonic ion-exchange process. This behavior was confirmed at different temperatures and at physiological conditions. Overall, the combined DFT–MD–ITC approach developed in this project provided a detailed picture of the thermodynamics and mechanism of ion chelation. It was shown that Decorporol favors Sr^{2+} over Ca^{2+}. The results demonstrate that the established method is suitable for future studies on more complex systems, including biological adsorption or macromolecules for ion chelation.

NIMORAZOLE vs isoNIMORAZOLE

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Nitroimidazoles are an important class of active compounds consisting of an imidazole ring substituted with a nitro (–NO_2) group and additional organic fragments. They are widely used as antimicrobial agents against Gram-positive and Gram-negative bacteria, protozoa, and helminths responsible for infectious diseases [1-2].
Nimorazole (formerly nitrimidazine) is a well-established antiprotozoal drug [2] and clinically relevant hypoxic cell sensitizers, with proven efficacy in the treatment of supraglottic and pharyngeal tumors [3]. Despite its introduction in 1970 [4] and continued therapeutic relevance, its single-crystal X-ray structure has not yet been reported.
In this communication, we present for the first time the X-ray structures of nimorazole and its isomer, isonimorazole, providing new insights into their molecular geometry and solid-state architectures. In addition, coordination complexes with selected biometals (Cu and Zn) were successfully synthesized and structurally characterized. These findings expand the structural chemistry of nitroimidazoles and open new perspectives for understanding their physicochemical properties and potential biological activity. Ongoing studies aim to evaluate the biological properties of the newly obtained crystalline forms of nimorazole.

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EFFECTS OF DEOA CONCENTRATION AND ABIOTIC DEGRADATION ON THE STRUCTURAL INTEGRITY AND ECOTOXICITY OF POLYURETHANE FOAMS

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Flexible polyurethane (PUR) foams are widely used in industrial and consumer products, leading to the generation of significant amounts of waste [1]. The environmental degradation of these materials may result in the release of potentially hazardous compounds, raising concerns regarding their ecological impact [2]. This study investigates three water-soluble amine catalysts commonly used in the production of polyurethane foams (1,4-diazabicyclo[2.2.2]octane (DABCO 33LV), bis(2-dimethylaminoethyl) ether (Jeffcat ZF-22), and N,N-bis(2-hydroxyethyl)amine (Tegoamin DEOA 85)), which may leach from PUR foams during their lifecycle [3]. The catalysts are assessed both individually and as mixtures representative of their occurrence in commercial formulations, with particular focus on identifying potentially critical components from ecotoxicological perspective.

To better understand potential environmental risks, PUR foams containing N,N-bis(2-hydroxyethyl)amine (DEOA) at different concentrations were prepared and subsequently subjected to simulated environmental stressors, including ultraviolet (UV) radiation, leaching, and mechanical fragmentation. The experimental design aims to evaluate how DEOA concentration and environmental exposure influence the microstructural, mechanical, and ecotoxicological properties of the materials. This work aims to provide insight into the role of amine catalysts in affecting the environmental behavior of PUR foams and to support the development of safer additive formulations, highlighting the importance of formulation accuracy and improved end-of-life management strategies.

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FROM ADSORPTION TO REGENERATION: INVESTIGATION OF THE ADSORPTION CAPACITY, REGENRABILITY, AND STABILITY OF ZIRCONIUM-PILLARED MONTMORILLONITE

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We applied zirconium-pillared montmorillonite in an *Escherichia coli* bacterial suspension as an adsorbent for binding microorganisms. The performed measurements showed that it is capable of efficiently adsorbing bacterial cells and that the adsorbent can be reused with the same efficiency after regeneration by heat treatment [1]. These investigations were extended to additional microorganisms (three further single-component systems), and moving toward more complex systems, adsorption capacity values were also determined in mixed bacterial suspensions. Based on the outstanding capacity numbers obtained, a natural river water sample was subsequently evaluated to test the applicability of the pillared adsorbent in a complex matrix. At this stage of research, the regeneration-reuse cycle was extended to five. As no decrease in adsorption capacity was observed, the regenerated adsorbent was re-characterized, and the results were compared with the initial properties. FTIR, DLS, XRD, SEM and ICP analysis indicated that no significant chemical or physical changes occurred in the adsorbent during the sterilization-adsorption-regeneration processes.
Overall, these results demonstrate that a zirconium-pillared adsorbent prepared from raw montmorillonite is a promising alternative for novel water treatment technologies, as it not only effectively removes microorganisms from the system but also exhibits excellent stability.

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HEMICRYPTOPHANE MACROCYCLES FOR WATER PURIFICATION: TARGETING CHLORO- AND FLUOROCARBON CONTAMINANTS

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The increasing environmental persistence of chloro- and fluorocarbon compounds has raised serious concerns due to their detrimental effects on human health and ecosystems, necessitating efficient strategies for their detection and removal. Although macrocyclic hemicryptophane (Hm) systems are well known for their roles in catalysis and energy-related applications, their potential as selective hosts for halogenated pollutant capture remains largely unexplored. In this study, the sensing capability and selectivity of hemicryptophane macrocycles toward a series of freon-type molecules, including CCl_4, CF_3Cl, CH_3Cl, CH_2Cl_2, CF_3Br, C_2F_6, and CF_4, are systematically investigated using computational approaches [1]. The host-guest interactions are analyzed through interaction energy calculations, natural bond orbital (NBO) analysis, frontier molecular orbital (FMO) studies, and interaction region indicator (IRI) analysis. The results demonstrate that the intrinsic cavity of hemicryptophane provides a favorable and selective binding site. The calculated interaction energies confirm strong thermodynamic stability, while the HOMO–LUMO energy gaps decrease to as low as 1.95 eV, indicating enhanced electronic responsiveness relevant for sensing applications. Chlorinated freons, particularly CCl_4 (-128.32 kJ mol^{-1}), CCl_3F (-109.37 kJ mol^{-1}), and $CHCl_3$ (-92.65 kJ mol^{-1}), exhibit the strongest interactions, primarily governed by non-covalent forces. Therefore, hemicryptophane-based systems emerge as promising platforms for the selective detection and capture of hazardous halogenated pollutants.

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$AgNO_3$ LOADED POLYURETHANE FOAMS AS LIGHT RESPONSIVE MATERIALS: MECHANICAL PROPERTIES, OPTICAL RESPONSE AND ALGAL TOXICITY

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Polyurethane foams (PUFs) are frequently used in structural, cushioning and insulation applications, yet we know not much about their potential for light-responsive functionality. In order to create mechanically reinforced and photo-sensitive foams that could detect light exposure through macroscopic optical changes, flexible PUFs were combined with silver nitrate ($AgNO_3$) at different loadings (0.5-2.0 parts per hundred resin, phr) using a one-shot foaming technique [1]. The samples were characterized using mechanical testing, thermal analysis, Fourier-transform infrared spectroscopy and color measurements. Additionally, the toxicity of the samples were tested by using algal organisms [2]. The foams showed increased mechanical strength and thermal stability at lower $AgNO_3$ concentrations (0.5-1.0 phr) while retaining their distinctive urethane chemical structure. While high compressive strength was maintained, photo-induced structural rearrangements were seen at greater concentrations (2.0 phr), indicating more complex degradation behaviour after irradiation. Effective light-induced optical response was demonstrated by colorimetric analysis, which showed a monotonic increase in colour difference with increasing $AgNO_3$ content. $AgNO_3$ loaded PUFs are promising multifunctional materials for smart packaging, insulation and environmental monitoring applications where both service history and sustainability considerations are crucial because of the combination of tunable mechanical strength, optical sensitivity and thermal stability.

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MACHINE LEARNING–GUIDED PREDICTION OF RUTINOSIDASE ACTIVITY TOWARD THE DESIGN OF GLYCOSYLATED FLAVONOIDS WITH ANTIBACTERIAL POTENTIAL

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Rutinosidases are enzymes involved in flavonoid glycoside metabolism and represent useful tools for generating glycosylated flavonoid derivatives with improved biological and pharmacological properties. The biosynthetic potential of rutinosidases as regioselective enzymes for flavonoid glycosylation can be modulated by mutagenesis of the +1 subsite and side tunnel residues [1, 2].

Glycosylation significantly improves the solubility and stability of flavonoids and reduces the toxicity of these compounds, which is important for their application as an antibacterial agent in medicine [3]. We used molecular dynamics and docking to characterize the binding affinity of several modified rutinosidase substrates, and to model interactions with wild-type (WT) and mutant enzymes. The *in silico* dataset we collected includes more than 15 substrates and four enzyme mutants, and the computational predictions were validated by measuring enzyme' activity experimentally. In many cases, we observed clear structural and energetic explanations for changes in enzyme affinity; the binding of several substrates was influenced by numerous enzyme-ligand interaction parameters.

Machine learning (ML) methods for data analysis are developing rapidly and are becoming increasingly powerful tools in computational enzymology and drug design. In this study, ML approaches were used to analyze a large dataset obtained from docking and molecular dynamics simulations. This dataset included information on interaction energies, substrate stability in the active site, hydrogen-bonding patterns, geometric descriptors, and solvent exposure parameters. Supervised learning models were then trained to correlate these structural descriptors with experimentally measured enzyme activities and ligand affinities. Feature-selection techniques were applied to identify the most informative descriptors and reduce model complexity, determining a minimal, unbiased set of parameters.

An integrated computational workflow combining molecular docking, molecular dynamics, and ML analysis was used to predict substrate–enzyme interactions and to identify key determinants of catalytic efficiency. The results contribute to the rational design and functional optimization of flavonoid-derived bioactive molecules currently investigated as modulators of multidrug resistance.

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IN SEARCH OF THE STRUCTURE-ACTIVITY CORRELATION FOR SELECTED THIOSULFONATES – SPECTROSCOPIC STUDIES COMBINED WITH MOLECULAR MODELLING

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Antimicrobial resistance (AMR) has become one of the key healthcare problems in recent years [1]. This negative trend provides the necessity to analyse the antibiotics market on drugs` effectiveness and to develop new medicines. Thiosulfonates are one of promising potential antibiotics, but the scientific literature provides limited information on their structure-activity relationships [1,2]. To expand the available data on the thiosulfonate group, three derivatives were studied: 4-aminobenzene-1-sulfonothioate (1), S-ethyl 4-acetamidobenzene-1-sulfonothioate (2), and S-methyl 4-acetamidobenzene-1-sulfonothioate (3). The crystal and molecular structures of 1-3 thiosulfonates were studied experimentally at 100 K. Theoretical analysis, using density functional theory (DFT) on their molecular structure and vibrational IR, Raman, as well as NMR parameters was provided. Electronic properties of all studied compounds are explored using predicted geometric and magnetic aromaticity indexes, as well as substituent push-pull effects. Additionally compounds 1-3 antibacterial properties were studied on two model bacteria strains: Gram-positive *Staphylococcus aureus* ATTC 6538P and Gram-negative *Escherichia coli* ATTC 8739. A general mechanism of thiosulfonates 1−3 biochemical actions was proposed according to the literature data [1,2]. Its feasibility was analysed using DFT theoretical studies. The obtained results provide a deeper insight into compounds 1-3 molecular structure and IR/Raman and NMR spectroscopic and chemical reactivity properties. A direct correlation between some NBO parameters and the S-S bond energy in compounds 1−3 with their activity against both studied bacterial strains was observed.

Acknowledgments

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LARGE-SCALE PHYSICOCHEMICAL ANALYSIS OF DEFECT FORMATION MECHANISMS IN PARAFFINIC ORGANIC SYSTEMS USING DSC

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This study presents a large-scale physicochemical analysis of defect formation mechanisms in paraffinic organic systems subjected to various thermal histories, employing differential scanning calorimetry (DSC) and infrared (IR) spectroscopy. The research focused on analyzing the crystallization and melting processes, alongside changes in the structural organization of the system that dictate its microstructural stability [1-3]. The aim of the study was to determine the impact of processing conditions and storage temperature on the thermal properties and phase stability of the investigated systems. The analysis was conducted on samples obtained via two technological variants (a low-temperature process – L43, and a high-temperature process – L8), which were examined immediately after production as well as following storage at 15 °C, 25 °C, and 40 °C. The obtained results revealed a significant influence of thermal history and storage conditions on the course of phase transitions. This was observed as alterations in the DSC profiles, encompassing shifts in phase transition temperatures, enthalpy changes, and additional thermal effects associated with phase reorganization [2,4].

It was observed that the most profound destabilization phenomena occurred in samples conditioned at 15 °C. Conversely, exposure to 25 °C yielded the highest microstructural stability of the system, whereas elevating the storage temperature to 40 °C induced accelerated degradation processes and advanced phase reorganization of its components. These findings demonstrate the critical impact of technological parameters and storage conditions on shaping the overall physicochemical stability of paraffinic organic systems.

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COMPUTATIONAL STUDY OF SIDEROPHORE PYOVERDINE AND METAL INTERACTION

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Siderophores are specialized macromolecules produced by microorganisms and plants to counteract potential iron shortages in the environment. Siderophores have a strong chelating ability. Due to this, they are not only scavenge iron but also other metals, such as Ni^{2+}, Cu^{2+}, Cd^{2+}, Pb^{2+}, $Zn^{2+,}$ In^{3+}, V^{3+}, Ga^{3+}, Co^{3+}, Al^{3+}, Mn^{3+}, Th^{4+}, U^{4+}, and Pu^{4+}.[1] There are four major types of siderophores according to their functional groups. The four major groups are hydroxamate, catecholate, phenolate, and carboxylate. Furthermore, there is a mixed type of group as well. Pyoverdines are mixed type siderophores with catecholate and hydroxamate functional groups.[2] There are various types of pyoverdine produced by *Pseudomonas sp.,* but all of them have a similar structure and functional groups.[3]

For the proper understanding of the pyoverdine-metal interaction, computational methods have been used. Five metals were studied: ferric (Fe^{3+}) and ferrous (Fe^{2+}) iron, cobalt (Co^{3+}), copper (Cu^{2+}) and zinc (Zn^{2+}). Molecular dynamics simulations have been carried out by using Gromacs version 2025.3 and Amber 22. The metal ions and the interactions with pyoverdine were specifically examined.

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DRUDE-POLARIZABLE WATER FOR PROTEX: THE IMPACT OF DRUDE CHARGES ON COLLECTIVE PROPERTIES

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Designing a cost-efficient water model that reproduces collective properties and interaction properties across diverse conditions with high accuracy remains challenging. In preparation for integrating water into Protex – the Python-based utility for fast, large-scale molecular dynamics with proton transfer in OpenMM [1] – a polarizable model without additional virtual sites is required to avoid complications during proton exchange. Prior applications of Protex have successfully used Drude-polarizable force fields for ionic liquids, motivating its extension to aqueous systems [2].

As a first step, the Drude-polarizable SWM4-NDP model [3] was analyzed to assess how the Drude charge influences dynamic properties. Although a reasonable range of Drude charges should not have a major impact, provided that the Drude force constants are adjusted accordingly [4], the preliminary results indicate that increasing the Drude charge causes the model to behave more like point dipoles. However, SWM4's massless M site complicates proton transfer, as its position would need to "teleport" upon exchange, rendering it unsuitable for Protex without modifications. Consequently, development has focused on SWM3 [5], a Drude-polarizable alternative without additional virtual sites, which is being re-parameterized to reproduce experimental density and diffusion with adjusted Drude charge. Additionally, dielectric spectroscopy is used for validation against experimental data. This talk will present progress toward a Protex-compatible SWM3 model, highlighting the sensitivity of various properties to the Drude charge.

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DEVELOPMENT OF A METHOD FOR THE DETERMINATION OF CITRININ IN FOOD SUPPLEMENTS

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Citrinin (CIT) is a secondary toxic metabolite of benzopyrene that is formed mainly during post-harvest storage of raw materials. It is most commonly found in stored grains, but it is also present in various plant-derived products (including rice, wheat, barley, rye, beans, fruits, juices, nuts, and spices) as well as in spoiled dairy products [1-3]. This compound poses a significant health risk, particularly in tropical countries, where it is often responsible for food poisoning associated with mold contamination. Although red yeast rice is widely used as a natural method for lowering lipid levels, the presence of CIT as a toxic by-product of fermentation raises concerns about its safety [4]. Therefore, EU regulations (EC No 212/2014) established a maximum level of CIT in such products at 2000 µg/kg [5], which was later reduced to 100 µg/kg based on more recent data [6].

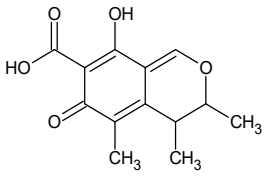

Figure 1. Chemical structures of CIT.

For this reason, a quick and simple method for the determination of CIT in food supplements, based on µ-QuEChERS, has been developed. The experimental study used certified reference materials to verify the accuracy of the method developed.

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MOLECULAR DYNAMICS SIMULATIONS REVEAL THE STRUCTURE AND STABILITY OF FOUR APOLIPOROTEIN E (APOE) VARIANTS

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Apolipoprotein E is a lipid-binding protein involved in the transport and metabolism of fats in human and other mammals. The three most common mutations in the ApoE gene lead to the three most observed isoforms of ApoE: ApoE2, ApoE3, and ApoE4. These isoforms differ in the amino acid residues at two positions: ApoE2 with Cys112 and Cys158, ApoE3 with Cys112 and Arg158, and ApoE4 with Arg112 and Arg158. Compared to individuals with no ApoE4 alleles, those with one copy of ApoE4 carry a 2-to-3-fold increase in risk for Alzheimer's disease (AD), whereas those that carry two ApoE4 alleles demonstrate a 12-fold increase in risk for developing AD. To date, the connection between the main genetic risk factor, ApoE, and the phenotypic hallmark of AD progression and diagnosis, the oligomers of the Aβ peptide, has yet to be established. Structural analysis of the ApoE isoforms could shed light on how structural differences between the three ApoE iosoforms affect the progression of AD. As a starting point, we compare the 'wild-type' ApoE2, ApoE3 and ApoE4 isoforms, as well as the site-directed mutant form of ApoE3 most often used in experimental studies. Molecular dynamics simulations are used in this study to investigate the more prevalent global structures, secondary structures, hydrogen bonding interactions, as well as the solvent exposure of Aβ, lipid, and receptor binding sites. Discrepancies between the structures of wild-type ApoE3 with the mutated 'experimental' ApoE3 variant are also examined as a first step in establishing a connection between ApoE and Aβ in AD.

Acknowledgments

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ENERGY-ENTROPY ANALYSIS OF PROTEIN-LIGAND INTERACTIONS

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As non-covalent association processes are ubiquitous in biology, their quantification is crucial. One approach for calculating binding free energies consists of energy-entropy methods. The energy of a system gives information concerning the strength of molecular interactions and can be easily computed, while entropy relates to dynamics within the system, but is often overlooked and more difficult to calculate in a computationally efficient and accurate manner. [1,2] However, assessing this term is also important for understanding these processes as protein and solvent dynamics have been established to play a significant role in governing whether binding occurs. [3] Multiscale cell correlation (MCC) yields the entropy of a system by discretizing configuration space into different length scales, as well as vibrational and topographical terms, thus giving rise to lower order terms which are easier to compute. This approach allows for detailed insights into contributions to entropy changes occurring upon binding, as well as for scalability and fast convergence. Another advantage of this method is that it treats all molecules in a system equivalently and hence, can be used for a complete analysis of the system, including both solutes and solvent. [1,4] The thermodynamics of the streptavidin-biotin system, widely studied due to its very high binding affinity [5], as well as those of two CLR/RAMP complexes binding to small molecule antagonists [6,7] have been studied. MCC has allowed a detailed breakdown of changes in configurational entropy terms of the protein-protein complex, ligands and solvation water molecules. Furthermore, the different length scales have allowed for assessing local entropy changes and gaining insights into residues' individual contributions to binding. Trends have been compared with experimental trends.

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SYNTHESIS AND CHARACTERIZATION OF INTERMOLECULAR INTERACTIONS IN A MULTICOMPONENT SYSTEM COMPRISING AN ANTIDIABETIC DRUG AND A COFORMER DESIGNED TO ENHANCE ITS AQUEOUS SOLUBILITY

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The drug tolbutamide (1-butyl-3-(4-methylphenylsulfonyl)urea, TB, Fig. 1) is employed in the pharmacological management of type II diabetes mellitus [1]. However, its clinical utility is constrained by its low aqueous solubility [2]. One strategy to ameliorate this limitation involves the formation of a multicomponent solid system with an auxiliary molecule specifically selected to enhance tolbutamide solubility [3]. The design and preparation of such cocrystals primarily depend on the establishment of favorable noncovalent interactions, which organize into characteristic supramolecular synthons [4].
The selected coformer is *N,N'*-dimethylurea (DMU, Fig. 1), which exhibits enhanced aqueous solubility when incorporated into a multicomponent system with the active pharmaceutical ingredient (API) [5]. In the present study, the TB:DMU cocrystal was isolated and subjected to comprehensive structural characterization. Furthermore, an in-depth examination of the intermolecular interactions was conducted employing a range of computational approaches, including Density Functional Theory (DFT), Symmetry-Adapted Perturbation Theory (SAPT), and Non-Covalent Interaction (NCI) analysis. Moreover, the molecular electrostatic potential (MEP) was computed to characterize the charge distribution in the individual API and coformer molecules, as well as in the resulting cocrystal system. In addition, periodic quantum-chemical calculations were conducted, facilitating a detailed analysis of the crystal structures and lattice energies of the co-crystals under investigation.

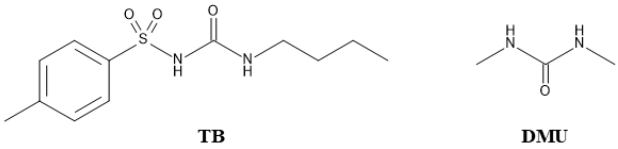

Figure 1. Structural formulas of 1-butyl-3-(4-methylphenylsulfonyl)urea (TB) and *N,N'*-dimethylurea (DMU).

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ELECTRONIC STRUCTURE AND NONLINEAR OPTICAL PROPERTIES OF FUNCTIONALIZED CUBANE DERIVATIVES

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Nonlinear optical (NLO) materials have attracted considerable interest due to their potential applications in optical communication, photonic technologies, and optoelectronic devices. In this work, density functional theory (DFT) calculations were performed to investigate the structural, electronic, optical, and nonlinear optical properties of a series of cubane-based derivatives functionalized with NH_2, OH, COOH, and Cl groups. Geometry optimization and vibrational frequency analysis confirmed the structural stability of all investigated species, while the calculated vertical ionization energies (7.50-9.18 eV) indicate high electronic robustness. Frontier molecular orbital (FMO) and density of states (DOS) analyses reveal that substitution significantly reduces the HOMO-LUMO energy gap compared with pristine cubane (9.12 eV), leading to enhanced charge transfer interactions and improved electronic responsiveness. Time-dependent DFT calculations show structure-dependent absorption spectra with longer wavelengths corresponding to lower excitation energies. The nonlinear optical properties were further evaluated through dipole moment (μ), polarizability (α_0), and first hyperpolarizability (β_0) calculations. Among the investigated derivatives, the IID exhibits the highest hyperpolarizability (β_0 = 132.10 a.u.), followed by the VE (β_0 = 117.68 a.u.), indicating their promising NLO behavior. Frequency-dependent calculations demonstrate significant second- and third-order nonlinear responses, with nonlinear refractive index values on the order of 10^{-18} cm^2/W. These findings suggest that functionalization of the cubane framework effectively tunes its electronic structure and significantly enhances its nonlinear optical performance, providing useful insights for the design of advanced NLO materials.

Acknowledgments

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MODELING OR5A2 INTERACTIONS: MACHINE LEARNING AND DOCKING APPROACHES TO MUSKY ODOR PREDICTION

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Olfactory perception of musky odor arises from interactions between structurally diverse small molecules and specific receptors such as OR5A2, yet the relationship between chemical structure and odor quality remains poorly understood [1]. Here**,** we present a combined machine learning (ML) and structure-based framework for predicting musky odor and evaluating receptor–ligand interactions.

A dataset of 7,744 odorants (256 musky) was constructed by integrating 59 public sources and 14 literature compounds. The dataset was partitioned based on similarity to musky chemical space to ensure representative coverage. Multiple TensorFlow-based classification models [2] were trained on molecular representations derived from 3D structures using SOAP descriptors, with stratified cross-validation. In parallel, the structure of OR5A2 was predicted using AlphaFold [3] and sampled by molecular dynamics simulations in GROMACS [4] to generate an ensemble of binding site conformations. Ligand binding was evaluated using ensemble docking in AutoDockGPU [5] with a composite score accounting for thermodynamic stability.

Screening performance of ML and docking approaches was evaluated using ROC curves, enrichment factors, and Matthews correlation coefficient under class imbalance. ML prediction quality improved with appropriate partitioning of chemical space, yielding robust global performance. However, docking models outperformed ML predictions for specific musky families, suggesting that OR5A2 is not a universal receptor and highlighting complementary strengths of AI-driven and structure-based approaches.

Acknowledgments

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MAGNETIC NANOPARTICLES AS AN EXTRACTION TOOL IN MODERN ANALYTICAL CHEMISTRY

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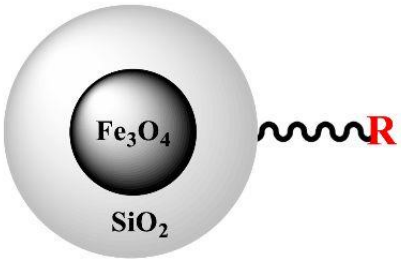
Extraction using modified magnetic nanoparticles is a modern tool in analytical chemistry, enabling the efficient preparation of samples for further analysis [1,2]. This technique relies on the use of magnetic nanomaterials whose surfaces have been functionalized to increase selectivity for specific analytes. From an analytical perspective, this method aligns with the trend of miniaturization and simplification of sample preparation procedures, while offering high extraction efficiency and the ability to work with small sample volumes [3]. A key advantage is the rapid and convenient phase separation using an external magnetic field, which eliminates the need for time-consuming filtration or centrifugation steps [4].

This presentation will discuss general aspects of this technique's application in the analysis of various sample types, with particular emphasis on its impact on improving sensitivity, selectivity, and repeatability. The role of appropriately selecting extraction conditions in optimizing analytical procedures will also be emphasized. This technique represents a promising solution supporting the development of modern analytical methods [4].



Schemat. Illustrative chemical structure of a modified magnetic nanoparticle.

Acknowledgments

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COMPUTATIONAL STUDY OF THE DEGRADATION OF URETHANE-TYPE MOLECULES

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Due to the limited recyclability of polyurethane (PUR), PUR waste is beig landfilled which can be environmentally dangerous, but it is problematic from a perspective of resources as well [1], [2]. There are environmentally friendly degradation methods which can give opportunities to recycle PUR. With the aid of these so-called degradation methods the growing tendency of the polyurethane plastic waste production can be slowed down by reusing the newly prepared raw materials in synthesis again. Among these degradation methods, biological degradation is a promising new approach for the environmentally friendly treatment of the polyurethane wastes, but this process is still in research phase, so the industrial application is not yet discovered making it an interesting research topic [3]. In this work the biological degradation of urethane-containing model compounds is being investigated with the help of computational chemistry methods. These computational chemistry methods include molecular docking, and molecular dynamics (MD) as well. All in all, 6 different PU-models were investigated, and their interactions with two different serine hydrolase enzymes were studied. The results can be the basis of future rational enzyme design studies for the purpose polyurethane degradation.

Acknowledgments

Financial support provided by the Co-Operative Doctoral Program (EKÖP-KDP 24/4) of the Ministry of Innovation and Technology is gratefully acknowledged. We acknowledge the Digital Government Development and Project Management Ltd. for awarding us access to the Komondor HPC facility based in Hungary. Calculations have also been carried out using resources provided by Wroclaw Centre for Networking and Supercomputing (http://wcss.pl).BF was supported by the János Bolyai Research Scholarship of the Hungarian Academy of Sciences.

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OPTIMIZATION OF GLYCOLYSIS PARAMETERS FOR RECYCLING POLYURETHANE WASTE INTO REPOLYOL AND ITS APPLICATION IN FLEXIBLE POLYURETHANE FOAM PRODUCTION

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Polyurethane (PU) waste management has become an increasing environmental concern due to its extensive industrial use and limited biodegradability. This study employed chemical recycling based on glycolysis, using ethylene glycol as solvent and potassium hydroxide as a catalyst, to cleave urethane bonds and produce recycled polyol (repolyol). The effects of reaction time (2 hr, 3 hr), mass ratio of PUF waste to ethylene glycol, and temperature (180 °C, 190 °C, 200 °C) on hydroxyl number, acid number, and viscosity of the repolyol were examined. Fourier Transform Infrared Spectroscopy (FTIR), Thermogravimetric Analysis (TGA), and Nuclear Magnetic Resonance (NMR) spectroscopy techniques were used to compare and analyze the structural and thermal properties of the obtained repolyol with those of the reference polyol. The repolyol was then used at 20%, 30%, 40%, and 50% as a substitute for the reference polyol to produce flexible polyurethane foam (FPUF). The produced foams were analyzed by FTIR and TGA, and their density, hardness, compression set, resilience, and tensile strength were tested. Characterization results confirmed successful depolymerization of PU and recovery of polyol with functional groups comparable to virgin polyol. The results demonstrated that incorporating repolyol up to 30% maintained acceptable foam characteristics, indicating that glycolysis is an efficient recycling method for polyurethane waste. Glycolysis effectively recovers polyol, which manufacturers can use to reduce their reliance on virgin materials during foam production, thereby supporting sustainable polymer waste management. However, increasing the repolyol ratio beyond 30% led to reductions in air permeability, compression set, and resilience performance of the produced FPUFs.

Acknowledgments

This study was funded through the Stipendium Hungaricum Scholarship Programme, financed by the Hungarian government and coordinated by the Tempus Public Foundation. BF thanks the support by the János Bolyai Research Scholarship of the Hungarian Academy of Sciences.

INFLUENCE OF RADIATION ON THE CRYSTALLIZATION OF THE TTCA-PYRIDAZINE SYSTEM

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In recent years, increasing attention has been paid to the influence of electromagnetic radiation on the crystallization of various compounds. Previous studies have shown that ultraviolet (UV) irradiation can significantly affect crystal morphology and internal structure, promoting the growth of larger bis(thiourea) cadmium chloride crystals [1] and inducing structural rearrangements within the crystal lattice of cobalt–thiourea complexes [2]. These findings suggest that UV irradiation may serve as an external stimulus capable of modifying crystal growth pathways.
In this work, we investigate the effect of electromagnetic radiation on the crystallization of multicomponent systems composed of trithiocyanuric acid (TTCA) and pyridazine. Experiments performed under different illumination conditions resulted in the formation of four previously unreported co-crystals, which have not yet been deposited in the Cambridge Structural Database (CSD) [3] (Fig. 1).

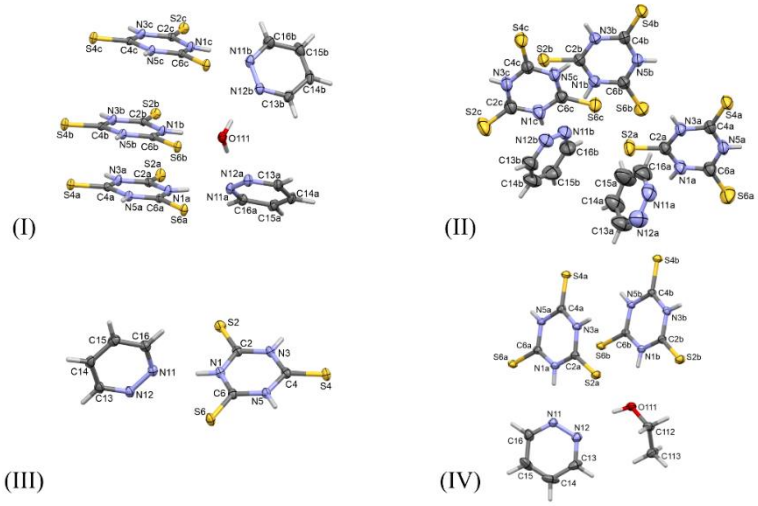

Figure 1. The diagram illustrates the molecular arrangement in the co-crystal structures of trithiocyanuric acid with pyridazine, obtained under darkroom conditions (I, II), visible light irradiation (III) and UV irradiation (IV), respectively.

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Poster Presentation

ARE RIBOSE-BINDING PROTEINS ABLE TO BIND OTHER SIMPLE SUGARS? A COMPUTATIONAL STUDY

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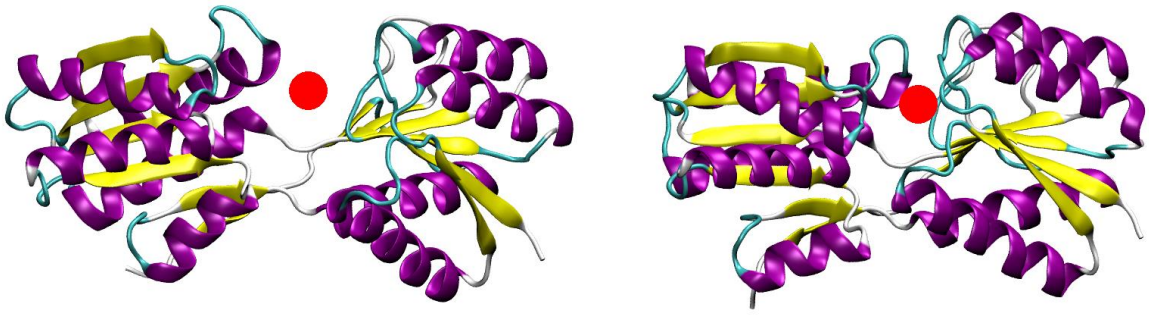
Ribose-binding proteins (RBPs) constitute a broad class of receptors and transporters necessary for handling the ribose fate in the cell. Our special interest in extremophilic organisms has brought our attention to the case of RBP from *Thermotoga maritima*, a hyperthermophilic Gram-negative bacterium able to grow in the temperature range of 55 – 90° C. The 3D structure of the RBP from this bacterium has been determined, and ligand-induced conformational changes have been observed as different from the mesophilic *Escherichia coli* RBP homolog [1]. The protein can attain two forms – open and closed – where part of the backbone acts as a hinge opening the sugar binding pocket, as shown below (the red dot indicates the ribose residue):



The current study aims at elucidating the possibility of other monosaccharides being bound to the RBP from *Thermotoga maritima*. First, docking with NVIDIA DiffDock was carried out, then molecular dynamics simulation with GROMACS served as a tool for analysing the dynamical nature of the binding. The 2FN8 PDB deposit [1] was taken as the initial structure of the complex, and the following ligands were tested: ribose (original ligand), fructose, galactose, glucose. The results show the unique strength of ribose binding, but do not exclude other sugars from binding. Structural and energetic implications of sugar binding to the receptor are discussed.

Acknowledgments

Authors gratefully acknowledge generous grants of computational time and the use of HPC resources of Wrocław Centre for Networking and Supercomputing (grant no. 206) as well as the Polish HPC infrastructure PLGrid (ACK Cyfronet AGH, grant no. PLG/2025/018939).

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MULTISCALE COMPUTATIONAL STUDY OF THE NORBORNADIENE QUADRICYCLANE (NBD7/QC7) MOST SYSTEM: ENERGY STORAGE IN SOLUTION AND SURFACE-CATALYZED CYCLOREVERSION ON Pt(111)

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Molecular solar thermal (MOST) systems undergo photoisomerization upon irradiation, forming a metastable, high-energy isomer capable of storing solar energy in chemical bonds. These molecules can subsequently be converted back to their original state, releasing the stored energy in the form of excess heat. The unsubstituted parent frameworks of MOST systems are not suitable for solar energy storage. However, by preserving the core scaffold and introducing appropriate substituents, ideal MOST systems can be designed. An ideal MOST molecule exhibits efficient photochemistry, high energy storage density, and a controllable, highly efficient back-reaction. The aim of this work is to establish a computational protocol capable of predicting or estimating the key properties of arbitrary MOST systems. The protocol is demonstrated through a well-known and promising Norbornadiene Quadricyclane pair (NBD7/QC7).

To assess energy storage properties, absorption spectra were calculated in implicit solvent using a multilevel quantum chemical method (STEOM-DLPNO-CCSD), yielding absorption maxima and spectral overlap of the isomers. The isomerization potential energy surface was examined with high-accuracy ab initio calculations (DLPNO-CCSD(T1)), enabling estimates of storage energy and activation barriers.

To model the heterogeneous catalytic back-reaction and energy release at the interface, adsorption free energy profiles were first computed on a Pt(111) surface in dichloromethane solvent using classical molecular dynamics simulations. The resulting adsorbed geometries were then used as starting structures for mechanistic investigation of the back-reaction pathways. The potential energy surfaces were explored using density functional theory (MN15), in which a finite slab model of the Pt(111) surface was treated explicitly at the quantum mechanical level. An external electric field was applied within this framework to represent the platinum surface as an electrode, enabling analysis of catalytic and electrochemical effects on the cycloreversion reaction.

Acknowledgments

Financial support was provided by the National Research, Development, and Innovation Fund (Hungary) within the TKP2021-NVA-14 project. LC is grateful for the Bolyai János Research Scholarship (BO/365/23/7) provided by the Hungarian Academy of Sciences. We acknowledge the Digital Government Development and Project Management Ltd. for awarding us access to the Komondor HPC facility based in Hungary.

DESIGN AND CRYSTALLISATION OF FORMAMIDINE SALTS – STRUCTURAL ANALYSIS BY X-RAY CRYSTALLOGRAPHY

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In the face of the deepening energy crisis and ongoing climate change, there is a growing need to develop modern technologies based on renewable energy sources [1]. One key research area is photovoltaics, which enables the direct conversion of solar radiation into electricity. In recent years, perovskite solar cells (PSCs) containing the formamidinium cation (FA^+) have attracted particular attention (Fig. 1) [2]. Owing to their high power conversion efficiencies, comparable to those of conventional silicon cells, these systems are regarded as one of the most promising solutions in modern photovoltaics [2,3].

The aim of this work was to obtain new, previously undescribed crystalline structures containing FA^+. For this purpose, a series of crystallization experiments was carried out using formamidinium iodide and selected organic acids. The resulting materials may provide a basis for the design of new compounds with desirable optical and electronic properties.

The poster presents three new crystalline structures based on FA^+: formamidinium 2-hydroxy-3,5-dinitrobenzoate, formamidinium pyridine-2,3-dicarboxylate, and formamidinium 4-nitrobenzoate. Single-crystal X-ray diffraction studies enabled detailed determination of their structural features and the geometrical parameters of non-covalent interactions in the obtained salts. In addition, quantum-chemical calculations provided deeper insight into the nature of the intermolecular interactions.

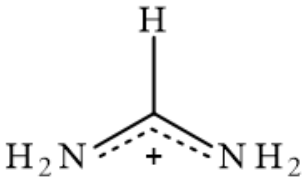

Fig. 1. Structural formula of the formamidine cation (FA^+)

Acknowledgments

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THERMODYNAMICS AND MOLECULAR INSIGHTS INTO β-CYCLODEXTRIN INCLUSION COMPLEXES WITH ANTI-ASTHMATIC DRUGS

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β-Cyclodextrin (β-CD) is widely used as a host molecule in drug delivery systems due to its ability to form inclusion complexes with various pharmaceutical compounds, thereby improving their solubility, stability, and bioavailability [1]. In this study, the inclusion complexation of β-cyclodextrin with two anti-asthmatic drugs, salbutamol (SAL) and tulobuterol (TUL) (Fig.1), was investigated using a combination of experimental and theoretical approaches [2].

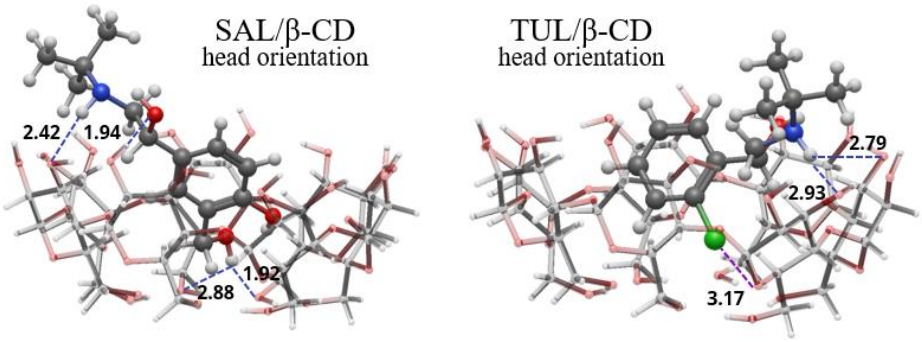

Figure 1. SAL/β-CD and TUL/β-CD complexes optimized using the M06-2X/6-311+G(d,p) method in water (SMD). The lengths of the intermolecular interactions are given in Å.

Isothermal titration calorimetry revealed that salbutamol exhibits a stronger binding affinity toward β-cyclodextrin than tulobuterol, as evidenced by higher stability constants and more favorable thermodynamic parameters. Differential scanning calorimetry confirmed the formation of inclusion complexes and demonstrated enhanced thermal stability of both drugs upon encapsulation. DFT calculations showed that the lowest-energy conformers of both drugs are stabilized by intramolecular hydrogen bonding and preferentially form head-first inclusion complexes with β-cyclodextrin. SAPT analysis indicated that dispersion interactions dominate host–guest binding, with higher interaction energies observed for salbutamol complexes, what is in agreement with experimental results. In summary, the stability of the complexes is governed by molecular conformation and dispersion interactions, providing insight into the design of cyclodextrin-based drug delivery systems.

Acknowledgments

The calculations were performed using computational resources provided by the Wroclaw Centre for Networking and Supercomputing (WCSS).

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ELECTROREDUCTION OF HETARYL KETONES AND THIOKETONES: A COMPARATIVE STUDY

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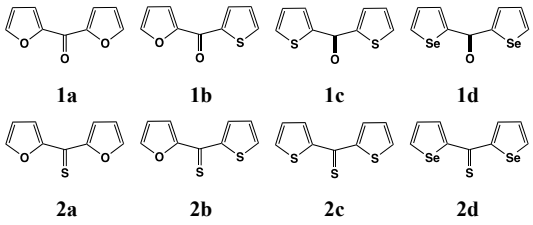
Ketones, especially aromatic ketones, form a well-known class of organic compounds widely applied in organic synthesis and other fields of organic chemistry [1]. Much less has been established for sulfur analogs of ketones (that is, thioketones), which are characterized by the presence of the functional thiocarbonyl group C=S [2]. In recent decades, thioketones have been reported as universal building blocks in the synthesis of sulfur heterocycles, proceeding mainly from [3+2] and [4+2] cycloaddition reactions. Due to their high reactivity towards 1,3-dipoles and dienes [2], thioketones were named as 'superdipolarophiles' and 'superdienophiles', respectively. Additionally, aromatic and cycloaliphatic thioketones found numerous applications as ligands in coordination chemistry [3]. From an electrochemical perspective, both ketones and thioketones are known as electroactive compounds and for that reason they are attractive models for diverse electrochemical studies.

The presented studies compare the electrochemical properties of hetaryl ketones **1a–d** (Scheme 1) with their sulfur analogs **2a–d**. The electroreduction of these compounds in two solvents (CH_3CN and CH_2Cl_2) was examined by means of the cyclic voltammetry (CV) and theoretical calculations based on the density functional theory (DFT). Additionally, the surface of the Au electrode used in the electroreduction of **2a–d** was studied by the atomic force microscopy (AFM).



Scheme 1. Studied ketones **1a–d** and thioketones **2a–d**

Acknowledgments

We gratefully acknowledge Polish high-performance computing infrastructure PLGrid (HPC Centers: ACK Cyfronet AGH and WCSS Wrocław) for providing computer facilities and support within computational grant no. PLG/2026/019341.

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AutoPocket2CREST: AUTOMATED GENERATION OF PROTEIN–LIGAND POCKETS FOR CREST CONFORMATIONAL SAMPLING

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Accurate conformational sampling of protein–ligand systems requires reliable preparation of the binding environment. While CREST[1] provides an efficient framework for semi-empirical or force-field based conformational sampling, its application to protein-bound ligands typically involves manual steps such as pocket definition, hydrogenation, and constraint setup. Here, we present AutoPocket2CREST[2], an automated workflow for generating CREST-ready protein-ligand pocket models. Starting from a protein and a ligand structure, the method uses the ligand to construct a binding pocket, removes unphysical residues, adds missing hydrogen atoms, and optional backbone constraints to maintain structural integrity during sampling. The workflow also post-processes CREST conformers by restoring residue and atom annotations from the reference structure, enabling direct analysis and visualization. By integrating these steps into a single pipeline, AutoPocket2CREST reduces user intervention and improves reproducibility. AutoPocket2CREST provides a practical approach for semi-empirical as well as force-field based conformational sampling of protein–ligand systems and facilitates the analysis of local binding-site dynamics.

Acknowledgments

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PREDICTION OF MOLECULAR DOCKING SCORES USING SOAP-BASED MODELS AND GRAPH NEURAL NETWORKS

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The search for computationally efficient methods for initial screening of candidate molecules in traditional in silico drug design workflows remains highly relevant, particularly when such methods can achieve accuracy comparable to molecular docking at a fraction of the computational cost. In this study, we focus on the prediction of docking scores for inhibitors targeting the SARS-CoV-2 main protease (M^{pro}). Reference docking scores were obtained using AutoDock Vina 1.2.2 with the standard AutoDock scoring function [1].

Building on our previous work [2,3], which investigated strategies for improving predictive performance through model optimization, the present study shifts focus to a systematic comparison of different machine learning architectures. Specifically, we evaluate four models: two neural network models based on SOAP (Smooth Overlap of Atomic Positions) descriptors using molecular and atomic representations, and two graph neural network (GNN) models, DimeNet and GemNet, which operate directly on molecular structures.

All models were trained on the *in vivo* dataset (~60,000 compounds) and evaluated on the independent *in vitro* dataset (~170,000 compounds), ensuring a realistic assessment of generalization performance. The SOAP-based models were implemented using the Keras/TensorFlow (molecular representations) and Pytorch (atomic representations) framework, while the GNN models were trained using state-of-the-art architectures designed to capture geometric and topological features of molecular systems.

The central objective of this study is to assess the relative performance of descriptor-based and graph-based approaches in docking score prediction, and to determine whether increased model complexity leads to improved predictive accuracy. Our results provide a comprehensive comparison of these methodologies and offer practical insights into the trade-offs between computational efficiency and predictive performance in large-scale virtual screening workflows.

Acknowledgments

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SENSITIVITY OF POLYURETHANE FOAM PROPERTIES TO CONTROLLED VARIATIONS IN ADDITIVE AND CATALYST RATIOS AND SUBSEQUENT AGEING

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Polyurethane (PU) foams are highly versatile materials whose structural and functional properties are strongly influenced by formulation parameters and processing conditions. In this study, the effects of systematic variations in additive and catalyst concentrations on the morphology, mechanical performance, and acoustic behavior of flexible PU foams were investigated. Starting from a reference formulation, selected components—including cell-opening polyol, blowing agent (water), surfactant, and different catalysts—were varied within a ±10–20% range to evaluate their impact on foam properties.

The results demonstrate that even moderate formulation changes significantly influence foam density and compressive strength, reflecting alterations in reaction kinetics and cellular structure. Increased blowing agent content led to lower density and reduced mechanical strength, while decreased water content resulted in denser, mechanically stronger foams. Variations in surfactant and catalyst concentrations affected foam stability and cell morphology, indicating the importance of maintaining a balance between blowing and gelling reactions [1].

Ageing studies under both dry and wet conditions revealed further modifications in foam performance. Wet ageing generally induced softening and reduced compressive strength [2], whereas dry ageing caused less pronounced changes [3]. The observed trends highlight the sensitivity of PU foam properties to both formulation parameters and environmental exposure. Overall, this work emphasizes the critical role of precise compositional control in tailoring PU foam performance and provides insight into the interplay between formulation variability and ageing effects.

Acknowledgments

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CRYSTALLIZATION OF THYMINE WITH CARBOXYLIC ACIDS: STUDIES OF SUPRAMOLECULAR INTERACTIONS

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The aim of this thesis was to obtain and characterize cocrystalline systems composed of thymine and selected carboxylic acids, including 3-hydroxybenzoic acid and 3,5-dinitrosalicylic acid. Thymine, or 5-methyluracil, is a pyrimidine derivative and one of the canonical nucleobases present in DNA, where it is involved in the storage and transmission of genetic information. Owing to their biological significance, thymine-based derivatives are of considerable interest in the development of antiviral and anticancer compounds. Moreover, thymine represents a polymorphic compound, capable of crystallizing in different structural forms [1–3].

Within the experimental part of the study, two crystalline forms of thymine were obtained, displaying different macroscopic morphologies. Furthermore, two solvated thymine–carboxylic acid cocrystals were prepared. The obtained crystal structures were examined in terms of their supramolecular organization, with particular attention paid to intermolecular hydrogen-bonding motifs responsible for the stabilization of the crystal lattice.

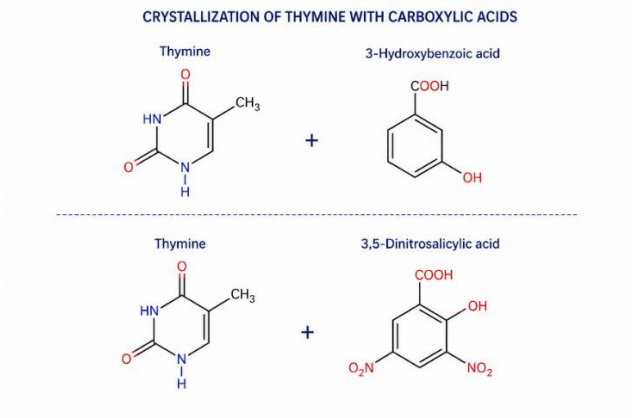

Figure 1. Crystallization scheme of thymine with carboxylic acids.

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COMPARING ATOMIC- AND MOLECULAR-LEVEL REPRESENTATIONS FOR THE MOST POTENT SARS-COV-2 M^{PRO} INHIBITOR IDENTIFICATION

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The study investigates the prediction of binding affinities for inhibitors of the main protease (Mpro) of SARS-CoV-2, comparing atomic- and molecular-level machine learning approaches (using SchNet [1], PaiNN [2] and XGBoost [3] models). Although molecular-level models yield lower mean square error (MSE) across the entire data set, they systematically underestimate the binding affinity of the top binders. In contrast, atomic-level models—which predict molecular properties as the sum of contributions from each atom based on its local environment—were significantly more accurate at identifying the most active compounds (higher Recall and F1 score), which is critical in drug discovery screening. The results indicate that the superiority of the atomic-level approach stems from error compensation: the general trend towards underestimating binding affinity, typical of machine learning predictions for rare, high- (or low-)affinity compounds, counteracts overestimation that arises from the cumulative effect of atomic contributions, particularly for compounds with a number of atoms exceeding the average of the training dataset.

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NOISE IN THE DATA AND ITS CONTRIBUTION TO PREDICTION ACCURACY OF MACHINE LEARNING.

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Machine learning (ML) is increasingly applied in the field of chemistry. In practice, there are two critical components of a successful implementation: a suitable architecture of the ML algorithm to describe the problem and high quality data [1,2]. Here, we have investigated the dataset quality acquired from the ZINC15 database and its influence on the ML predictions of docking scores [3]. Structures from *in vivo* and *in vitro only* subsets of ZINC15 were docked against the active site of a SARS-CoV-2 main protease (M^{pro}) in AutoDock Vina 1.2.2 software and calculated docking scores were used to train and test the neural network model (Atomwise prediction block and SchNet descriptor) [4,5,6].

Training set is constructed with respect to the charge of the molecule and its protonation state and created training sets are used to train multiple neural networks. Predictions of these neural networks are compared to predictions by neural network trained on the original training set and to each other. More focused training sets contain a lower amount of contradictory data and therefore allow for more accurate predictions on relevant molecules. Moreover, comparison of the obtained predictions reveals information about level of noise and the overall sensitivity of learning to this noise.

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SYNTHESIS OF 1,2,4-TRIAZOLYL RADICALS FOR STRUCTURAL STUDIES

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1,2,4-Triazolyl radicals (TRs) represent a little-known group of stable open-shell compounds that have recently attracted attention due to their potential practical applications, for example, in organic synthesis, polymerization processes, and pharmacological studies [1–4].

Surprisingly, no fluorinated analogues are reported up to date, even though the introduction of fluorine atoms or fluoroalkyl groups into organic molecules is well known to significantly (and often desirably) tune their physicochemical and biological properties. Hence, this project aims to develop a general protocol for the synthesis of trifluoromethylated 1,2,4-triazolyl derivatives based on the condensation of highly reactive, *in situ*- generated CF_3-nitrile imines, with suitable primary amines as key starting materials, followed by oxidation of the initially obtained 1*H*-1,2,4-triazoles.

The resulting products characterized by different electronic properties depending on the substituent located on the phenyl ring (e.g., alkoxy, alkyl, halogen, ester, cyano, nitro, etc.), will be used as model compounds for further structural studies supported by DFT calculations and, in the longer term - for preliminary biological screening tests.

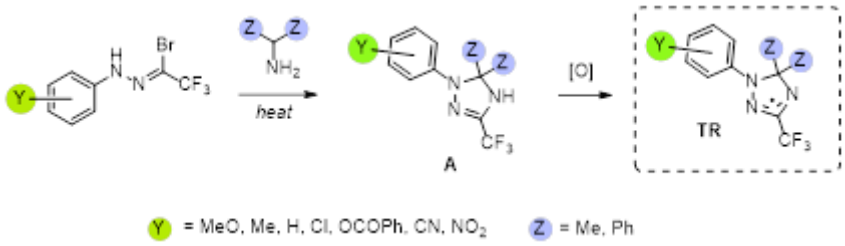

Fig. 1. The synthesis of the title 1,2,4-triazolyl radicals (**TR)**

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HETEROGENEOUS PAIR INTERACTION COEFFICIENTS IN β-CYCLODEXTRIN – ORGANIC SOLVENT SYSTEMS

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Enthalpic pair interaction coefficients describe the interactions between two molecules, including the competitive contribution of the solvent as they approach each other. They are derived from the McMillan–Meyer theory [1], according to which interactions between molecules in solution are related to the second osmotic virial coefficient by the following relationship:

$$B^* = -\frac{1}{2} L \int [g_{\alpha\beta}(r) - 1] 4\pi r^2 dr$$

where:

L – Avogadro constant ,

$g_{\alpha\beta}(r)$ – radial distribution function of molecules α i β

Theoretical calculations of the radial distribution function, $g_{\alpha\beta}(r)$, present significant computational challenges, primarily due to the complexity of accounting for many body forces and solvent mediated effects. Consequently, Kozak and co-workers [2] implemented a statistical mechanical approach that enables the formal separation of pair interaction effects from higher order contributions, such as triplet or quadruplet molecular interactions. This simplification is crucial for interpreting the behavior of dilute solutions, where pair interactions predominate. Building on this foundation, Friedman and Krishnan [3] further refined the McMillan–Meyer theory. Their key modification involved a thermodynamically rigorous transition from the activity scale to the Lewis–Randall molality scale, which is more practical for interpreting experimental data in multicomponent systems.
The objective of this study was to determine the energetic effects of interactions between β-cyclodextrin and various organic solvents, namely dimethylformamide, dimethyl sulfoxide, ethylene glycol, propylene glycol, and glycerol, as well as their aqueous solutions at 298.15 K. The thermal effects associated with the dissolution of β-cyclodextrin in the selected solvents were measured using a non-isothermal, non-adiabatic calorimeter. The enthalpies of solution obtained from these calorimetric measurements were used to calculate the standard molar enthalpies of solution ($\Delta_{sol}H°$). Based on the obtained data, heterogeneous pair interaction coefficients (h_{xy}) between β-cyclodextrin and the selected solvents were determined. These coefficients provide a measure of the energetic effects of interactions between heterogeneous molecular pairs (cyclodextrin–solvent) occurring within the competitive environment of water molecules.

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