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The 17th Edition of the Conference

NEW TRENDS IN CHEMISTRY RESEARCH

NOI TENDINȚE DE CERCETARE IN DOMENIUL CHIMIEI

BOOK OF ABSTRACTS

NewChemRes 20$_2$5

September 24-26, 2025
TIMIŞOARA

Dear colleagues from Romania and abroad,

It is our great pleasure to warmly welcome you to the 17th edition of the International Conference **"New Trends in Chemistry Research"** / "**Noi tendințe de cercetare în domeniul chimiei**" (**NewChemRes 2025**), held in Timişoara between 24–26 September 2025. This traditional scientific event is organized by the "Coriolan Drăgulescu" Institute of Chemistry of the Romanian Academy, in partnership with the Romanian Chemical Society and Politehnica University Timișoara.

This year's event emerges as an international platform for dialogue and collaboration, bringing together researchers from more than 11 countries, doctoral students from Romania and abroad, as well as professionals from the industrial sector. Participants will have the opportunity to exchange ideas, present research findings, share recent discoveries, and put forward innovative visions, thereby contributing to shaping new directions for a more sustainable and valuable future of chemistry.

The conference is not only a venue for showcasing the latest achievements, but also an occasion for collaboration, networking, and the initiation of joint projects, opening pathways towards scientific and technological partnerships at both national and international levels.

The scientific program includes plenary lectures, oral presentations, poster sessions, research equipment promotion, and a visit to the **Interdisciplinary Center for Intelligent Specialization in Biological Chemistry**, **RO-OPENSCREEN** (https://ro-openscreen.ro/). Moreover, a special section entitled **"Chemistry for a Sustainable Tomorrow – Romania Joins the Global Conversation,"** organized under the umbrella of the **IUPAC project "Global Conversation on Sustainability"** (https://iupac.org/project/2021-034-2-041/), will underscore the urgent need for a transition to sustainability and highlight the central role of chemistry in advancing the Sustainable Development Goals.

We would like to express our sincere gratitude to all the speakers, scientific committee members, chairpersons, sponsors, and everyone who contributed to the organization of this event and to the presentation of valuable results and perspectives.

Best wishes for a professionally rewarding conference!

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CASE STUDIES IN BIOINORGANIC COORDINATION CHEMISTRY: INTERPLAY BETWEEN ELECTRONIC PROPERTIES, DYNAMICS, AND BIOLOGICAL RELEVANCE

Radu SILAGHI-DUMITRESCU

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Using the cobalamin, hemes (e.g., as seen in globin systems), platinum (IV) and others as test cases of complexes with small molecules relevant for catalysis and/or biomedical processes, we explore the ability of computational methods to reproduce trends in stability, biologically-relevant interactions, and spectral properties (especially UV-vis, EPR, NMR) – and then to make practically useful predictions. On one hand, differences in charge, hardness, spin state, kinetic lability and isomeric and conformational space complicate the chances of successful simulations with any single computational method – be it semiempirical, TD-DFT, or variations therefrom, including those that account for the second sphere of coordination (e.g., QM/MM) and/or solvation. On the other hand, the complex reactivity of transition metals puts strains on some very basic and widely-employed experimentally-derived concepts, such as the spectrochemical series.

SUSTAINABLE STRATEGIES FOR THE PROCESSING OF PLATFORM MOLECULES TO POLYMERIC MATERIALS

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Renewable bio-based polyesters are one of the effective answers that the bioeconomy offers to solve the environmental emergency connected to fossil-based plastics. The next generation of plastics are expected to contribute to a massive reduction in the carbon footprint by the exploitation, in industrial productive processes, of renewable monomers such as polyols and dicarboxylic acids obtainable via biotechnological production. More specifically, there is a rising demand for advanced materials displaying new functional properties while meeting higher sustainability criteria. This talk will highlight new greener strategies for a more environmentally friendly synthesis of various polyester-based materials and their potential application.

Acknowledgements
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CARBORANE-CONTAINING DRUGS: NEW KEYS FOR OLD LOCKS

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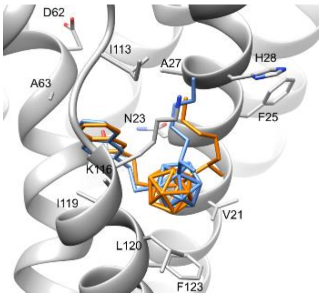
Since the discovery of polyhedral carboranes more than fifty years ago, their potential for various applications has been unlocked. Mainly, their use as pharmacophores is due to their remarkable biological stability and hydrophobicity. The cage framework of these clusters can be easily modified with a variety of substituents both at the carbon and at the boron atoms. It has been shown that the implementation of the carboranyl moiety, as a phenyl mimetic, in biologically active molecules results in compounds that can exhibit improved biological stability and activity in comparison to their generic paradigms. However, up to now, the use of carboranes as pharmacophores is limited to just a few examples. [1] Our research focuses on several types of enzyme inhibitors, such as cyclooxygenase (COX),[2] lipoxygenase (LOX) [3] or ABCG2 inhibitors [4] as well as cannabinoid receptor Type 2 (CB_2R) ligands [5].

A highly coveted approach in the design of novel nonsteroidal anti-inflammatory drugs that are applied in the treatment of various inflammatory processes is achieving cyclooxygenase (COX) 2 selectivity. By implementing a carboranyl moiety in the structures of known COX inhibitors more selective and robust COX-2 inhibitors were obtained. [2] 5-Lipoxygenase (5-LOX) is an enzyme of the extracellular matrix and plays a role in increased metastasis and angiogenesis. Numerous reports show the overexpression of 5-LOX in several cancer cell lines. For the activation of 5-LOX, the 5-LOX-activating protein (FLAP) is necessary. Therefore, inhibition of 5-LOX or FLAP could inhibit tumour growth and angiogenesis. Replacement of phenyl rings in selected 5-LOX inhibitors by carboranes resulted in a similar enzymatic inhibitory behaviour but markedly increased cytotoxicity against several melanoma and colon cancer cell lines. [3]



Selected examples also for other biological targets [4,5] will also be presented.

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WITH A LITTLE HELP FROM COMPUTER-AIDED DRUG DESIGN: NEW ANTITUMOR AGENTS AS TUBULIN POLYMERIZATION INHIBITORS

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Tubulin polymerization inhibitors are a cornerstone of anticancer drug development, as they disrupt microtubule dynamics essential for cancer cell growth. This lecture highlights our multi-year research efforts in designing, synthesizing, and evaluating novel benzazole-based compounds as potent tubulin-targeting agents (Figure 1). These tunable chemical scaffolds, vital in modern medicinal chemistry, [1,2] display versatile chemical and biological properties, making them ideal for innovative bioactive molecules.

Using classical and microwave-assisted synthesis, we developed *N*-substituted benzimidazole acrylonitriles (Figure 1, X = C–H) with submicromolar antiproliferative activity (IC_{50} 0.2–0.6 μM) against diverse cancer cell lines, with favorable selectivity over normal cells. [3,4] Mechanistic studies confirmed their ability to inhibit tubulin assembly and induce mitotic arrest. Computational analyses revealed structural features that enhance antitumor potency, and revealed critical protein-ligand interactions, guiding the strategic replacement of the benzimidazole phenyl ring with pyridine, yielding imidazo[4,5-*b*]pyridine analogues (Figure 1, X = N).[5,6] These showed improved activities (IC_{50} as low as 0.04 μM), alongside reduced toxicity, and migration inhibition, with computations uncovering unique binding patterns at the colchicine site and allosteric regions (Figure 2), underscoring the versatility of these nitrogen-rich ligands.

Our research validates the benzazole-acrylonitrile framework as a promising platform for tubulin inhibitors, offering valuable insights for rational drug design. By integrating synthetic chemistry, biological profiling, and computational modeling, we aim to advance next-generation anticancer therapies with improved efficacy and selectivity. Since microtubule anomalies are, beyond oncology, linked to neuropsychiatric illnesses, future directions, including repurposing for post-COVID neurological sequelae, will be discussed to drive from discovery to clinical impact.

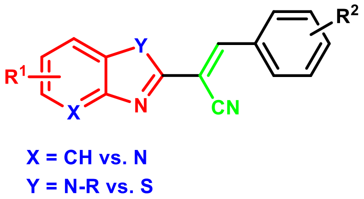

Figure 1. General chemical structure of studied ligands that interfere with the tubulin polymerization.

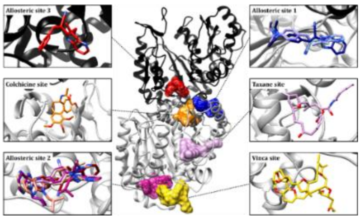

Figure 2. Various ligand binding sites on the α- (in black) and β-subunits (in gray) in the tubulin dimer, as identified through the docking and molecular dynamics simulations.

Acknowledgment
This work was supported by Croatian Science Foundation (grant number IP-2024-05-3953)

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RADU BACALOGLU – THE MAN, THE TEACHER, THE CHEMICAL ENGINEER – IN MEMORIAM

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The review will evoke the scientific life of my teacher, supervisor, head and friend Radu Bacaloglu, a great Romanian organic chemist, who recently left us. I will talk about a great personality having an important impact on overall organic chemistry. Despite the challenges, the flavor of the review will be offered in a more personal and unusual style, i.e., with emotion, with respect, and a lot of consideration.

The Radu Bacaloglu' scientific work is impressive and brilliant. His experimental and theoretical research enhanced the knowledge on micellar catalysis and aromatic substitution and resulted in revisiting the Chapter 13 of the fundamental book «*March's Advanced Organic Chemistry*». He created and developed the Romanian School of Carbonic Acid Derivatives. With his visionary approach he successfully started to work in Biocatalysis and Liquid Crystals. Nonetheless he performed creative research with a huge impact on day-by-day industrial applications finding new procedures for polyvinyl chloride catalytic stabilization and new polymer formulations.

The research work started with his PhD experimental studies in the 60's at the Organic Chemistry Department of Polytechnic Institute of Timisoara. He was assistant between 1959 and 1979, and (just) associate professor of organic chemistry, between 1979 and 1985. He was the founder and Director of the Research Group in homogeneous and enzymatic catalysis of Institute for Chemical Energetics, Bucharest (1981-1985).

After the emigration to the US, Radu Bacaloglu covered different research and teaching positions: Research associate at the University California, Santa Barbara (creative collaboration with prof C. A. Bunton's group) 1985 – 1989, and Assistant professor at the Rutgers State University, New Brunswick, New Jersey, between 1989 and 1991. Then, he moved to Witco Corporation, Oakland as Group leader in the Research and Development Vinyl Group, 1991—1997, Manager of Research and Development Vinyl Group in Tarrytown, New York, 1997—2003, and Research Fellow, 2003—2004. Retired in 2004 Radu Bacaloglu ended his career as Member of Faculty Bergen Community College, Paramus, New Jersey. He continued to work until the last days of his life.

Radu Bacaloglu published more than 220 scientific papers in journals and conference proceedings, 4 books, and a huge number of patent applications. He has participated and presented research papers in a number of academic and industrial - research conferences.

EMERGENCE OF CONFORMATIONAL DIVERSITY IN SUPRAMOLECULAR ASSEMBLY AT SURFACES

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We present a remarkably complex on-surface structures and networks that form spontaneously from molecular modules taking up multiple site-specific conformations. Based on these observations we analyze the different physicochemical interactions at surfaces contributing to the symmetry breaking of the building blocks in their conformational adaptation. We compare the binding motifs observed in 3D crystal structures obtained from X-ray diffraction with high-resolution scanning tunneling microscopy and spectroscopy data and chemical information from x-ray photoelectron spectroscopy. Density functional theory of the molecular modules on different substrates evidence that the complex interplay of different possible interactions on the flexible molecules is the cause of the complexity observed: Molecular conformational flexure facilitates the site-specific adaption of molecules and its relocation to the most energetically favoured site on the corrugated surface potential. Further, the molecules interact with the surface state electrons in the underlying substrate and via intermolecular binding through hydrogen bonds linking molecular units at different elevations above the substrate surface. Notably also, the molecule is showing conformational diversity in comparison between one and another substrate. In conclusion we discuss surfaces and interfaces as a possible cause for the emergence of quasi degeneracy of molecular configurations in supramolecular self-assemblies. The adsorbate-adsorbent interface is recognized as the driver for this system to behave counterintuitively to equilibrium thermodynamics.

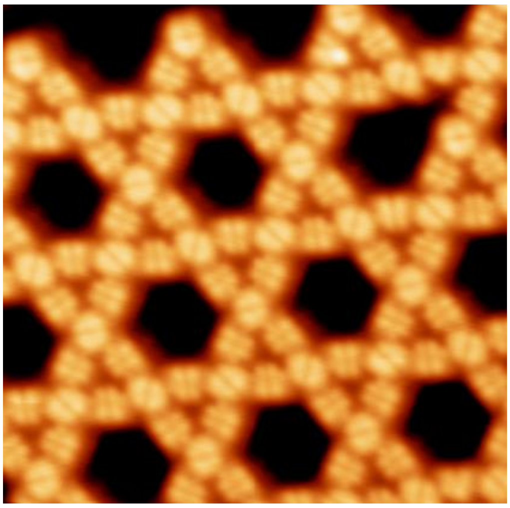

Fig. 1) Tetrakis(3,4,5-trimethoxyphenyl) porphyrin forms spontaneous assemblies of molecular modules with up to three conformers co-existing on the same substrate, Ag(111) in this case. Conformational identification by Scanning Tunneling Microscopy allows for deep insights into the site-specific conformational adaptation which is recognized as the key element for conformational diversity and a pre-requisite for the formation of more complex supramolecular structures – like the Kagome network shown here.

AZULENE-BASED ARCHITECTURES: FROM PHOTOSWITCHES AND MOLECULAR CAGES TO CO-CRYSTALS AND COORDINATION POLYMERS

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Azulene, a vibrant-blue 10-π-electron isomer of naphthalene, shows unique electronic and structural characteristics such as a dipolar structure with the dipole moment around 1.0 D, high electron affinity, low ionization energy and unusual S_2−S_0 fluorescence. [1,2] The large dipole moment arises from the electron drift from the seven-membered ring to five-membered ring, forming an intrinsic dipolar structure with the five-membered ring carrying the negative charge and, the seven-membered ring the positive charge, respectively (Figure 1). Thus, azulene is reactive towards both nucleophiles and electrophiles, making it a versatile building block for constructing diverse multifunctional materials. [3] As a result, azulene derivatives have been investigated for various applications, including organic semiconductors, solar cells, light-emitting diodes, sensors, and molecular switches. [4]

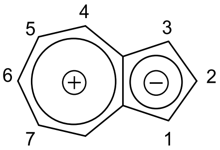

Figure 1. Dipolar structure of azulene with the numbering scheme

Given the demonstrated potential of azulene to yield valuable materials, [3,4] we developed a rich chemistry using azulene derivatives as building blocks for constructing hydrogen- and halogen-bonded co-crystals [5,6], fluorescent switching compounds [7], terpyridine-based receptors [8], and magnetic materials.[9] To leverage both covalent and noncovalent interactions, the azulene-1,3-carbaldehyde derivative played a key role. Initially employed as a halogen bond acceptor [6], it subsequently facilitated the isolation of discrete organic and metal-organic cages. [10,11] Structural characterization involved single-crystal X-ray diffraction, complemented by NMR spectroscopy where feasible. Our ongoing investigations concentrate on understanding the structural contributions of azulene derivatives to molecular assembly, discrete structure formation, and crystal packing interactions within the resulting solids.

Acknowledgement
This work was supported by a grant from UEFISCDI, project number PN-IV-P8-8.3-ROMD-2023-0045, within PNCDI IV. The theoretical calculations of the Moldova' team lead by G. Duca is gratefully acknowledged.

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ORGANIC CARBONATES - GREEN SOLVENTS AND REAGENTS FOR BIO-BASED PLATFORM CHEMICALS

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The integration of basic sciences into sustainable development has become a central objective for numerous global initiatives, including the International Year of Basic Sciences for Sustainable Development and the United Nations Agenda 2030, which outlines 17 Sustainable Development Goals (SDGs). Organic synthesis plays a pivotal role in addressing sustainability challenges by emphasizing the use of non-toxic reagents, reducing energy consumption and waste, and encouraging recycling practices. These principles align with the missions of key international organizations such as the International Union of Pure and Applied Chemistry (IUPAC).

The discovery, development, and mechanistic understanding of innovative organic synthesis methods remain critical research areas. In this context, dialkyl carbonates (DACs) have attracted growing attention over the past decades due to their environmentally benign properties. Among them, dimethyl carbonate (DMC) stands out as a sustainable alternative to traditional chlorine-based reagents in various chemical transformations. Although halogenated compounds typically exhibit higher reactivity, they often suffer from poor selectivity. DACs, by contrast, offer improved selectivity in alkylation reactions, even if their reactivity is lower. [1] Green synthetic methodologies employing DMC have been successfully applied in the production of anti-inflammatory agents, polymers, fragrances, and solvents. [2] Additionally, DACs serve as fuel additives, lithium battery electrolytes, and intermediates in the synthesis of pharmaceuticals, pesticides, plastics, coatings, electronic materials, and agrochemicals. [3]

This lecture will highlight the use of DMC and related DACs as greener alternatives to halogenated reagents in the synthesis and functionalization of bio-based platform chemicals, including isosorbide, galactaric acid, and furanic compounds derived from D-fructose. The environmental performance of these synthetic procedures has been critically assessed using green chemistry metrics.

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SILICA ADSORBENT FOR ENVIRONMENTAL REMEDIATION-DEVELOPMENT, TESTING AND FUTURE PERSPECTIVES

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Numerous studies have recently been published focusing on the removal of various pollutants from both gaseous and liquid phases using adsorbent materials. These works explore the efficiency, selectivity, and mechanisms of adsorbent-contaminant interactions, contributing to the development of more effective and sustainable pollution control methods. Our primary goal is to develop efficient silica adsorbents for water purification within a circular economy framework. To achieve this, we are designing silica materials with specialized functionalization and/or incorporating biomolecules. We aim to better understand how the structure of these adsorbents influences their activity and selectivity towards various pollutants, as well as their ability to capture precious metals.

For this purpose, we have developed methyl-, ethyl-, vinyl-, methacrylate-, and epoxide-functionalized silica aerogels for removing oil, organic solvents, and pharmaceutical compounds from wastewater. Benefiting from the functionality of the organic groups and the high surface area and stability of the inorganic silica host, these hybrid materials demonstrated excellent adsorption properties against these organic pollutants [1-3]. We have also developed silica-biopolymer hybrid adsorbents with high adsorption capacity for the removal and recovery of precious heavy metals (PHMs) and rare earth elements (REEs) from secondary resources. Various polysaccharides (chitosan, alginate, cellulose, gelatin, and carrageenan) bearing different functional groups (amino, carboxyl, and sulfate) were hybridized with a new-generation biocompatible silica source. These novel composite structures were found to effectively adsorb various heavy metal ions (e.g., As(III, V), Cu(I, II), Pb (II, IV), Cd(II)) and rare earth elements (Nd(III), Eu(III)), exhibiting sorption capacities exceeding 50 mg/g and repeatable sorption performance over five cycles.

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METAL PHOSPHONATE CHEMISTRY; FROM CRYSTAL CURIOSITY TO APPLICATION

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Since the first reports in the 1970's [1] metal phosphonates have evolved. Those first reports demonstrated that organophosphorus derivatives of zirconium phosphate could be prepared wherein the organic functionality could imbue properties such as acidity, or basicity into layered materials. Over the intervening period, advances in the variety of organophosphates available and the reactions use to make them have opened the doors to many other areas through the incorporation of functional groups which allow co-ordination of metallic species, catalytic centres, the inclusion of photo-optically or biologically active groups which in addition to the much wider variety of metals that can be included has led to an exponential growth in the number of papers appearing in the literature. In those early days of metal phosphonate chemistry their application often came from investigation a material after it had been made.

Early synthetic methods often polycrystalline materials whose structure was often implied from powder XRD and other data, more often than not based on layered systems. Deducing the structure of more complex 3D systems was difficult. The use of hydrothermal methods provided the single crystals and hence structural characterization, and that insight allowed a better understanding of how these materials could be 'designed' and synthesized with the properties required for a particular application.

This paper will review the evolution of metal phosphonate chemistry from the early simple methods of synthesis and characterization through to the complex structures and cutting-edge applications we now see some 47 years after they were first reported, and pose some questions as to the future direction of this rich and interesting class of materials.

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BORON STRUCTURAL SPECIATION CHEMISTRY IN THE PHYSIOLOGY AND PATHOLOGY OF PLANTS

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Inorganic elements have long been known to be essential to the physiology and pathology of organisms in the entire hierarchy of species on the planet. Their presence has been undisputed over the ages, with recent decades being devoted to research pertaining to the delineation of their role at the (bio)chemical role in bacteria, plants, and humans. [1] Key among those elements are main group elements in the Periodic Table, with boron being a representative example that has been at the forefront of interest and practical applications, yet its role in the (bio)chemistry has eluded scrutiny of its chemistry with biological components in the cellular machinery of energy production and survival. [2] In that respect, the need to understand that element's chemistry and biology has prompted our Lab to investigate its reactivity at the chemical and biological level.

Cognizant of the fact that boron is encountered in its B(III) oxidation state, physiological substrates active in the cellular metabolism could serve as viable organic ligands capable promoting coordination bond formation with that Lewis acid ion. [3,4] In that respect, a select group of organic α-hydroxycarboxylic acids (e.g. citric acid from the Krebs cycle) was employed in the exploration of the aqueous structural speciation of appropriately designed binary and ternary systems involving boron. The aqueous synthetic chemistry of such binary systems was investigated in a pH-specific manner, leading to the isolation of crystalline materials, which have been further characterized through elemental analysis, FT-IR, ESI-MS spectrometry, and X-ray crystallography. Physicochemical characterization of the derived materials reveals that all species isolated contained B(III) in a tetrahedral environment, with the α-hydroxycarboxylato moiety acting as a bidentate chelator, bringing about considerablestability to the emerging complex assemblies. The accrued experimental data justified employment of the new materials in *in vitro* biological experiments on eukaryotic cell cultures. To that end, cytotoxicity studies (morphology, viability, proliferation, chemokinetic behavior, etc.) were looked into in a concentration- and time-dependent fashion, with the results projecting clear atoxicity of the new species over a wide concentration range.

The collective data on the investigated binary systems formulate a well-defined (bio)chemical reactivity profile of hybrid boron(III)-organic acid complexes, which prompts further use in *in vitro* biological experiments assessing their potential and merit as future pharmaceuticals in bacterial, human, and plant (patho)physiologies.

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CHEMO-ENZYMATIC SYNTHESIS OF NOVEL MACROMOLECULAR ARCHITECTURES BY USING BIO-BASED FUNCTIONAL MONOMERS

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In the context of a circular economy, the valorisation of industry byproducts is considered as a fundamental step of the green transition. Produced every single day on a multi ton scale, one of the main Italian industry byproducts is dairy whey from cheese production. The major component of cheese-whey is lactose (165,25 g/L), a disaccharide composed by D-Glucose and D-Galactose linked by glycosidic bond [1]. As widespread natural platform molecules, carbohydrates constitute a valid alternative for the design and synthesis of novel macromolecular architectures. D-Glucose and D-Galactose from dairy whey are useful for the synthesis of carbohydrate derivatives that could be used for the synthesis of novel materials [2]. In fact, bicyclic carbohydrate-derived difunctional compounds can be used as the constituent building blocks for the synthesis of terephthalate-substituting polymers and, at the same time, they could be used as the starting material for the synthesis of innovative bio-based nucleating additives and plasticisers [3].

Usually, when diols and dicarboxylic acids (or their esters) are used as monomers, polyesters are obtained by polycondensation in the presence of a metal catalyst. However, when these kind of catalysts like dibutyltin dilaurate and dioctyltin mercaptide ester (Metatin) are used on functional and/or carbohydrate-derived monomers, several side reactions occur leading to a loss of functionality and difficulties in the material's processing [4]. As a valid alternative to process functional monomers, hydrolytic enzymes such as *Candida antarctica* Lipase B (CaLB) can be considered as valid alternatives. Biocatalysts can if fact work at mild conditions (T<100 °C) in bulk conditions or in more sustainable, biomass-derived solvents [5]. In this work the enzymatic synthesis of carbohydrate-derived polyesters in novel green solvents was developed using various aliphatic diesters and GluX as monomers and immobilized CaLB as the biocatalyst. The obtained polymers were fully characterized via nuclear magnetic resonance, gel permeation chromatography and thermal analysis.

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VALORIZATION OF BAMBOO BIOMASS VIA CHEMO-ENZYMATIC PROCESSES FOR SUSTAINABLE PRODUCTS DEVELOPMENT

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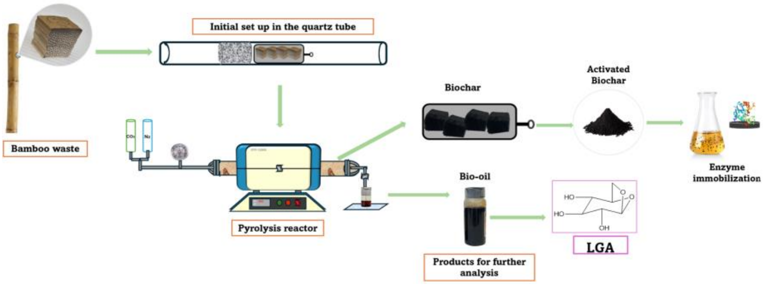
Bamboo, an abundant source of lignocellulosic biomass, has a chemical composition and fibre structure similar to wood, offering high potential for sustainable material synthesis. This work reports on the implementation of an integrated biorefinery strategy utilising pyrolysis process to extract high-value platform chemicals such as levoglucosan (LGA) as monomeric precursor. This molecule is subsequently transformed via a chemo-enzymatic procedure, combining selective enzymatic esterification to prepare bio-based surfactants and emulsifying agents. The process integrates the products valorisation from bamboo pyrolysis (bio-oil and biochar) at different temperatures from 400° to 800°C (Fig.1). The untreated bamboo (*Dendrocalamus giganteus*) was pyrolyzed in slow and fast thermal treatments under different gases (N_2 and CO_2) controlling pressure and flow rate eliminating the need for toxic reagents and chemically intensive routes. [1-2] The characterization via Gas Chromatography–Mass Spectrometry (GC-MS), Nuclear Magnetic Resonance (NMR), and High-Performance Liquid Chromatography–Mass Spectrometry (HPLC-MS) confirms the presence of high purity of the LGA, and further esterification takes place employing *Candida antarctica* lipase B (CaLB) enzymes as biological catalyst. [3] To enhance catalytic efficiency and reusability, the enzyme was immobilized onto biochar providing a stable and effective heterogeneous biocatalytic system. The synthetic approach prioritizes low-energy inputs, non-toxic solvents, and minimal by-product formation. Guided by the Twelve Principles of Green Chemistry, our process minimizes waste and avoids hazardous reagents, significantly enhancing the sustainability and scalability of bio-based additives and polymers production. This work underscores the viability of bamboo biomass as a circular feedstock for next-generation polymers, surfactants, and emulsifying agents, contributing to the transition towards renewable materials.

Figure 1. Diagram of the pyrolysis set up used in the integrated biorefinery process, including product collection (bio-oil and biochar)



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FUNCTIONALIZED NANOMATERIALS WITH ANTIOXIDANT PROPERTIES

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Over the past decade, a wide range of nanomaterials have attracted attention as artificial enzymes (nanozymes) to perform specific tasks due to their intrinsic enzyme-like catalytic activities. [1]
Compared to natural enzymes, nanoenzymes have many advantages, such as higher stability, greater design flexibility, and lower production costs. Nanozymes can be used to mimic natural antioxidant enzymes to treat diseases caused by oxidative stress. [2]
The present study aims to investigate the antioxidant properties of some all-carbon and hetero-substituted fullerenes. The computational methods are applied for characterizing the stability and properties of these nanomaterials.
Some of the investigated fullerenes containing 52 atoms, with the general formula $C_{49}N_3$ are presented in figure below:

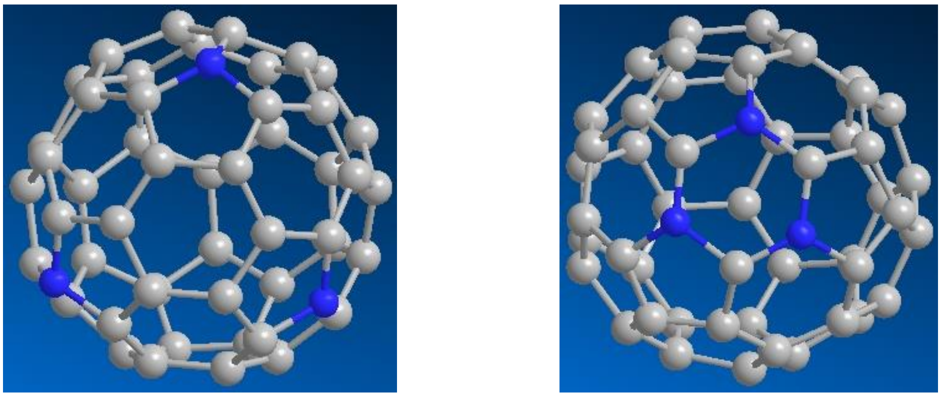

Figure 1. $C_{49}N_3$ fullerenes

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FLOW CHEMICAL SYNTHESIS OF BIOLOGICALLY ACTIVE COMPOUNDS AND ACTIVE PHARMACEUTICAL INGREDIENTS

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Flow chemistry exceeded in pharmaceutical industry in the 2010s, thanks to the expansion of organic chemistry and the development of technology, creating a wealth of new opportunities. In flow systems, compounds can be produced faster, safer, and with consistent quality, as well as processes can be easily controlled, scaled up and automated.[1]

One of our aims was to develop a telescopic microwave-assisted flow chemical method for the synthesis of (1,2,3-triazol-4-yl)methyl phosphoramidates, as a new family of bioactive compounds by the preparation of the two key intermediates of prop-2-inylphosphoramidates and organic azides followed by azide-alkyne cycloaddition.[2]

We have also developed the first flow synthesis of capsaicin derivatives [3] and 6-amino-6-deoxy-β-cyclodextrin by three reaction steps.[4] Both flow methods elaborated are generally greener, safer, faster and more atom-efficient processes than their batch alternatives described.

Flow chemistry has several advantages as mentioned, however it has also a few drawbacks, for instance, commercially available flow chemical equipment and reactors are quite expensive. Fortunately, there is a way for a cheaper, customizable, yet reliable flow chemistry, which can be realized via Fused Filament Fabrication (FFF) 3D printing. [5] For 3D printed flow reactors, however, it is important to choose a thermoplastic that is thermally and chemically compatible with the organic reactions to be carried out. For this reason, comprehensive chemical, thermal and pressure stability studies were performed on flow reactors printed from different polymers and polymer composites. Finally, the performance of the 3D printed reactors has been demonstrated in the flow synthesis of several drug intermediates (e.g. cetirizine, paliperidone and tamoxifen) based on the results of chemical resistance studies.[6]

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NANOPLATFORMS BASED ON METALLIC NANOPARTICLES FOR BIOMEDICAL APPLICATIONS

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Gold and silver nanoparticles (NPs) can be used in the development of nanoplatforms for the delivery of phytochemicals due to their properties such as controlled size, biocompatibility, antimicrobial activity, anti-inflammatory etc.[1,2] By combining the capabilities of Ag and Au NPs with those of mesoporous silica, whose surface can be easily functionalized with various organic groups, nanoplatforms with tailored properties can be developed for various biomedical applications such as phototherapy for cancer treatment, imaging, antimicrobial treatment against drug resistant pathogens, wound dressings, lateral flow immunoassays etc. [3-5]

The aim of this research was to obtain functionalized mesoporous silica-based carriers in which Ag or Au NPs were incorporated. The mesoporous supports were characterized by nitrogen adsorption-desorption isotherms, FTIR spectroscopy, X-ray diffraction, as well as scanning and transmission electron microscopy coupled with energy dispersive X-ray analysis.

The resulting supports were further used to incorporate a wild bilberry leaf extract prepared by solvothermal method under inert gas pressure. The extract was characterized by various spectrometric methods such as the total content of polyphenols, flavonoids, anthocyanins, condensed tannins, radical scavenger activity and α-glucosidase inhibitory potential, while the identification of components from the extract was performed by high-performance liquid chromatography.

The extract encapsulated in proposed carriers did not show cytotoxicity on human HaCat keratinocytes up to a treatment dose of 50 µg/mL. An improved antioxidant activity of the designed composites, evaluated on HaCat keratinocytes, was observed compared to that of the free extract. Inflamed THP-1 monocytes treated with free wild bilberry extract free and encapsulated in mesoporous supports secreted a lower amount of pro-inflammatory TNF-α cytokines.

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AMPHIPATHIC PEPTIDES WITH BIOLOGIC ACTIVITIES

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As longevity increases, there is a growing demand for solutions to combat health challenges such as cancer, neurological disorders, and infections from bacteria and viruses. Antimicrobial peptides are a class of peptides recognised for their capacity to eliminate microorganisms. They are currently being investigated as novel vehicles for delivering bioactive substances to address ailments such as cancer, genetic disorders, cardiovascular diseases, infectious diseases, and inflammatory conditions.

Antimicrobial peptides (AMPs) exhibit distinct structural characteristics, including amphipathic configurations and specific amino acid residues, which facilitate selective interactions with various membranes.

Ten new peptides derived from established antimicrobial peptides (AMPs) were synthesised via solid-phase peptide synthesis (SPPS) and characterised using MALDI-TOF-MS analysis. At the same time, their purity was evaluated through analytical HPLC. Using the broth microdilution method, the minimum inhibitory concentrations of these peptides were determined for several bacterial strains, including *Salmonella typhimurium, Pseudomonas aeruginosa, Escherichia coli, Staphylococcus aureus,* and *Bacillus subtilis subsp. spizizenii*. Designing peptides with advantageous properties, such as the ability to cross biological barriers, enter cell membranes, sustain prolonged circulation, and prevent toxicity or immunogenic reactions in humans, is crucial to the advancement of peptide-based medicinal systems.

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TARGETED CANCER THERAPY: CHALLENGES, SUCCESS AND HOPE

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Targeted cancer therapy is one of the greatest achievements of modern biomedicine – a personalized approach that allows for selective recognition and attack of tumor cells and sparing of healthy cells and tissues. A magic bullet that Paul Ehrlich and generations of brilliant minds dreamed of. Introduced at the end of the 20th century with the first monoclonal antibodies approved for the treatment of some leukemias, targeted therapy revolutionized the control of a number of malignant tumors and gave a chance for life and happiness to millions of people and their loved ones.

What is targeted antitumor therapy? What are some of the most successful examples, but also stumbling blocks on its way? Will synthetic biology help us to bridge the gap between hope and reality? Do we still need conventional antitumor agents and is it worth working on improving them? Is there a place for cell cultures in our quest to overcome one of the greatest health and social challenges of our time – cancer.

New data on tumor biology will be presented as well as the most important lessons learned from targeted anticancer therapy (including melanoma and breast cancer); our experience in searching for new antitumor agents and creating and applying cell model systems for the needs of experimental oncology and oncopharmacology will be also summarized.

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BIOMASS ACTIVATED CARBON AS SUSTAINABLE WAY FOR HYDROGEN STORAGE

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Climate change and constant increase in energy demand in the last decades made the transition from fossil fuels to green solutions and more sustainable energy systems necessary. A suitable solution has been represented by Hydrogen (H_2), an alternative and clean fuel to be applied to store energy, as solution to intermittent from coming from renewable energy sources and/or for mobility and transport systems. However, storing H_2 safely, economically, and efficiently is undoubtedly a major technological challenge. An interesting alternative to the classical storage methods as liquid and/or compressed to high pressure could be represented by the adsorption into porous materials. Among the different available materials, nanostructured carbon with high specific surface area and optimized porosity are particularly promising because are easy to prepare, cheap and effective [1]. Of particular interest are the activated carbon (Ac) which can be obtained starting from economic precursors using eco-sustainable synthesis processes appears to be a particularly interesting research field nowadays [2], allowing the reintroduction of waste materials (lemon peel, peach pit, walnuts shell, coffee ground etc.) into the economic system, transforming them into a new resource [3,4,5]. Resulting activated carbons, in fact, show interesting nanostructure in terms of specific surface area (S_{BET}), total pore volume (V_T) and an excellent microporosity that make them functional not only for H_2 storage but also for other applications such as gas separation (CH4, CO2, N2), filters, sensors, super capacitors etc. In the present experimental work, ACs were produced by pyrolysis, through two main phases, i.e. carbonization and physical activation of the raw material.

The main goal was to study how the key process parameters (gas type and temperature) and the starting form of biomass influence the structural properties and, consequently, the hydrogen adsorption capacity. Chemical and morphological properties were investigated through different energy dispersive x-ray (EDX) analysis, scanning electron microscopy (SEM) while textural features and H_2 adsorption capacities were determined using volumetric techniques. All porous carbons derived show interesting specific surface area (more than 1000 m^2/g) and total pore volume higher than 0.5 cm^3/g with microporosity percentage (< 2nm) between 85-100% and excellent H_2 adsorption capacity.

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HIGH PERFORMANCE POLYAMIDES FOR ENERGY STORAGE SMART WINDOWS

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Smart windows that can electrically modulate the light transmission while maintaining single or multiple color states with minimal or no energy consumption contribute significantly to improving building energy efficiency by reducing the energy needed for heating, cooling, and lighting. [1] To enhance energy efficiency, efforts have been made to integrate electrochromism with energy storage within a single system, leading to the development of electrochromic energy storage devices (ECESDs), also known as electrochromic supercapacitors (ECSs), energy storage smart windows (ESSWs), or electrochromic capacitive windows (ECWs). [2] These systems can perform both functions simultaneously, allowing the optical response of the electrochromic material under applied voltage to visually indicate the stored energy level.

Recently, we have reported on the electrochromic behavior of a series of polyamides [3], demonstrating that non-conjugated polymers containing electroactive units can compete with conjugated polymers when used as electrode materials in ECW applications. To improve solubility, processability, and solid-state packing of the polymers, which directly influence ion diffusion and transport, we modified the structural pattern of the diamine segments. Thus, bulky fluorene groups, flexible hexafluoroisopropylidene units, and fluorophenyl-substituted oxadiazole fragments anchored on triphenylamine (TPA) were incorporated into the polyamide chains to reduce molecular aggregation and enable the processing of these polymers into uniform, transparent films capable of reversible color change under an applied voltage. First, the structural, optical, thermal, and electrochemical properties of these polymers were investigated to establish structure-property relationships, which were supported by DFT calculations. Chronopotentiometry was employed to perform galvanostatic charge-discharge studies for evaluating the polymers' energy storage capabilities, followed by spectroelectrochemical and chronoamperometric analyses to determine electrochromic performance indicators, such as optical contrast, switching time, coloration efficiency, and stability. Throughout the study, we discussed how structural variations within the polymers influence their capacitive and electrochromic properties, and the best-performing polyamide was tested in a prototype electrochromic capacitive device. Given its effective dual functionality as a smart color-changing and energy-storing electrode, this polymer represents a promising material for energy storage smart windows with potential applications in green and sustainable technologies. [4]

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TOWARDS GREENER POLYMERS: ADVANCING THE SYNTHESIS OF FURAN-BASED MATERIALS FROM RENEWABLE RESOURCES

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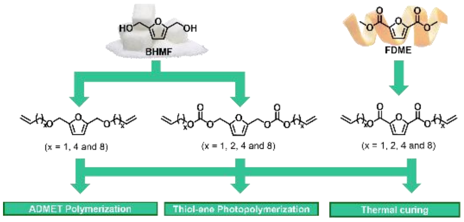
The increasing interest in utilizing renewable resources for the production of polymeric materials is primarily driven by environmental concerns and the need for sustainable solutions to the challenges faced by the current generation. [1] Consequently, the plastic industry is shifting toward more sustainable methods for developing new monomers and materials. Among these innovations, furan-based polymers derived from renewable sources have garnered significant scientific attention in recent years. However, their use remains limited, with the majority of research focusing on polymers derived from 2,5-furandicarboxylic acid (FDCA). [2] To date, the few furan-derived polymers that have been synthesized typically utilize polycondensation methods, which often require harsh reaction conditions, involving environmentally hazardous procedures, and providing limited control over the polymer structure. [3] In contrast, there are other polymerization techniques – namely Acyclic Diene Metathesis (ADMET) polymerization, Thiol-ene photopolymerization, and thermal curing – that allow for the synthesis of polymeric materials with precise control over polymer structures under mild conditions. These techniques have been extensively used in the synthesis of bio-based polymers, however, despite the ever-growing interest in furan-based monomers, the application on these compounds is still scarcely explored. In this study, we present the development of novel furan bio-monomers derived from D-fructose, specifically 2,5-bis(hydroxymethyl)furan (BHMF), and galactaric acid, namely dimethyl furan-2,5-dicarboxylate (FDME). Through etherification, transcarbonylation and transesterification reactions different lengths aliphatic chains with terminal olefins were incorporated in BHMF, 2,5-diylbis(methylene) dimethyl bis(carbonate) furan (BACMF) and FDME respectively. These new furan-based α,ω-diene monomers are then polymerized via ADMET polymerization, Thiol-ene photopolymerization, and thermal curing, allowing for the production of a variety of both homo and co- polyethers, polycarbonates and polyesters with a wide range of thermal properties under mild conditions[4]. Overall, this work underscores the importance of integrating renewable feedstocks with sustainable synthetic strategies when developing novel polymeric materials. The versatility and tunability of the furanic monomers presented here highlight their promise for future applications across diverse fields, including coatings, packaging, and recyclable thermosets.



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CONTINUOUS FLOW: A NEW APPROACH TO THE ETHERIFICATION OF BIO-BASED FURANIC COMPOUNDS

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The ultimate goal of biorefinery is to move away from a fossil-based industry aiming to a more sustainable one centered on the use of renewable feedstocks; on this way, in chemistry, Bio-based platform chemicals play an important role. Bio-based platform chemicals derived from hemicellulosic materials are extensively investigated to synthesize several value-added molecules, useful for different applications in the polymer sector [1] such as composites, thermosets [2] and coatings. [3] Among them, biomass-derived C6 carbohydrates are of particular interest since they lead to furanic building blocks such as 5-hydoxymethyl furfural (HMF), 2,5-furandicarboxylic acid (FDCA) and 2,5-bis(hydroxymethyl)furan (BHMF) [3]. In the last years, a family of HMF and BHMF derivatives - 5-(alkoxymethyl)furfurals (AMFs) and 2,5-bis(alkoxymethyl) furans (BAMFs), respectively - has attracted increasing attention due to their potential applications as bio-diesel additives. [4] In addition, HMF, when subjected to self-etherification, leads to 5,5′-[oxybis(methylene)]bis-2-furfural (OBMF), another bio-based monomer of growing interest due to its exploitation in the synthesis of macrocycles (16-crown-6) [5] and as a precursor of polyurethanes, polyamides, and polyamines. [6]

In this work, a comprehensive investigation on the etherification of Bio-Based furanic compounds promoted by a commercially available ion exchange resin - Purolite CT275DR - is conducted using a continuous flow apparatus. The reaction conditions are initially optimized for the etherification of BHMF with ethanol and then extended to achieve a library of BAMFs. The long-term stability of Purolite CT275DR was investigated using the optimized reaction conditions for BEMF synthesis and with other two alcohols, i.e., 2-propanol - a more sterically hindered alcohol - and allyl alcohol, too. In addition, HMF etherification and self-etherification are studied. HMF self-etherification to form OBMF is conducted using dimethyl carbonate as green solvent in the presence of both heterogeneous and homogeneous acid catalysts, with the latter being the most effective. Finally green metrics are calculated for the optimized etherification of BHMF with ethanol and the values are compared to previously published procedures. [7]

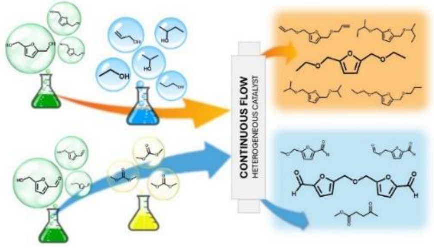

Figure 1. Etherification of furanics via Continuous Flow

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R-NADES AS GREEN SOLVENTS FOR BIOCATALYSIS: IMPROVING LIPASES STABILITY AND SELECTIVITY

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Natural deep eutectic solvents (NADESs) have emerged as sustainable, green alternatives for biocatalytic reactions, providing high substrate solubility while improving enzyme stability and efficiency.

In our studies, the design of reactive natural deep eutectic solvents (R-NADESs) and their effect on the esterification activity and thermal stability of free and immobilized lipases in the synthesis of polyol- and carbohydrate-based biosurfactants was investigated. A total of 16 binary and ternary R-NADES systems were synthesized using choline chloride (ChCl) as hydrogen bond acceptor (HBA) and carbohydrate polyols, including mono-, di-, and oligosaccharides, urea, N-methyl urea, and water as hydrogen bond donors (HBDs), in various molar ratios. These systems were characterized based on their physicochemical properties, including viscosity, polarizability, hydrogen bonding, and thermal behaviour.

The results showed that lipases, both free and immobilized, exhibited high stability and catalytic performance in R-NADESs during esterification reactions. In particular, R-NADESs consisting of ChCl and sugar alcohols (D-sorbitol, xylitol, D-arabitol) were efficient in catalyzing the esterification of polyols with fatty acids, with Candida antarctica lipase B immobilized on acrylic resins exhibiting exceptional thermal stability. A Box-Behnken factorial design optimized the reaction conditions, resulting in an 80 mol% conversion of lauric acid (LA) to D-arabitol, yielding the product 1,5-dilauryl-D-arabitol with >99.9% purity.

In addition, the esterification of glucose was investigated and only lauroylcholine chloride was obtained due to strong interactions in the H-bond network of a ChCl:Glc:H2O R-NADES. Molecular dynamics simulations provided insight into these reaction results and explained the observed selectivity and stability of the lipase-catalyzed reactions in R-NADES media.

Acknowledgements
This study was supported by a grant of the Romanian Ministry of Education and Research, CCCDI-UEFISCDI, project number PN-III-P4-ID-PCE-2020-2177, within PNCDI III, contract number PCE 157/2021.

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SYNTHESIS OF 2,5-FURANDICARBOXYLIC ACID ESTERS AND THEIR APPLICATION IN MACROCYCLES FORMATION

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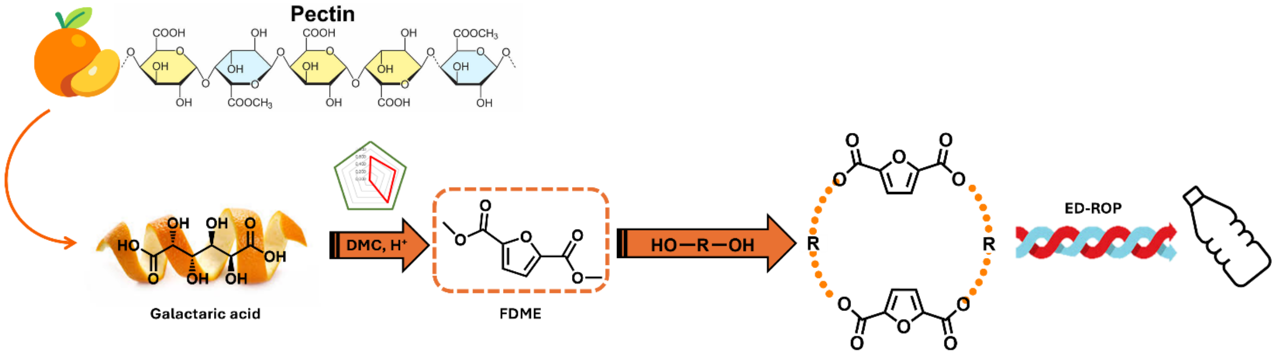
2,5-Furandicarboxylic acid (FDCA) and its ester 2,5-furandicarboxylic acid dimethyl ester (FDME) have been extensively studied as monomers for the production of polyesters[1] such as polyethylene furanoate (PEF), considered as one of the most valuable bio-based substitute of the petroleum-derived polyethylene terephthalate (PET).[2] FDCA and FDME can be synthetized starting from aldaric acids, which can be obtained either via oxidation of sugars or directly extracted from citruses peel.[3,4] From these premises, the present study reports an alternative synthetic procedure for the production of FDME starting from galactaric acid via dimethyl carbonate (DMC) chemistry. FDME was retrieved as a white crystalline solid with an isolated yield of up to 70% without any chromatographic purification. In addition, the greenness of the herein discussed synthetic procedure was evaluated using the most common green metrics and compared with other available synthetic pathways.[5]
The obtained FDME was then employed for the production of bio-based polyesters (PEs) via entropically-driven ring opening polymerization (ED-ROP). Macrocycles were prepared by reacting FDME with diols such as tetraethylene glycol (TEG) and hexaethylene glycol (HEG) via pseudo-high dilution condensation (PHDC) using CPME as recyclable green solvent. Isolation of the pure macrocycles was achieved by simple crystallization/precipitation from the reaction mixture. Subsequent ED-ROP of pure macrocycles was also investigated as viable route to prepare the related PEs in mild reaction conditions.



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EU-OPENSCREEN – AN OPEN ACCESS INITIATIVE TO IDENTIFY NEW BIOLOGICAL ACTIVITIES OF YOUR COMPOUNDS

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Compounds and natural products synthesized by chemists represent a rich, untapped source of novel chemical diversity. In many cases, chemists have limited opportunities to test these compounds against a variety of drug targets or for them to be accessed by biologists who have developed suitable assays. EU-OPENSCREEN enables chemists to share their compounds within a transparent framework, making them available for screening in diverse bioassays. **This opportunity allows compounds to be tested against many biological targets, uncovering unknown bioactivities and facilitating new collaborations with EU-OPENSCREEN** users from across Europe and beyond. Submitted compounds are quality-controlled, stored, and reformatted at the Central Compound Management Facility in Berlin. They undergo initial "bioprofiling" (cell-based, biochemical, and physicochemical assays) free of charge to the chemist. The bioactivity data are shared with the respective chemist. After the initial 'bioprofiling', compounds are tested exclusively at official EU-OPENSCREEN partner sites and are not passed on to third parties without consent, so that the chemists retain control over the use of their compounds.

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CHEMISTRY FOR A SUSTAINABLE TOMORROW - ROMANIA JOINS THE GLOBAL CONVERSATION

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Aligned with the IUPAC Project *"Global Conversation in Sustainability (GCS)"* [1] and *UN SDG Day* [2], the first edition of the Global Conversation in Sustainability event series in Timişoara will take place on 25 September 2025 at the *Romanian Academy, "Coriolan Drăgulescu" Institute of Chemistry (ICCD)*, as a special section of the *New Trends in Chemistry Research 2025 Conference* [3].

The concepts of sustainability and sustainable chemistry have gained increasing attention, particularly among the younger generation of chemists. This special section reflects on how chemists can contribute to the sustainable transformation of the discipline, not only by proposing specific research directions, but also by inspiring engagement across education, outreach, policymaking, research culture, and publishing. Emphasis is placed on empowering young scientists with resources and opportunities to act as catalysts and ambassadors for change, while acknowledging the challenges and complexities associated with sustainability. Although focused on early-career chemists, the discussion also provides insights relevant to the wider scientific community, encouraging collective action toward a more sustainable future. [4,5]

This session will highlight the role of chemistry in advancing the UN Sustainable Development Goals (SDGs), foster dialogue and networking, and showcase 20 posters on green chemistry and sustainable practices across diverse domains. By combining lectures and poster presentations, the program seeks to promote knowledge exchange, interdisciplinary collaboration, and the dissemination of best practices at local, national, and international levels.

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HYBRID MATERIALS BASED ON METAL COMPLEXES WITH POLYPHENOLS FROM *TARAXACUM OFFICINALE* FOR UV RADIATION SHIELDING APPLICATIONS

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Scientific interest in the valorization of natural compounds for the synthesis of functional materials and biologically active agents has increased significantly in recent decades. Among these compounds, polyphenols hold a prominent position due to their antioxidant, anti-inflammatory, and antimicrobial properties. *Taraxacum officinale* (common dandelion), a widely distributed species in spontaneous flora, represents an inexpensive natural source of polyphenols. The interaction of these compounds with transition metal ions leads to the formation of metal complexes with potential applications in the pharmaceutical, biomedical, and environmental fields. [1–4]

This study aims to highlight the possibilities for the synthesis, characterization, and application of metal complexes formed through the reaction of polyphenols extracted from *Taraxacum officinale* with metal ions such as Cu^{2+}, Zn^{2+}, and Ag^{+}. Polyphenols were extracted from plant biomass (flowers, leaves, and roots) through maceration or ultrasonic process in alcoholic solvents (ethanol and methanol). After extraction, the solutions were filtered and concentrated, yielding polyphenol-rich extracts. These extracts were used in complexation reactions by gradually adding metal salt solutions, adjusting the pH from neutral to slightly basic, and varying the metal ion concentration in the alcoholic medium.

The resulting metal complexes were deposited onto an inorganic support (sericite, a mica derivative) through adsorption processes carried out under controlled temperature and time conditions. Both the metal complexes and the hybrid materials obtained by their deposition on sericite were characterized using specific analytical techniques, including FTIR spectroscopy, UV-Vis spectroscopy, diffuse reflectance spectroscopy, scanning electron microscopy (SEM), and thermogravimetric analysis (TGA). The antibacterial properties of these structures were also investigated and confirmed.

The analyses revealed that leaf-derived extracts contained the highest concentration of polyphenols and provided the greatest efficiency in complexation reactions. The hybrid materials obtained by immobilizing the metal complexes onto sericite exhibited high thermal stability and showed lower transmittance values compared to the inorganic support alone. These properties make the hybrid materials suitable for potential applications in various fields, such as cosmetics, coatings, packaging, or functional textiles designed for UV radiation shielding.

Acknowledgements

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SYNTHESIS OF LEVOGLUCOSENONE-BASED AMPHIPHILIC MOLECULES

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Current European sustainability policies are driving the chemical industry to reduce its reliance on fossil-based raw materials, which are often associated with environmental pollution and ever growing CO_2 emissions. In response, synthetic chemistry is increasingly aligning with the principles of Green Chemistry, promoting the use of renewable feedstocks, shorter and more streamlined reaction steps, minimal use of solvents and reagents, and the adoption of more energy-efficient technologies. In this context, levoglucosenone (LGO), a platform molecule obtained from cellulose, has been explored as a Michael acceptor in the sustainable synthesis of amphiphilic derivatives. This work presents the development of a green, solvent-free protocol for the conjugate addition of LGO with various bio-based malonate esters (R = Me, Et, Bu and Bn), using microwave irradiation and an inorganic heterogeneous catalysts. Among several inorganic bases tested ($Ca(OH)_2$, MgO, NaOH, K_2CO_3), calcium hydroxide proved to be the most effective, enabling high conversion without the need for hazardous reagents like KF/alumina and organic complex nickel-based typically reported in literature. [1,2] Optimization of the reaction conditions was carried out using a Design of Experiment (DoE) approach, evaluating the influence of reaction time (2, 8.5, 15 min), microwave power (5, 13, 20 W), and malonate equivalents (1, 1.5, 2 eq). The combination of high power/short time (20 W–2 min) or moderate power/long time (13 W–15 min) provided optimal conversions. The best results (conversion >95%) were achieved using 10% w/w $Ca(OH)_2$. Given their amphiphilic structure, the hydrophilic–lipophilic balance (HLB) values of the synthesized compounds were calculated using Griffin and Davies methods. Both approaches consistently identified dibuthyl-malonate (DBuM-LGO) adducts as wetting agent, dimethyl-malonate (DMM-LGO) and diethyl-malonate (DEM-LGO) derivatives as o/w emulsifying agents while producing divergent outcomes in the case of benzyl malonate (DBnM-LGO). To support the theoretical HLB predictions, emulsification tests and contact angle measurements were performed in various liquid media. These experiments confirmed the amphiphilic behavior and surface activity primarily for the adducts bearing longer alkyl chains, such as the butyl and benzyl derivatives, highlighting their potential as effective bio-based surfactants. [3]

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f-ORBITAL ELECTRONIC STRUCTURE: COMPLETE, *AB INITIO* DERIVATION OF CRYSTAL FIELD PARAMETERS FOR THE f^1-CONFIGURATION

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The seminal book of Abragam and Bleaney provides a deep yet challenging-to-grasp overview of the elementary theory of the crystal field. [1] Given a lanthanide ion, the standard approach to deriving crystal field parameters (CFPs) involves constructing an analytical matrix in the basis of the ground-state J-manifold using Stevens equivalent operators, and extracting the parameters based on a numerical matrix built from *ab initio* quantum chemistry calculations. [2] This approach yields parameters that exclude contributions from off-diagonal matrix elements between blocks of different J-manifolds associated with the same spin-free ground orbital term. Although widely used in the molecular magnetism community, this method has a significant limitation: The resulting CFPs may be effectively biased by those second-order crystal field effects, potentially hindering the identification and rationalization of trends.

In this presentation, inspired from our previous work on the extraction of CFPs based on the effective Hamiltonian theory and multiconfiguration wavefunction theory calculations on transition metal complexes [3], we propose the first theoretical approach that accounts for both the ground and excited state manifolds of a reference f^1 ion in a consistent way, with *ab initio* demonstration of the occurrence of sizeable second-order crystal field effects. By doing so, we show that the exact same parameter values can be extracted regardless of the absence or presence of the spin-orbit coupling, validating the correctness of the newly proposed extraction strategy. Our findings for this configuration challenge the common assertation in the literature that spin-orbit coupling affects CFPs – an assertion that stems from the widespread use of the pseudospin approach, which inherently neglects contributions from off-diagonal elements of the crystal field.

Acknowledgement
This work was partially supported by the "PHC Brancusi" Romania-France bilateral research program (code: PN-IV-P8-8.3-PM-RO-FR-2024-00-22), funded by the Romanian National Authority for Scientific Research and Innovation (UEFISCDI).

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RATIONAL DESIGN OF LANTHANIDE AND TRANSITION METAL COMPLEXES WITH POLYDENTATE SCHIFF BASE LIGANDS

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Polydentate Schiff base ligands derived from N-(1-naphthyl)ethylenediamine and substituted salicylaldehydes were used for the synthesis of mono- and heteronuclear complexes with 3d, 4d and 4f metal ions. These ligands, characterized by extended π-systems and multiple coordination sites, enable the formation of structurally and functionally diverse metal complexes. [1]

Mononuclear complexes with Zn(II), Cu(II), Pd(II), Eu(III), and Tb(III) were synthesized and characterized through spectroscopic methods and single-crystal X-ray diffraction, which confirmed coordination geometries ranging from tetrahedral and square-planar to square-antiprismatic. A schematic synthetic route for 3d complexes is shown in Figure 1.

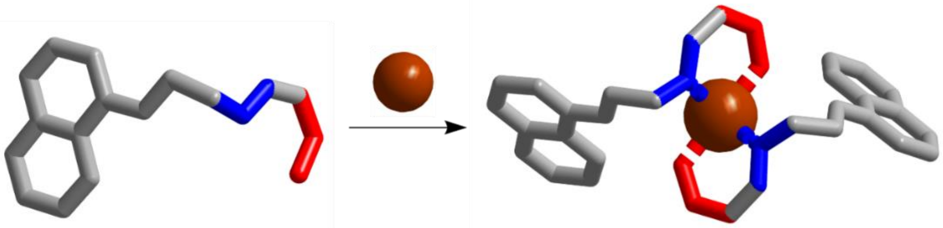

Figure 1. Schematic synthesis of 3d complexes using Schiff base ligands.

Luminescence studies revealed emission for Eu(III) and Tb(III) complexes, facilitated by ligand-to-metal energy transfer. Additionally, sequential synthetic strategies allowed the formation of heterometallic Zn–Ln complexes, which exhibited enhanced luminescence.

A particular focus was placed on Pd(II) complexes due to their potential interaction with biomolecules. Owing to their planar geometry, previous DNA-binding studies suggest a possible intercalative mechanism, making these compounds promising candidates for further investigation as intercalation agents. [2] Figure 2 presents the X-ray crystal structures of two Pd(II) complexes, each exhibiting different metal-to-ligand stoichiometries.

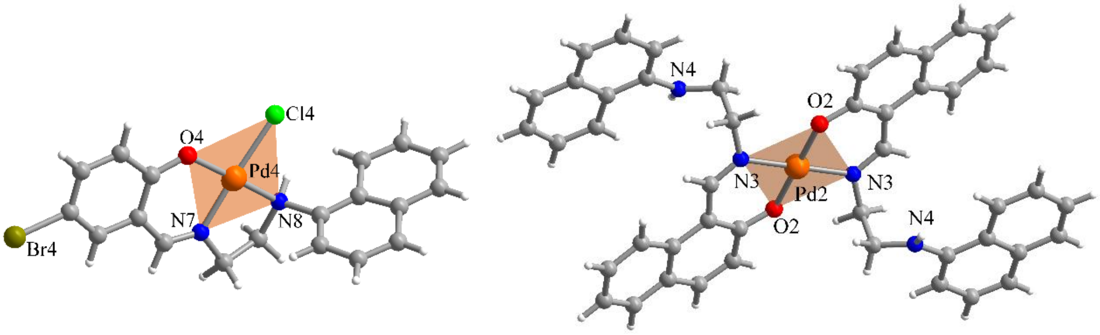

Figure 2. X-ray crystal structures of two Pd(II) complexes featuring 1:1 and 1:2 metal-to-ligand ratios.

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ENCAPSULATION OF DNA IN POLYMERIC NANOPARTICLES FOR TARGETED GENE DELIVERY

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In recent years, targeted drug delivery has been considered to be a very rational and desired requirement in the treatment of human pathophysiologies or even neurological disorders. Nanotechnology has introduced new pathways providing improved therapeutic delivery of drugs, using different types of nanoparticles (i.e. polymeric, liposomic, inorganic) without inducing toxicity or affecting healthy tissue. The main requirements for such types of nanocarriers include biocompatibility, drug compatibility, and biodegradability. One of the most known disorder, namely Charlot-Marie-Tooth Disease (CMT), remains an incurable neuropathy [1]. It is known for causing axonal degeneration, sensory loss, muscle weakness and atrophy. To address this issue, we have developed in our Lab, PLGA (poly (lactic-co-glycolic acid)) based nanoparticles for encapsulation of plasmid DNA. The work focused on the nature of the therapeutic plasmid (appropriately modified), thus achieving all the requirements. PLGA is one of the most commonly and effectively used biodegradable polymers for the development of nanocarriers. The atoxicity of PLGA polymer nanoparticles is attributed to the hydrolysis of lactic and glycolic acid, both products of the Krebs cycle. [2] Furthermore, to enhance the stability and control the size of the nanoparticles, PVA (polyvinyl alcohol) was added as an emulsifying agent. [3]

To achieve specificity toward the target cells (Schwann cells), a "guiding rod" was attached to the surface of the nanoparticle in order to target specific transmembrane protease serine 5 receptor, which is expressed in Schwann cells compared to different tissue cells. [4] To that end, conjugation to the surface of the nanoparticle though an RNA-aptamer was achieved using EDC (ethyl(dimethylaminopropyl)carbodiimide) – NHS (N-hydroxysuccinimide) chemistry. Aptamers provide a huge range of flexibility toward the targeted cell surface protein, since they are specifically engineered to firmly bind to the protein. [5]

Following the design and synthesis of the nanoparticles, the next step included validation of the proposed nanoparticle, using characterization with physicochemical techniques for verification of all of the aforementioned steps (size, conjugation, stability, encapsulation of DNA) through Fourier Transform Infrared Spectroscopy (FT-IR), Dynamic Light Scattering (DLS), particle size and shape analysis using Confocal Microscopy, and Transmission Electron Microscopy (TEM). Finally, the produced and characterized nanoparticles were lyophilized and introduced to *in vivo* experiments for further evaluation of their potential therapeutic effects in the specified neuronal disease.

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SYNTHETIC EFFORTS EXEMPLIFY STRUCTURAL SPECIATION OF BIOLOGICALLY-RELEVANT Zn(II)-AMINO ACID ZWITTERIONIC SPECIES

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Metal ions and especially zinc (Zn(II)) play a key role in human (patho)physiology as cofactors of numerous enzymes and proteins. Zn(II) is often included in dietary supplements and medicines for various illnesses. Furthermore, clinical studies have demonstrated that zinc influences immune response and oxidative stress, thus being highly effective in addressing pathological conditions [1]. Linked to zinc (bio)chemical reactivity is a huge family of substrates, including high molecular mass as well as low molecular mass molecules, which interact with that metal ion and give rise to complex assemblies exerting biological activity. One such group of low molecular mass molecules involves amino acids, the interactive chemistry of which with metal ions is intimately associated with compounds essential to protein synthesis and other important nitrogen-containing compounds, such as creatine, peptide hormones, and neurotransmitters. Among those, glycine, as the simplest amino acid, possesses an uncharged side chain and is of vital importance to the biosynthesis of many pharmacologically relevant biomolecules, serving a crucial role in many neurochemical processes [2]. Thus, the need for well-defined metal-organic complex species capable of exerting biological activity under pathologically aberrant conditions rises, thereby presenting a challenge to the scientific community.

Guided by the aforementioned need to develop alternative molecular drugs encompassing physiologically active and indigenous metal ions, research was launched in our lab to design and synthesize new Zn(II)-amino acid complexes, with glycine as the lead amino acid and its N-derivatives as bound zwitter ionic substrates capable of seeking (sub)cellular targets [3, 4]. It is excepted that new such hybrid zinc-zwitterionic species will ensure solubility and bioavailability facilitating zinc transport and utilization by cells. To that end, new hybrid zincoform species have been synthesized through multiparametric synthetic procedures in a pH-, concentration- and temperature-dependent manner. The isolated crystalline materials have been further characterized though elemental analysis, FT-IR, UV-Visible, and X-Ray Crystallography. The collective data formulate the chemical reactivity profile of hybrid metal-organic complexes, which justifies further use in *in vitro* biological experiments assessing their potential and merit as future metallodrugs in the protection of human physiology.

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DERIVATIVES OF NATURAL PRODUCTS WITH DIAMINES PROVIDING ENHANCED ANTI-INFLAMMATORY AND ANTIBACTERIAL PROPERTIES

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Naringin (4′,5,7- trihydroxyflavanone-7-rhamnoglucoside) and its aglycone form naringenin belong to flavanones (flavonoid class). They are found mainly in citrus fruits, including lemon, orange, mandarin and grapefruit. [1] Their anticancer activities are pleiotropic, and they can modulate different cellular signaling pathways, suppress cytokine, and arrest the cell cycle. [2] The pharmacokinetic properties and bioavailability of naringin and naringenin have recently been studied and shown that naringin is poorly absorbed through the gastrointestinal tract and epithelial cells of the oral cavity and the small intestine. Moreover, intestinal microorganisms generally convert naringin to its aglycone form, naringenin.

Cognizant of the fact that the antioxidant properties of flavonoids are distinct in their own nature and application(s) in each plant (parts and products), thereby affecting human nutrition, dietetic habits and cellular protection at the molecular level, the possibility was explored that appropriate derivatization of a select group of such molecules could be modified in vitro so as to exhibit potentially new properties or enhanced properties with respect to their antioxidant-therapeutic potential [3], thereby averting deleterious cellular chemical reactions from taking place. In this specific research work, a select group of flavonoids was chosen, essentially targeting improvement of antioxidant potential through derivatization. The so chosen flavonoids, naringin and naringenin [4], have been further modified in their substituents peripheral to the C ring, including diamines (i.e. putrescine, spermine, spermidine). The derived products, mainly involving ether and oxime moieties, were fully physicochemically characterized, showing enhanced luminescence properties and subsequently employed in microbiological studies, essentially seeking to determine their antimicrobial properties and evaluate the extent of their anti-inflammatory capacity through BSA denaturation assay. At the same time in vitro studies in bacterial cultures show promising results against Gram(+) and Gram(–) bacteria.

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GREEN OXIDATION OF GLYCEROL TO GLYCERIC ACID USING IMMOBILIZED LACCASES ON FUNCTIONALIZED SUPPORTS

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The surplus of glycerol from biodiesel production has driven interest in its conversion into value-added chemicals such as glyceric acid, used in food, medicine, and cosmetics. [1] Conventional chemical oxidation is effective but costly and poorly selective, whereas biocatalytic methods using laccases provide a greener alternative but face challenges with enzyme stability and reuse. [2] This study explores glycerol oxidation with four commercial laccases, emphasizing *Trametes versicolor* and *Aspergillus sp.*, and introduces Ni-Zn ferrite as a novel immobilization support to enhance enzyme performance, reusability, and glyceric acid yield.

Four laccases were screened with five mediators for glycerol oxidation. The top candidates (*T. versicolor* and *Aspergillus sp.*) were covalently immobilized on six supports: three magnetic ferrites (Fe_3O_4, Ni-Zn, Ni-Zn-Co) and three polymethacrylate-based Lifetech™ resins with amino or epoxy groups. Immobilization used glutaraldehyde crosslinking followed by $NaBH_4$ reduction to stabilize Schiff bases. Enzyme activity was assessed with 2,6-dimethylphenol assays, while glycerol oxidation was monitored by HPLC over 96h under optimized conditions. Characterizations by SEM and XPS validated immobilization and stability.

T. versicolor laccase immobilized on Ni-Zn ferrite (MG-Zn2) and on epoxy-butyl resin exhibited the best performance, retaining activity across pH 5-8 and up to 50°C. Covalent immobilization improved reusability, with magnetic biocatalysts maintaining ~80% activity after five cycles. Glycerol conversion reached 50% to glyceric acid within 72-96 h - far surpassing prior covalent immobilization studies (<10%). SEM and XPS confirmed stable 3-4 nm enzyme layers with no morphological degradation. Among resin supports, the epoxy-butyl spacer provided superior stability compared to amino- or epoxy-functionalized variants without spacers.

A robust biocatalytic platform for glycerol valorization was developed using covalently immobilized laccases on Ni-Zn ferrite and epoxy-butyl supports. This system achieved high stability, reusability, and unprecedented glycerol-to-glyceric acid conversion, addressing key limitations in laccase applications. The approach holds promise for sustainable biorefinery integration, with future work focused on optimization and scale-up.

Acknowledgements

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PVC-BASED COORDINATION POLYMER MEMBRANES FOR IMPEDIMETRIC DETECTION OF PHENOL

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Metal-organic frameworks are known as a class of porous coordination polymers containing metallic nodes (most of the time divalent cations such as Zn^{+2}, Co^{+2}, Ni^{+2}, Cd^{+2}, Cu^{+2} etc.) and organic linkers (for example: carboxylates, phosphonates, N donating linkers). Because of their structure and its proprieties, the area of MOFs became one of the fastest growing fields in chemistry. [1,2]

Our objective is creating a PVC-MOF membrane that can detect different kind of compounds, in this case phenol, by using impedimetric measurements. By using PVC as the matrix we are guaranteed to obtain a chemical and mechanical stable product. [3] This leads us to a mass ratio of 1:0.16 PVC:MOF of the final product with a thickness of approximately 170 µm. The membrane was deposited on the surface of iron and copper working electrodes. The test was made possible using a potentiostat/galvanostat 302N in order to analyze the absorption capacity of phenol on the membrane surface by analyzing the Nyquist and Bode graphics in the concentration range of 10^{-10}-10^{-1} M phenol solutions at a pH of 9.11. The Fe/PVC-MOF electrode was successful in determining the phenol absorption on de surface with a linearity of 0.9938 (R^2=0.9938) in the range concentration of 10^{-10}-10^{-6} M.

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NEW Ti(IV)-METAL ORGANIC COMPOUNDS WITH Α-HYDROXYCARBOXYLIC ACIDS

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Titanium is a metal of particular biomedical and technological interest. Due to its remarkable biocompatibility, it is employed in a number of medical applications, such as in the manufacturing of orthopedic and dental implants. [1] In its soluble form, it appears mainly in the Ti(III) and Ti(IV) oxidation states and it has been shown that it can form stable complexes with various organic substrates-ligands, resulting in the generation of new hybrid metal-organic compounds capable of affecting critical biological processes, such as enzyme catalysis or cell signaling. [2] A class of compounds, with which titanium could form chelate complexes are the α-hydroxycarboxylic acids, which due to their structure (the α-hydroxy group is in the α-position to the carboxy group) can and do complex with metal ions. They are widely used in pharmaceuticals due to their exfoliating, keratolytic and anaplastic properties, while their participation in titanium chelates attracts therapeutic and diagnostic interest. In the past, attempts have been made to complex titanium with α-hydroxycarboxylic acids that have afforded positive results in combating human pathophysiologies.

In the context of the synthesis of new metal-organic titanium compounds, research in our Laboratory has focused on two potential ligands: citramalic acid and benzylic acid. Citramalic acid is an α-hydroxycarboxylic acid that occurs in nature and is structurally a methylated derivative of malic acid. [3] It occurs in some microorganisms and plants, where it participates in alternative metabolic pathways, such as the biosynthesis of secondary metabolites. On the other hand, benzylic acid is an aromatic α-hydroxycarboxylic acid, which is of particular interest in medicinal chemistry, as it is used as a precursor molecule in the development of anticonvulsant and anticholinergic drugs. The use of these promising ligands led synthetically to the isolation of crystalline materials that were further characterized through elemental analysis, FT-IR, UV-Visible, and X-ray crystallography. The results obtained formulated a well-defined chemical profile of these hybrid metal organic complexes, thus setting the grounds for promising foundations for their possible biological activity and their use in disease diagnosis and treatment. [4]

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MILD AND EFFICIENT POLYESTER SYNTHESIS VIA CaLB-CATALYZED POLYCONDENSATION OF 1,8-OCTANEDIOL AND VARIOUS DIESTERS

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Polyesters are versatile materials with applications in various industries, such as automotive, furniture, coatings, packaging, and biomedicine. They are typically synthesized through chemical processes that require high temperatures (>180°C). These conditions can promote excessive oxidation, which reduces product stability and limits the range of polymers that can be obtained especially when working with functional monomers. [1] Furthermore, chemical catalysts, which are often metal-containing oxides or organometallic compounds based on aluminum, zinc, or tin, may leave behind toxic residues if they are not completely removed. This can compromise the biosafety and biocompatibility of the resulting polymers. [2]

Enzymes are a sustainable alternative to toxic metal catalysts in polycondensation reactions. They enable solvent-free polymerization and allow the synthesis of functionalized, biodegradable polyesters with well-controlled architectures under mild conditions (40-90°C). Although enzymatic synthesis usually produces polymers with moderate molecular weights, this issue can be resolved with a two-step process: first, enzymatic polymerization to create oligomers; then, a second step conducted at an elevated temperature and/or reduced pressure after the biocatalyst is removed. [3]

Lipases are particularly important among industrial enzymes and are extensively employed in detergents, cosmetics, fragrances, food processing, leather treatment, and fine chemical synthesis. *Candida antarctica* lipase B (CaLB) is the most used lipase in organic synthesis due to its high enantio-, chemo-, and regioselectivity. [4]

In this work, the polymerization of 1,8-octanediol with dimethyl glutarate, dimethyl 2-oxoglutarate, dimethyl 3-oxoglutarate, and dimethyl adipate using CaLB in solvent-free systems was performed. The resulting polyesters–poly(1,8-octyleneglutarate), poly(1,8-octylene-2-oxopentanedioate), poly(1,8-octylene-3-oxopentanedioate), and poly(1,8-octylene adipate) were fully characterized using FT-IR and NMR techniques. GPC analysis also demonstrated the formation of the polymer while TGA and DSC analyses were used to confirm their thermal stability. [5]

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ADVANCED SYNTHESIS AND CHARACTERIZATION OF MESOPOROUS SILICA USING IONIC LIQUIDS FOR ENHANCED HYDROGEN STORAGE

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Three series of mesoporous silica particles were synthesized using the sol-gel method, with variations in the preparation methods (stirring, microwave, sonication) and employing an Ionic Liquid (IL) as a co-solvent and directing agent. [1] The IL, Butyl-3-methylpyridinium hexafluorophosphate ([BMPyr][PF6]), was added to the silica precursors in an aqueous solution. For half of the synthesized samples, an ethanol-washing treatment was performed to remove the IL.

The samples were investigated using Scanning Electron Microscopy (SEM) combined with energy-dispersive X-ray Spectroscopy (EDX) and Fourier-transform Infrared Spectroscopy (FTIR) to evaluate their morphological and chemical properties. [2] Structural and textural properties, such as specific surface area, pore distribution, and total pore volume, were calculated from nitrogen adsorption/desorption isotherms at 77 K up to a relative pressure of p/p0=1 by employing the Brunauer–Emmett–Teller (BET) and Barrett-Joyner-Halenda (BJH) models. [3] Among all the samples studied, a more detailed analysis was conducted only on those with distinct characteristics

Preliminary hydrogen (H2) adsorption and desorption tests were conducted to evaluate the performance of the samples for potential storage applications. H_2 isotherms were acquired at liquid nitrogen (LN2) temperature and low pressure (up to 1 bar). The synthesized nanostructures that exhibited promising performance in gas adsorption at low pressure were further tested at higher pressures, up to 80 bar, and at different temperatures: 77 K (liquid nitrogen), 193 K (dry ice), 273 K (ice), and 298 K (room temperature). This additional analysis enabled the calculation of the isosteric heat of adsorption at low coverages. [4]

The research aimed to understand how preparation methods, IL concentrations, and IL extraction influence material properties, particularly focusing on the relationship between surface characteristics, structure, and gas adsorption behavior of the produced materials samples.

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ACETOLACTATE SYNTHASE - CASE STUDY FOR MODELLING HERBICIDE RESISTANCE

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Acetolactate synthase (ALS) is an enzyme found in plants, fungi, bacteria, and archaea, but not in animals. [1] ALS is a target for herbicides, making it highly relevant in agriculture. Several classes of herbicides, such as sulfonylureas and imidazolinones, inhibit ALS, disrupting amino acid synthesis and ultimately leading to plant death. However, intensive use of these herbicides has contributed to the development of herbicide resistance over time.

Specific mutations in ALS—such as P197L/A/S/E, S653T, W574L, A122T, A205V, and D376E—have been identified in several invasive plant species and are responsible for acquired resistance. [2] Comparative analysis of these mutations using sequence alignment provides a useful overview, but for a more in-depth understanding, the three-dimensional structures of ALS—both wild-type and mutant forms—are essential.

For plant species lacking experimentally determined 3D structures, comparative models were constructed. Structural superposition of these models revealed differences in the herbicide-binding pockets of the enzymes. To evaluate structural stability and intermolecular interactions, molecular dynamics simulations were employed, enhancing the scope of *in silico* studies. Additionally, Molecular Mechanics Generalized Born Surface Area (MM/GBSA) computations were conducted to estimate the binding free energy between herbicides and ALS.

Beyond the residues affected by known mutations, this study also identified additional key amino acids influenced by these changes. These residues play a significant role in stabilizing herbicides within the binding site.

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THE WATER ELECTROLYSIS ACTIVITY OF CARBON-BASED ELECTRODES MODIFIED WITH Co-DOPED $YMnO_3$ PEROVSKITE AND 5,10,15,20-TETRAKIS(4-METHOXYPHENYL)-21H,23H-PORPHINE

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Environmentally friendly hydrogen generation methods constitute a promising solution to a couple of important problems humanity is presently confronted with: climate warming and the energy crisis. [1] However, the extent to which a hydrogen-based economy is desirable depends on several key factors. In the case of hydrogen generation via electrochemical water-splitting, one of these factors is the material used to catalyze the hydrogen evolution reaction. [2] So far, researchers have studied a large number of materials as part of their attempt to identify highly active, stable, Earth-abundant, and low-cost electrocatalysts for the cathodic half-cell reaction unfolding during water electrolysis. [3,4] Considering the specified context, this work describes the investigation of the water-splitting electrocatalytic activity of carbon-based electrodes modified with Co-doped $YMnO_3$ perovskite and the A_4 free-base 5,10,15,20-tetrakis(4-methoxyphenyl)-21H,23H-porphine. Catalyst inks were prepared by adding the perovskite material into porphyrin solutions of different concentrations. The solvent was tetrahydrofuran, the substrate was glassy carbon, and the electrode modification method was the drop-casting method. The anodic and cathodic linear sweep voltammograms were recorded in 1 M KOH electrolyte solution during hydrogen evolution reaction (HER) and oxygen evolution reaction experiments. The obtained data reveal that the highest electrocatalytic activity is displayed during the HER by the electrode manufactured with the catalyst ink containing 5 mg Co-doped $YMnO_3$ in 15 mM porphyrin solution. A HER overpotential of 0.53 V at the -10 mA/cm^2 current density and a Tafel slope of 0.21 V/dec ($R^2 = 0.9993$) were found. This study contributes to the domains of water-splitting, perovskite chemistry, and porphyrin chemistry. It also increases the current understanding of the applicative potential of electrodes modified with both perovskites and free-base porphyrins.

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EXPLORING MOLECULAR MECHANISMS OF XYLITOL IN SALIVARY STIMULATION

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A comprehensive analysis of how polyols interact with receptors involved in salivary flow regulation is crucial for improving formulations designed to prevent oral diseases. Present in sugar-free chewing gums and candies, these compounds can promote salivary secretion by engaging taste receptors and osmotic receptors, thereby alleviating dry mouth symptoms and reducing the risk of dental caries. Among these, xylitol stands out due to its well-documented benefits in stimulating saliva production and inhibiting cariogenic bacteria. Gaining insight into these mechanisms at the molecular level supports the development of more effective oral care strategies that enhance saliva's buffering capacity and remineralization potential. [1,2,3]

Molecular docking simulations were performed to evaluate xylitol's interaction with the human muscarinic acetylcholine receptor M1 (PDB ID: 5CXV) in the context of salivary stimulation. Xylitol demonstrated favorable binding energies ranging from –4.6 to –4.0 kcal/mol across multiple receptor conformations. Interaction analysis revealed a hydrogen bond between the 1-OH group of xylitol and Val127 (2.066 Å), along with close contacts involving Asn217, Asn1067, Phe1003, Glu1063, Thr128, and Val127.

These findings underscore xylitol's potential to engage critical residues within the receptor's binding site, supporting its role as a promising modulator of salivary secretion. The molecular interactions identified (Figure 1) offer new insights into the development of effective strategies for xerostomia management.

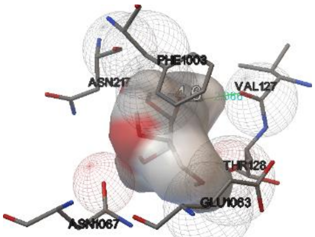

Figure 1. Xylitol binding interactions within the active site of M1 muscarinic acetylcholine receptor (PDB ID: 5CXV). Hydrogen bonds and residues in close contact are highlighted.

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SUPRAMOLECULAR ORGANIZATION OF TWO 2,4-DIAMINO-6-PHENYL-1,3,5-TRIAZIN-1-IUM SALTS WITH FLUORO-CONTAINING ANIONS

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Supramolecular chemistry defined by the Nobel laureate J-M Lehn as 'chemistry beyond the molecule' deals with studies of non-covalent interactions and molecular assemblies.[1] This knowledge serves as a basic tool for design of new multicomponent crystalline materials or supramolecular materials that find applications in nanotechnology, drug delivery, catalytic systems and so on. 2,4-Diamino-6-phenyl-1,3,5-triazine has a great potential in crystal engineering and was selected for this study as a useful supramolecular agent that contains a number of coordination/hydrogen bonding sites, and an aromatic fragment for the π-interaction abilities.[2] On the other hand, a series of 1,3,5-triazine based compounds revealed a wide range of biological activities.[3] Present work sheds light on the different types of non-covalent interactions in the supramolecular architectures of two newly synthesized salts of 2,4-diamino-6-phenyl-1,3,5-triazine. The 2,4-diamino-6-phenyl-1,3,5-triazin-1-ium trifluoroacetate, $C_9H_{10}N_5^+$ $C_2O_2F_3^-$ (**I**), and 2,4-diamino-6-phenyl-1,3,5-triazin-1-ium tetrafluoroborate monohydrate, $C_9H_{10}N_5^+$ BF_4^- H_2O (**II**) were characterized by single-crystal X-ray diffraction. Crystal data for **I**: Mr = 301.24, monoclinic, sp. gr. $P2_1/c$, a = 12.632(3), b = 11.3072(12), c = 9.957(2) Å; β = 109.58(3) °; V = 1340.0(5) Å^3; Z = 4. Crystal data for **II**: Mr = 293.05, triclinic, sp. gr. P-1, a = 7.3104(8), b = 9.6098(8), c = 10.4479(9) Å; α = 113.933(8), β = 106.900(9); γ = 92.819(8) °, V = 630.07(12) Å^3; Z = 2. The cation-anion pairing in **I** and **II** occurs *via* robust cyclic heterosynthon $R_2^1(6)$ with participation of two NH…O/NH…F hydrogen bonds (Fig. 1). The acid-base pairs are further interconnected into supramolecular H-bonded ribbons via alternation of homomeric (cation-cation) and heteromeric (cation-anion/cation-water-anion) H-bonded patterns through the supramolecular synthon sequences …$R_2^2(8)R_3^2(8)R_1^2(5)R_2^1(6)R_4^4(12)$… in **I** and …$R_2^2(8)R_2^2(9)R_2^1(5)R_2^3(6)R_3^2(8)$ $R_4^2(8)$… in **II**.

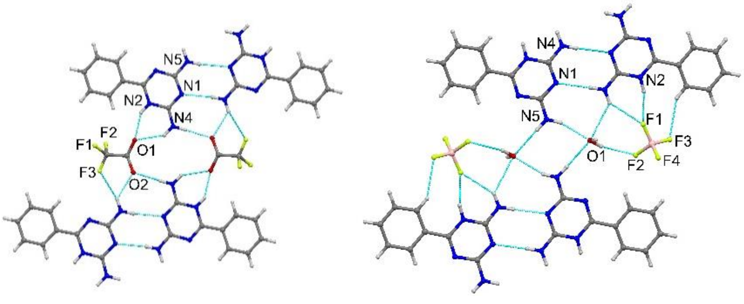

Figure 1. Fragments of supramolecular ribbons in **I** (left) and **II** (right).

Further stabilization of **I** and **II** via numerous intermolecular N(O, C)H…F short contacts as well as π···π interactions (triazine···triazine rings and triazine···phenyl rings) are also investigated.

Acknowledgement
The authors are grateful for support to the subprogram 011202 „Design and fabrication of intelligent materials with advanced magnetic, adsorption, luminescent and biologically active properties".

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ANTIOXIDANT AND ANTI-INFLAMMATORY ACTIVITY OF POLYPHENOLIC DERIVATIVES

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Over the past years, inflammation has become one of the most important processes under scrutiny in biomedical research, focusing on delineating correlations between with oxidative stress and implications in human physiology. Emphasis has thus been given to mechanisms of onset and progression of inflammation, with molecular pathways involving transduction of signals, leading to chronic phenotypic changes in the (patho)physiology of humans. Counteracting the pathological consequences of inflammation, natural products including flavonoids have been increasingly been employed in research, with dietary and pharmacological extensions attracting keen interest from the respective industries to impact the welfare of the greater society. To that end, based on the fact that the antioxidant properties of flavonoids are distinct in their own nature and affect human nutrition, dietetic habits, and cellular protection at the molecular level, flavonoids were selected in our Lab as molecules for further derivatization in an effort to enhance solubility and therefore their bioavailability. Such new derivatives of flavonoids could be investigated to influence antioxidant and anti-inflammatory actions at the genetic level (investigating neuronal cell lines), thereby contributing to the enhancement of their therapeutical potential.[1] Naringin and naringenin are the main bioactive polyphenols encountered in the plant kingdom including citrus fruit, lemon, orange, mandarin, and grapefruit.[2] Their anticancer activities are pleiotropic, and they can modulate different cellular signaling pathways, suppress cytokines, and arrest the cell cycle.[3]

The so chosen flavonoids, naringin and naringenin [4] have been further modified in their substituents peripheral to the C ring, including diamines (i.e. putrescine, spermine, spermidine). The derived products, mainly involving ether and oxime moieties, were fully physicochemically characterized, showing enhanced luminescence properties and subsequently employed in microbiological studies, essentially seeking to determine their antimicrobial properties and evaluate the extent of their antioxidant and anti-inflammatory capacity. To achieve that, two highly sensitive brain tissue cell lines (physiological mouse neuronal (N2a) and pathological human neuroblastoma (SH-SY5Y) were employed. After screening of their toxicity profile the antioxidant was determined in the presence of oxidative stress, while at the same time, the corresponding genes (NFE2L2, GCLM, HMOX1) and (TNF-α and IL-6) were examined using qPCR. The results of the study set the stage for the development of new hybrid flavonoids and derivatives thereof, so as to enhance the antimicrobial arsenal of options when bacterial insurgents find their way into a) nutritional resources, traditionally used in human diet or products destined for human consumption, and b) humans, thereby benefiting their health.

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SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF A THIOPHENE-DERIVED SCHIFF BASE COPPER(II) COMPLEX WITH POTENTIAL BIOLOGICAL ACTIVITY

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Thiophene-derived Schiff bases and their metal complexes are gaining attention as promising antimicrobial and anticancer agents due to their notable biological properties. [1] Studies indicate that the metal complexes often exhibit superior activity compared to the free ligands, owing to chelation, which reduces metal ion polarity, enhances membrane permeability, and disrupts microbial enzyme function. [2]

This study reports the synthesis of a novel thiophene-derived Schiff base ligand, ethyl (E)-2-((2-hydroxy-3-methoxybenzylidene)amino)-6-methyl-4,5,6,7-tetrahydrothieno[2,3-c]pyridine-3-carboxylate (TSB), along with its corresponding copper(II) complex. Structural characterization was performed using spectroscopic techniques, including ^{1}H NMR, FT-IR, UV–Vis, and single-crystal X-ray diffraction. According to X-ray crystallography, TSB crystallizes in the orthorhombic space group, exhibiting an intramolecular hydrogen bond between the phenolic oxygen and the imino nitrogen (Figure 1).

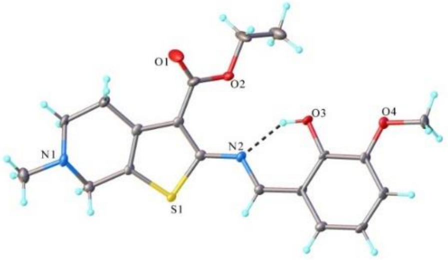

Figure 1. X-ray molecular structure of TSB ligand

The copper(II) complex exhibits a molecular crystal structure comprising one binuclear $[Cu_2TSBCl_4H_2O]\cdot1.5H_2O$ unit in the asymmetric part of the unit cell. The Cu is five coordinated in distorted square pyramidal geometry with the basal plane formed by a tridentate NOO ligand and water molecule, while the apical position is occupied by a chloride ion bridging two Cu^{II} centers. By contrary, the Cu_2 atom has a distorted tetrahedral coordination formed by four chloride atoms.

Further studies will be conducted to assess the potential biological properties.

Acknowledgement
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SUSTAINABLE VALORIZATION OF WHEY THROUGH ITS APPLICATION IN BAKERY PRODUCTS

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Whey represents a valuable by-product of the dairy industry, resulting from the processing of milk to obtain cheeses. Traditionally, it has been considered an industrial waste, but recent research highlights its potential for valorization in various food industries, especially in baking.

The whey from milk is a valuable resource that can be efficiently used in baking, both for its technological and sensory benefits, as well as for its nutritional advantages. Its integration into bread and pastry recipes supports the development of sustainable and innovative food products, in line with the current demands of the modern food market.

In this regard, the present study aims to demonstrate the possibilities of utilizing whey in baking by including whey powder in various proportions in the recipe for producing bread, as well as studying the nutritional, functional, and rheological properties of the composite flours and obtained bread based on wheat flour with added whey in different proportions. The topic addressed presents practical importance considering the current trends in utilizing food by-products in the context of the circular economy. The proximate composition, the macro and microelements content and the MIXOLAB profile of dough with different percent of whey powder (10-30%) in wheat flour was studied. The obtained data highlight the positive impact of the addition of whey powder on the nutritional value of composite flours and bakery products, especially through the increase in protein and mineral content, alongside a reduction in carbohydrate content. Also, the macro and microelements profile of fortified flours and bread shown an increase in Mg, Ca, Cu and Zn. The analysis of the Mixolab radar charts confirms the progressive impact of the addition of whey powder on rheological behavior. Although it tends to diminish kneading resistance and protein stability, negatively affecting gluten structure and starch gelatinization, these effects are balanced by a high functional potential, especially from a nutritional standpoint.

SILIBININ LINOLEATE AS A NATURAL LIPOPHILIC ANTIOXIDANT FOR THE STABILIZATION OF EDIBLE VEGETABLE OILS IN FOOD INDUSTRY

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Lipid oxidation is one of the primary factors affecting the stability, nutritional value, and shelf life of vegetable oils. Conventional synthetic antioxidants such as butylated hydroxytoluene (BHT) and butylated hydroxyanisole (BHA), though effective, are increasingly questioned due to health concerns and regulatory restrictions. In this context, naturally derived compounds with antioxidant properties represent a promising alternative. This study investigates the potential application of **silibinin linoleate (SIL-L)**, a lipid-soluble ester of the flavonolignan silibinin and linoleic acid, as a natural antioxidant in vegetable oils. Due to its amphiphilic structure, SIL-L exhibits enhanced solubility in lipid matrices and a strong ability to scavenge free radicals and chelate transition metal ions, both of which are critical in preventing lipid peroxidation.

This study includes the obtaining of SIL-L using green technology and the behavior of sunflower oil when heated for different times of 4 and 8 hours at 180 degrees in the presence of SIL-L at different concentrations, compared to BHT and in its absence of natural or synthetic antioxidants. The investigated parameters to control the oxidation processes were: the peroxide value (PV), the **p-anisidine value (p-AV)**, the **total oxidation value (TOTOX) and the profile of fatty acids before and after termal process.** Saturated fatty acids (SFA), monounsaturated fatty acids (MUFA), polyunsaturated fatty acids (PUFA) and unsaturated fatty acids (UFA) were calculated. The changes in inhibition of sunflower oil oxidation during heat exposure following supplementation with SIL-L and BHT show that the inhibition effect, after 4 and 8 hours compared to the control decreases in order SFSL3>BHT>SFSL2>SFSL1. The obtained data confirm that heating the oil leads to a decrease in PUFA to a greater extent than MUFA, and the addition of antioxidants can slow down this process, but the effectiveness depends on the concentration and chemical structure. When compared to BHT, SIL-L demonstrated superior efficacy in maintaining a stable lipid profile, indicative of a potentially lower atherogenic and thrombotic risk associated with its consumption. These findings support the application of SL as a potent natural antioxidant capable of enhancing the thermal and oxidative stability of vegetable oils.

EXPLORING THE STRUCTURAL DIFFERENCES IN THE JAK FAMILY TO IDENTIFY SELECTIVE CANDIDATES FOR JAK1

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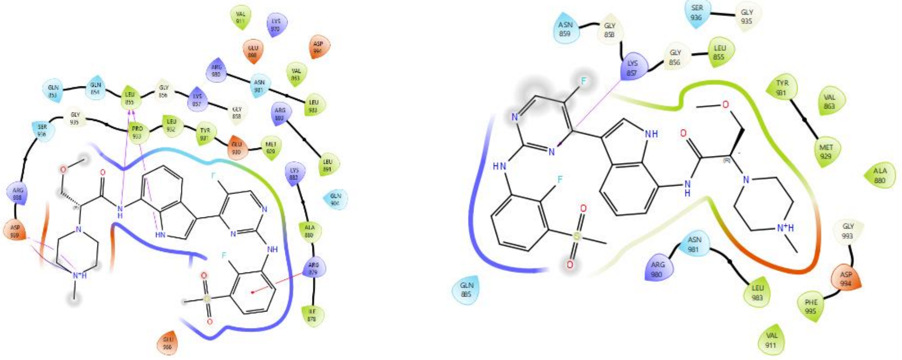
JAK1 and JAK2 are important tyrosine kinases involved in complex inflammatory processes and have been associated with rheumatoid arthritis and psoriasis. Presently available psoriasis therapies focus on immune suppression by blocking cytokines like TNF-α, IL-17 and IL-33. Recently, a novel approach targets the JAK family, especially JAK1 due to its important role in cytokine signaling.[1,2] JAK1 and JAK2 share high sequence similarity (~85%) in the catalytic domain, especially in the ATP-binding site - a key region for binding of Type I and II inhibitors. (6 different residues in a 5A radius around the ligands). Our analysis of three compounds with preferential activity towards JAK1, compared to 700 compounds active on both JAK1 and JAK2 showed several relevant differences. Specifically, three of the residue differences are found in the Glycine loop and affect the overall charge and tendency to form hydrogen bonds (Glu/Lys, His/Asn, Lys/Ser). Two other differences involve larger (Ser/Tyr, Phe/Tyr) amino acids in the JAK1 binding site which in turn reshape the binding pocket. The last difference is in the gatekeeper area (Val/Ile) where the amino acid in JAK1 allows the entrance of larger ligands. Based on these insights, compounds from a physical library were further screened through a virtual screening protocol to determine potential drug candidates that could be potentially tested on cells in the future.



A B

Figure 1. Jak2 (A) and Jak1 (B) interactions with londamocitinib

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CLOTRIMAZOLE DRUG LOADING AND RELEASE USING AS CARRIERS MERCAPTOPROPYL FUNCTIONALIZED MESOPOROUS SILICA

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In order to be tested for their drug loading and release properties, functionalised mesoporous silica particles were synthesized by sol-gel method, starting from mixed silica precursors, tetraethoxysilane and mercaptopropyltriethoxysilane, in two different concentrations. Also, a simple nonfunctionalised mesoporous silica of MCM-41 type, was sintetised. The obtained materials were evaluated for their textural properties. Subsequently, they were evaluated as carriers for a drug loading, clotrimazole, and they demonstrated enhanced drug loading capacity of around 99%, in all tested solvent media for loading. The loaded carriers were also tested for their release behaviour in different solvents with different pH values. The cumulative percent of drug release in hydrochloric acid solution 0.1 N, was 45.07% after 3 hours of release. The best results were obtained when the same buffer was used for the drug entrapment as well for the drug release. The percent of drug release in acidic buffered solution of pH= 2 was constantly in the 51-91% range of release and of pH= 4.5 was constantly in the 11-20% range of release, all during 3 hours.

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MULTIFUNCTIONAL Zn(II) COORDINATION POLYMER: PHOTOLUMINESCENT, ANTIMICROBIAL AND ANTICANCER PROPERTIES

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Recent advances in coordination polymers (CPs) have highlighted their promising potential in biomedical applications, particularly in antimicrobial and anticancer therapies. This work presents the synthesis, characterization and multifunctional evaluation of a Zn(II)-based laminated coordination polymer derived from $ZnSO_4 \cdot 7H_2O$ and a dihydrazone Schiff base ligand under ambient conditions. Comprehensive structural and spectroscopic analysis revealed diverse metal coordination environments along with photoluminescent behavior. Photoluminescence (PL) studies revealed emission maxima at 2.15 eV (576 nm), 2.35 eV (527 nm) and 2.45 eV (505 nm), with a twofold increase in PL intensity at 505 nm in the desolvated sample compared to the synthesized compound, offering valuable insights into structure-property relationships.

Biological assessments demonstrated strong antimicrobial activity of compound 1 against both Gram-positive and Gram-negative bacterial strains, including multidrug-resistant clinical isolates. Notably, it exhibited bacteriolytic effects on *Salmonella typhimurium* at all tested concentrations and inhibits biofilm formation. Furthermore, the compound displays selective antiproliferative activity against MCF-7 breast cancer cells while remaining biocompatible with healthy human fibroblasts.

This study highlights the synthesized CP as a promising candidate for future applications in luminescent materials and biomedical research, due to its combined photoluminescent properties, antimicrobial efficacy, and anticancer potential.

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RAPID SYNTHETIZED UIO-66 BY MICROWAVE METHOD AND ITS APPLICATION AS H_2 STORAGE MATERIAL

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In this study, we present a fast, simple and efficient microwave assisted synthesis method in the presence of acetic acid as modulator for obtaining zirconium-based metal-organic framework UIO-66. Characterization via X-ray diffraction confirms their crystalline structures, in agreement with the literature for UIO-66 architecture, any impurity in its crystalline structure is not seen, and all the spectra of the samples exhibit similar characteristic peaks. The samples are composed by small crystalline agglomerated nanoparticles, with irregular shape, as can be seen from SEM images and the EDX analysis of each sample confirmed the presence of corresponding elements of the UIO-66 framework, namely Zr, O and C. The materials showed relatively good values of specific surface area, the highest being 725 m^2/g, had a combination of porosity, given by microporosity and mesoporosity, and high thermal stability despite high linkers deficiencies per Zr_6 formula unit.

The results showed that higher specific surface area value led to an increase of microporous specific surface area, therefore an increase of H_2 absorption performance can be observed.

EXPLORING THE CHEMICAL PROPERTIES OF QUATERNARY PHOSPHONIUM SALTS

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In the context of aligning with the principles of green chemistry, which aim to reduce harm to the environment and human health, while making chemical processes more efficient and sustainable, the interest in quaternary phosphonium salts has significantly increased. The benefits of this family of organic compounds such as: their unique physicochemical qualities and simplicity of synthesis, make them attractive for use in a variety of sectors, including biology, medicine, and industry.

In this study, the synthesis of six quaternary phosphonium salts was performed, namely: ethyltriphenylphosphonium iodide, butyltriphenylphosphonium iodide, pentyltriphenylphosphonium iodide, ethyl-3-furyldiphenylphosphonium iodide, ethyl-di(3-furyl)phenylphosphonium iodide, and ethyl-tri(3-furyl)phosphonium iodide. These compounds were characterized using various one-dimensional and two-dimensional nuclear magnetic resonance (NMR) techniques: ^{1}H-NMR, ^{13}C-NMR, ^{13}C-APT (Attached Proton Test), ^{31}P-NMR, COSY (Correlation Spectroscopy), HSQC (Heteronuclear Single Quantum Correlation), and HMBC (Heteronuclear Multiple Bond Correlation). These methods provided information for accurate spectral interpretation. FTIR and elemental analysis further supported the structural confirmation of the synthesized compounds.

The results of this study show that adding more 3-furyl groups to the phosphorus atom causes the signal in the ^{31}P-NMR spectrum to shift to higher fields, which means it shows lower ppm values.[1] Furthermore, preliminary antimicrobial studies will be conducted. Existing research on this class of compounds has shown that they are effective against both Gram-positive (Staphylococcus aureus) and Gram-negative (Escherichia coli) strains, suggesting potential applications in biomedical and industrial fields.[2]

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PHOTOCATALYTIC ACTIVITY OF A 1D COPPER(II) COORDINATION POLYMER FOR DYE DEGRADATION FROM SINGLE AND BINARY AQUEOUS SOLUTIONS

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A major challenge in treating wastewater from the textile industry is the presence of a wide range of synthetic dyes. [1] During the dyeing process, approximately 11–15% of the dyes fails to bind to the fabric and is discharged into wastewater, causing environmental and ecological harm, including disruption of aquatic ecosystems, higher wastewater treatment costs, and potential risks to public health. [2] Photodegradation based on coordination polymers represents a new approach for the removal of dye from wastewater, combining tunable structures, efficient light utilization, and catalytic performance. [3]

Therefore, as a continuation of our work [4] in the present study the photodegradation efficiency of Acid Orange 7 (AO7) and Methyl Orange (MO) from single and binary system, using $^{1}_{\infty}[Cu_3L_2(H_2O)](ClO_4)_2$ (**1**), where H_2L stands for N,N'-bis[(2-hydroxybenzilideneamino)propyl]-piperazine) was investigated. The results obtained under visible light irradiation, both with and without H_2O_2, show slightly increased removal efficiency of AO7 and MO in the presence of hydrogen peroxide. In the binary dye solution, degradation efficiencies were lower (41.70%) compared to the single dye solutions (89.03% for AO7 and 54.45% for MO), which is attributed to competition between the dyes for active sites on the coordination polymer surface available for adsorption and degradation. Upon adding H_2O_2, the degradation efficiency of both dyes in the binary system improved to over 50%. The kinetics of dye photodegradation were analyzed using the Langmuir-Hinshelwood model, revealing that the process follows pseudo-first-order kinetics. The copper(II) coordination polymer demonstrated excellent stability throughout the photodegradation, evidenced by the consistency of the initial and final structure of the complex. Additionally, a photocatalytic oxidation mechanism was proposed for the degradation of AO7 and MO, based on a trapping experiment with disodium ethylenediaminetertaacetate (EDTA-2Na) as holes h^+ scavenger.

Continued research into novel coordination polymers and their mechanisms will further enhance their practical application in sustainable environmental remediation.

Acknowledgement
This work was partially supported by Program no 2, Project no. 2.2, and Program no. 4, Project no. 1.2 from the "Coriolan Dragulescu" Institute of Chemistry.

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ECO-FRIENDLY MATERIAL DEVELOPMENT FROM CAROB: SYNTHESIS AND STRUCTURAL CHARACTERIZATION

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In the current context of the transition to a sustainable economy, the valorisation of renewable natural resources is gaining increasing importance. This work explores the potential of carob (Ceratonia siliqua), a plant rich in polysaccharides and bioactive compounds, as a raw material for the development of ecological materials. Carbon materials were synthesized using carob powder by selecting standard sizes without the addition of solvents or synthetic additives. The structural characterization of the obtained materials was carried out by spectroscopic techniques such as FT-IR Spectroscopy, Raman Spectroscopy, Small/Wide Angle X-ray Scattering (SAXS/WAXS), Scanning Electron Microscopy (SEM + EDX) and analysis based on the Brunauer-Emmett-Teller theory (BET), highlighting the presence of amorphous structures and the properties of the materials. This research highlights the potential of waste plants in the development of biomaterials, offering sustainable solutions to reduce the negative impact of synthetic materials on the environment. The resulting carbon materials have a high surface area and a porous structure, which makes them suitable for various applications, including: adsorption (activated carbon from carob powder is effective at removing pollutants, such as dyes and heavy metals, from wastewater); energy storage or catalysis: They can be used as catalyst supports in various chemical reactions.

SUSTAINABLE SYNTHESIS OF ZINC AND SILVER OXIDE NANOPARTICLES MEDIATED BY ISOFLAVONE PUERARIN: CHARACTERIZATION AND BIOLOGICAL ASSESSMENTS

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Green nanotechnology has emerged as a sustainable approach to producing functional nanomaterials while reducing reliance on toxic reagents and energy-intensive methods. [1] Isoflavone puerarin, derived from *Pueraria lobata*, offers dual functionality as a reducing and stabilizing agent, providing an eco-friendly route for nanoparticle synthesis.

In the present work, zinc oxide (ZnO) and silver oxide/silver (Ag_2O/Ag) nanoparticles were successfully synthesized via a Puerarin-mediated pathway. [2,3] Structural analysis using X-ray diffraction (XRD) confirmed crystalline nature and phase purity, while electron microscopy (TEM,SEM) revealed uniform morphology and nanoscale particle dimensions (<100 nm). Atomic force microscopy (AFM) further provided three-dimensional surface profiles and height distribution, supporting the stability of the synthesized nanoparticles.

Biological evaluations demonstrated marked antioxidant activity, indicating potential for free radical scavenging and oxidative stress mitigation. Antimicrobial assays revealed significant inhibitory effects against both Gram-positive and Gram-negative bacterial strains (*Staphylococcus aureus*, *Streptococcus pyogenes*, *Escherichia coli*, *Pseudomonas aeruginosa*) and yeast *Candida parapsilosis*, highlighting broad-spectrum potential. Additionally, the Hen's Egg Test on the Chorioallantoic Membrane (HET-CAM) demonstrated low irritant response coupled with angiogenesis inhibition, supporting potential therapeutic relevance in medical and pharmaceutical fields.

Taken together, these findings establish Puerarin-assisted synthesis as a greener, safer, and more efficient alternative to conventional routes, offering enhanced stability, reduced environmental impact, and significant promise for biomedical applications, particularly in antimicrobial and antioxidant therapies.

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THE BIOLOGICAL RELEVANCE OF Pt(IV) PRODRUGS WITH SPECIFIC AXIAL LIGANDS

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Bifunctional assemblies featuring an organic ligand with therapeutic potential coordinated to a cisplatin-like Pt(IV) framework can act as prodrugs, as the cellular environment reduces platinum(IV) to platinum(II), thus liberating in situ cisplatin (or variations thereof) and the additional drug. Studying the interactions of potential drugs with proteins provides us with information regarding mechanisms of action, side effects and selectivity. [1]

The research presented here explores the behavior of Pt(IV) complexes in biologically relevant interactions with the aim of developing new selective anticancer drugs. Ligands such as fenbufen, benoxaprofen, ibuprofen, oxaprozin, nicotinic acid and capric acid were used for coordination.

The above- mentioned interactions were monitored using spectroscopy UV-Vis and fluorescence. A major component of blood, to which any therapeutic agent would be exposed, is hemoglobin (Hb). A range of compounds with therapeutic action/potential (anticancer and beyond), including Pt(II)-based compounds, have been shown to affect the oxidative reactivity of Hb – either by acting as antioxidants or as agents of oxidative stress that promote Hb autoxidation. [2] Thus, the oxy-Hb autoxidation reaction was studied, in the presence of Pt(IV) hexacoordinated complexes and also of ligands. The peroxidase reactivity of Pt(IV) complexes and ligands was assayed with ferryl-Hb. Binding of complexes to albumin as well as to Hb was confirmed by fluorescence measurements.

DNA binding was also studied by fluorescence assays for the same set of compounds. As expected, the ligands do not bind to DNA, while all Pt(IV) complexes do. We have identified compounds with high affinity for DNA, which suggests potential biomedical applications for the development of new cytostatic treatments.

Pt(IV) drug candidates are generally expected to be reduced to Pt(II) by thiol pools inside living cells [1], so the reaction between glutathione (GSH) and Pt(IV) complexes was spectrophotometrically followed. A decrease in absorbance was found, indicating reduction to Pt(II) – as also confirmed by TD-DFT calculations.

Acknowledgments

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SPECTROSCOPIC EVALUATION OF THE INTERACTION OF MYOGLOBIN WITH BIOMEDICAL RELEVANT COMPOUNDS

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This study investigates the redox behavior of myoglobin (Mb) in the presence of several bioactive compounds with biomedical relevance. These include the well-known Pt(II) drug, cisplatin, oxoplatin (a Pt(IV) compound representative for a newer-generation drugs based on platinum), capric acid, fenbufen, plumbagin and fisetin. These molecules were selected based on their structural diversity and documented biological effects, such as anti-inflammatory, chemotherapeutic, or antioxidant properties. The study aimed to evaluate how these compounds affect the structural and redox properties of Mb, particularly in terms of their capacity to bind to the protein and modulate its oxidation state.

Spectroscopic methods (UV-Vis absorption, fluorescence, and NMR) and docking calculations were used to monitor binding and modifications of the redox state of the Mb in reactions such as autoxidation, nitrite-induced autoxidation, and peroxide-induced damage. These experiments are designed to parallel previous findings with similar experiments on hemoglobin with small molecules of biomedical/therapeutic relevance. [1–4] Our results demonstrate a differential response: while some compounds induced minimal or no spectral changes - suggesting limited interaction or redox impact, while others, such as fisetin and plumbagin, displayed notable pro-oxidative effects.

These findings suggest that fisetin and plumbagin may act as pro-oxidants or interact with Mb through mechanisms that alter their redox state, while the other compounds may exhibit stabilizing or potentially antioxidant effects. The observed variability highlights the complex nature of small molecule-protein interactions and underlines the importance of assessing individual compound behavior in biochemical systems.

This work contributes to a better understanding of how diverse small molecules influence the redox chemistry of globins, with implications for pharmacology and redox biology.

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OXYGEN-CARRYING PROTEINS EMPLOYED IN BLOOD SUBSTITUTE CANDIDATES: DIFFERENCES IN INTERACTIONS WITH A MODEL ANTIOXIDANT MOLECULE

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Glutaraldehyde-polymerized hemoglobin (poly-Hb) has long been explored as a key candidate for blood substitute compositions, to be used in transfusions in order to supplement the oxygen-carrying capacity following severe blood loss. Bovine hemoglobin (bHb) has been the standard choice for such efforts, due to its reasonable availability and to its reduced dependence on organic allosteric effectors. We have recently shown that poly-Hb produced from ovine Hb (poly-oHb) outperforms poly-bHb in in vivo tests employing transfusion after up to 30 % blood loss in animals. This improvement was found to correlate with an increased resistance of ovine hemoglobin (oHb) and of poly-oHb towards oxidative and nitrosative stress agents in vitro. The molecular bases for these differences in reactivity offer an interesting challenge, given the high sequence homology between vertebrate hemoglobins. Reported here is an investigation of these molecular bases using different spectroscopic (fluorescence, resonance Raman, NMR, EPR) and computational (molecular docking) methods to assess the interaction with a convenient probe ligand representative of the class of natural antioxidants, caffeic acid. Fluorescence experiments reveal that ovine Hb fluorescence saturates above 25 μ M caffeic acid and indicating full occupancy of fluorescence-responsive binding sites, while resonance Raman and NMR data indicate signals for the heme and indicate the differences between the types of Hbs and the antioxidant binding behavior after polymerization. Computational docking corroborated the spectroscopic data by identifying aromatic residues and distinct affinity patterns for caffeate. The results show that structural differences in oHb may explain a higher redox stability.

COMPUTATIONAL APPROACHES TO FIND POTENTIAL AGENTS USED IN TYPE II DIABETES

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A computational study was performed to find potential compounds capable of lowering the glycemic index in type 2 diabetes. A number of 48 compounds were selected based on a virtual screening (VS) similarity search referencing the antidiabetic drug rosiglitazone. The VS was performed on ChEMBLdb v29, using a combination of multiple 2D and 3D chemical encodings and a similarity threshold of 0.85 (SwissSimilarity platform: http://www.swisssimilarity.ch). Further, the compounds were supplied to more advanced cheminformatics methods. Firstly, the dataset was docked in peroxisome proliferator-activated receptor gamma (PPARγ) protein bound to rosiglitazone (PDB 4EMA), using OpenEye's FRED software (http://www.eyesopen.com). Secondly, the top compounds showing the highest docking scores (ChemGauss4 scoring function) were further supplied to DFT analysis and described comparatively with rosiglitazone.

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3D BIOPRINTING SCAFFOLD DEVELOPMENT FOR ANTIBACTERIAL APPLICATIONS INVOLVING BIOINORGANIC COMPOUNDS

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Antibacterial surfaces linked to hybrid biopolymeric and composite materials have over the years attracted considerable interest from the scientific community, due to the plethora of applications in environmental and biomedical engineering. [1] Coupled to the requirement of such a materials development has been inevitably the introduction of 3D printing, which has provided technological tools for rapid advancements in the field. Consequently, the need to develop advanced materials, a) bearing surfaces capable of counteracting bacterial growth, b) eliciting interactions from tissues that render biocompatibility to human body rectification devices, and c) standing in line with the immune system response, thus contributing to biomedical engineering progress in the field of human health, emerges ostensible and challenging in contemporary science and engineering. [2]

Being cognizant of the interdisciplinary nature of the specific field, research was launched in our Lab to construct scaffolds that contain antimicrobial agents, which render the host resistant to bacterial growth. [3,4] In view of the fact that such materials should be well defined and manufactured to exhibit both (bio)chemical and mechanical strength properties, composite materials were first employed in the Lab that were based on PLA, with additional components complementing the polymeric milieu. Subsequently, introduction of antimicrobial agents was pursued, with the actual compounds emerging from a family of species generated in the Lab and fully characterized. To that end, titanium(IV)-containing materials extending from the simple oxide to citrato complexes were employed and introduced in the manufacturing process. The ensuing employment of a 3D printer constructed in the Lab was crucial in advancing the generation of scaffolds of known geometry, porosity and mechanical strength, thereby providing a substrate for further in vitro testing of cell growth. Cell culture growth of bacterial and eukaryotic cells was next attempted, with monitoring of the process extending over 24-72 h, with the results pointing toward optimization of the conditions used.

The collective experimental data on the design of the scaffolds and the associated in vitro testing of cell cultures denote the a) importance of factors influencing the efforts toward manufacturing such devices, and b) optimization required to achieve maximal antibacterial activity, thus projecting merit toward development of such composite materials, the function of which entails well-defined (bio)chemical support structures operating under the influence of (bio)inorganic complexes with enhanced bioavailability.

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PHOTOLUMINESCENT 2D Zn(II) COORDINATION POLYMERS BASED ON 2,6-DIACETYLPYRIDINE BIS(ISONICOTINOYLHYDRAZONE)

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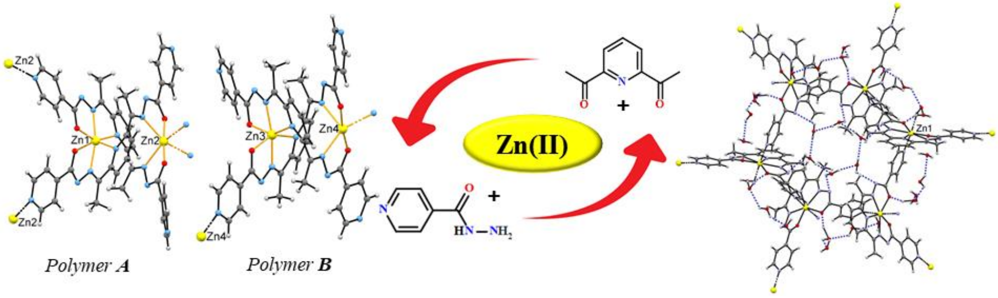
In recent times the coordination polymers (CPs) based on Schiff base ligands have proven to be excellent candidates for luminescent sensors. [1] Schiff bases derived from 2,6-diacetylpyridine are particularly suitable for the development of luminescent CPs. [2]

A template synthesis, in solvothermal conditions involving Zn(II) tetrafluoroborate, 2,6-diacetylpyridine and izonicotinic acid hydrazide in a methanol:DMF mixture at 120ºC led to the formation of elongated-prismatic and cubic yellow crystals of the CPs $[Zn_2L_2]_n$ (**1**) and $\{[ZnL]\cdot6H_2O\}_n$ (**2**), where H_2L = 2,6-diacetylpyridine bis(isonicotinoylhydrazone).

Coordination polymer **1** crystallizes in the monoclinic system, space group $P2_1/c$. In the asymmetric part of the unit cell there are two crystallographically independent 2D coordination polymers A and B. Each CP contains two zinc atoms Zn(1) and Zn(2) in **A** and Zn(3) and Zn(4) in **B**, connected by two H_2L ligands respectively (Figure).



$[Zn_2L_2]_n$ $\{[ZnL]\cdot6H_2O\}_n$

Figure. Schematic representation of the preparation of Zn(II) coordination polymers.

As a result, these coordination polymers have a similar formula $[Zn_2L_2]_n$. The coordination polyhedra of the Zn atoms in **A** and **B** are distorted tetragonal bipyramids formed by a set of N_4O_2 donor atoms.

Coordination polymer **2** crystallizes in the trigonal system, space group *R3*. In CP **2** the metal atoms are seven-coordinated (N_5O_2), adopting a symmetrical pentagonal bipyramidal geometry.

The coordination polymer **1** exhibits photoluminescent activity about 10 times more intense than the free luminophore coordination agent (H_2L). It is demonstrated by the fluorescent emission observed in the 550-650 nm range, which is visible even to the naked eye. $[Zn_2L_2]_n$ is proposed as a promising material for the development of green light sources.

Acknowledgement
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STYRENE-DIVINYLBENZENE COPOLYMER FUNCTIONALIZED WITH AMINO(4-HYDROXYPHENYL)ACETIC ACID GROUPS AND ITS POTENTIAL USE IN ENVIRONMENTAL REMEDIATION

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Worldwide environmental protection initiatives have stimulated a growing interest in functionalized polymeric materials for water decontamination. [1] Polystyrene-based polymers, valued for their chemical and physical stability, can be improved by introducing pendant functional groups. This study extends previous research on styrene-divinylbenzene copolymers functionalized with nitrogen-containing derivatives.

In this work, styrene-divinylbenzene copolymer supports were functionalized with amino(4-hydroxyphenyl)acetic acid groups using a phase-transfer catalysis method. [2] To confirm the successful functionalization of the copolymer with amino acid moieties, the obtained material (S-12%DVB, code: AM) was subjected to comprehensive characterization using Fourier transform infrared (FTIR) spectroscopy (see Figure 1), energy-dispersive X-ray (EDX) spectroscopy, scanning electron microscopy (SEM), and thermogravimetric analysis (TGA). The fraction of repetitive units functionalized with amino acid pendant groups grafted on S-12%DVB was determined by accepting the statistical structure of AM and is presented in Scheme 1. The functionalized copolymer shows promising potential for the adsorption of contaminants, such as silver ions.

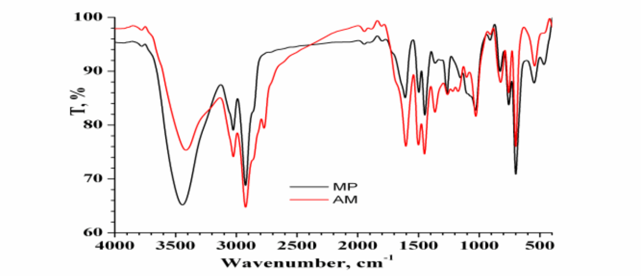
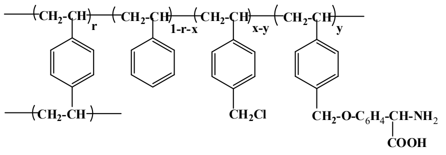


Figure 1. Comparison of FTIR spectra of raw material (MP) and final product (AM).

The observed decrease in the intensity of the γ-CH_2Cl band at 1213 cm^{-1}, along with the increased intensity of the bands at 1605–1610 cm^{-1} attributed to C=O group formation, provides evidence of successful functionalization.



Scheme 1. Styrene-divinylbenzene functionalized product structure (AM)
where: *y*-fraction of styrene units bearing pendant aminoacid groups; *x*-fraction of styrene units bearing pendant -CH_2Cl groups; *r*-fraction of divinylbenzene (DVB) units.

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COPOLYAZOMETHINES CONTAINING TRIPHENYLMETHAN AND THEIR OPTICAL ABSORBANCE CHANGES INDUCED BY NO_2 GAS

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Toxic vapors and gases resulting from human activities pose a global threat to both human health and the environment. Among these pollutants, nitrogen dioxide (NO_2) is particularly hazardous and is predominantly present in industrialized and urban areas, where it forms through the atmospheric oxidation of nitric oxide. As a polar and acidic oxide, NO_2 reacts with water vapor in the air to form nitric acid, contributing to acid rain. Industrially, NO_2 serves as an intermediate in the production of nitric acid. However, due to its corrosive nature, NO_2 can cause severe damage to the skin, eyes, and respiratory system, and is also associated with an increased risk of lung cancer. Therefore, the development of cost-effective, highly sensitive sensors capable of detecting low concentrations of NO_2 is essential. [1]

One of the key optical conducts that a material sensitive to NO_2 vapors should possess reversible color change upon exposure to this gas. We have previously reported several materials that exhibit reversible sensitivity to external stimuli, with the best results achieved using systems containing azomethine groups (named also imines or Schiff base). [2] The polyazomethine (PaZ) backbone features C=N bonds with lone pair electrons, enabling intra- and intermolecular interactions such as hydrogen bonding with other functional groups. Azomethine-based organic derivatives have already been investigated as porous films for NO_2 gas detection. [3]

However, similar to other conjugated polymers, PaZs often because of poor solubility in common organic solvents, which limits their processability, comprehensive characterization, and practical applications. Strategies to improve PaZs solubility include introducing packing-disruptive bulky groups, such as the non-polar triphenylmethane (TPM) moiety. Furthermore, structural modifications are essential to tailor the properties of PaZs for application as coatings in specific sensors, like Mach-Zehnder interferometer sensors. Using chemical design tools, various building blocks such as carbazole (CBZ), thiophene (Th), and benzothiadiazole (BTD) can be employed to develop organic sensing materials for nitric oxide detection, as already demonstrated [4]. In addition, synergistic impacts of integrating TPM and heterocyclic units in the same PaZ architecture have been already proved towards sensing applications. [2]

In our efforts to develop high-performance azomethine-based coatings, we present here novel sensing materials with a non-conventional design achieved through linear conjugated copolyazomethines (CoPaZs) incorporating Th, BTD, and bulky TPM substituted with CBZ moieties within the same copolymeric architecture. The synthesis of these CoPaZs and the methodology employed for NO_2 detection are detailed herein, with focus on polymers reusability.

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PHENOL-SENSITIVE MN-PORPHYRIN MEMBRANE-BASED POTENTIOMETRIC SENSOR

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Ionophore-based potentiometry is recognized as a valuable analytical technique owing to its high selectivity and straightforward instrumentation. This has facilitated its establishment in various fields, particularly in clinical and environmental analysis, physiology, and process control. [1]

Potentiometry utilizes an indicator electrode referred to as an ion-selective electrode (ISE). This electrode converts the activity of a specific target ion into an electric potential, which acts as the measured signal when paired with a reference electrode. Usually a "coated-wire electrode", employing a metallic wire coated with a polymeric sensing membrane was doped with various ionophore extended the application of coated-wire electrodes to many ions. [2] The coated-wire electrodes demonstrated a Nernstian response to their target ions; however, they experienced considerable potential drift. This drift can be primarily attributed to the formation of an aqueous layer at the metal/membrane interface, leading to transmembrane ion fluxes and an unstable phase boundary potential at the interface of the sensing membrane and the underlying metal.

The objective of the current research study is to prepare PVC membrane modified with porphyrin for the phenol quantification. The general performance characteristics of modified potentiometric membrane sensors responsive to phenol at basic pH were established. The technique was based on the employment of PVC, Mn porphyrin as an ionophore, and dioctyl sebacate (DOS) as a plasticizer for sensor. The sensors showed response over a wide concentration range (1×10^{-2} to 1×10^{-7} M), with detection limits of 1.25×10^{-7} M. The tested sensor exhibits the near-Nernstian response at 39 mV/decade and low relative standard deviations.

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AN ELECTROCHEMICAL STUDY OF METAL PHOSPHONATES BASED ON ZINC AND ETIDRONIC ACID AND FOSFONOACETIC ACID IN SALINE SOLUTION

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Phosphonates and phosphonic acids have recently been studied as potent corrosion inhibitors. Corrosion inhibition is typically achieved by applying phosphorus-containing compounds, which work by modifying the surface state of the protected metal. The main mechanism behind the effectiveness of corrosion inhibitors is their ability to adsorb onto the metal surface or to form insoluble compounds with metal cations. Additionally, phosphonic acids can react with metal cations to form stable, poorly soluble compounds, further reducing the corrosion rate [1,2].
The aim of this work is to investigate the efficiency of metal phosphonates inhibitors based on zinc and etidronic acid (ZnHEDP) and fosfonoacetic acid **(**ZnPA**)** in preventing the corrosion of metallic materials in saline solution**.** Electrochemical tests (figure 1) were performed to evaluate the corrosive effect of chloride ion on iron in the absence and presence of metallic phosphonates compounds.

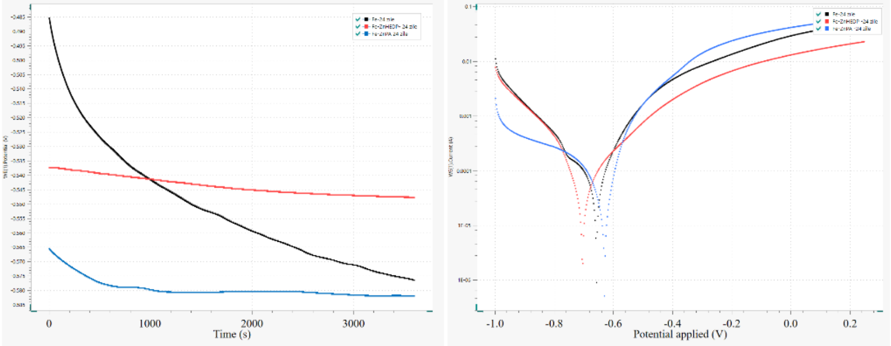

Figure 1. Polarization curves (CP) of the iron electrode immersed for 60 minutes in 3% NaCl solution (pH~2.5) and with 200 ppm metal phosphonates inhibitors

The variation of the potential at the open circuit potential (E_{OCP}) was monitored for electrodes immersed for one hour in a 3% NaCl solution, pH ~2.5, both without and with the addition of 200 ppm of an inhibitor. The CP tests were performed after one hour of immersion in solutions. It was observed that the iron immersed in the solution with the inhibitor exhibited less negative E_{OCP} values, suggesting the presence of a barrier layer on the metal surface that prevents corrosion of the metal. From the polarization curves, the parameters Rp (polarization resistance), Ecorr (corrosion potential), and Jcorr (corrosion current density) were determined. The corrosion inhibition efficiency (IE, %) was calculated to be approximately 48% for ZnPA and about 58% for ZnHEDP during the first hour of immersion. The corrosion process evolves over time. The effect can be visibly observed after 24 days of immersion. With increasing immersion time, the IE increases to approximately 57% in the case of ZnPA, indicating that the film formed on the steel surface grows over time. A more significant increase of about 71% was observed in the case of ZnHEDP, resulting from the formation of a more compact protective layer compared to the one formed with ZnPA.

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POTENTIAL ANTITUMOR ACTIVITY OF CU(II) COMPLEXES WITH SCHIFF BASES IN HUMAN TUMOR CELLS

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The interest of scientists and clinicians in the use of metal complexes as potential antitumor agents is constantly growing, due to their unique characteristics. It has been found that copper, administered in the form of various compounds, can effectively induce tumor cell death. Actively proliferating and metastasizing tumor cells exhibit a greater "demand" for copper, making this element suitable for diagnostic and therapeutic purposes in oncology. The antitumor activity of Schiff bases and their metal complexes are also promising.

That's why the aim of our study was to evaluate the influence of newly-synthesized Cu(II) complexes with Schiff-bases on viability and proliferation of human tumor cells.

Two groups of Cu (II) complexes with Schiff-base ligand derived from condensation reactions between o-vanilline (V) and amino acids (tryptophan, serine and tyrosine) were investigated. In one group, the coordination complex is bound with 1,10 –phenanthroline, and in the second group - with 2,2' – dipyridtlamine. As an experimental models were used two permanent cell lines, obtained from cervical carcinoma (HeLa) and melanoma (A375) in human. The complexes were applied at a concentration range of 1-200 µg/ml for 24, 48 and 72 hours. The influence of the compounds on cell viability and proliferation was examined by cytotoxicity assays with different mechanisms of action and cell targets - MTT test, Neutral red uptake cytotoxicity assay, Crystal violet staining technique, double staining with acridine orange and propidium iodide. The ability of tested compounds to inhibit 3D cell colony formation in a semi-liquid medium was examined by colony-forming method (up to 30 days). The results obtained reveal that all examined Cu(II) complexes with Schiff-base ligands decrease viability and proliferation of the treated tumor cells in a time- and concentration-dependent manner, as well as induce cythopathological changes and inhibit their 3D growth in semi-solid medium. Cu(II) complexes with 1,10 –phenanthroline exshibit higher cytotoxic activity compared to Cu(II) complexes with 2,2' – dipyridtlamine. The results obtained so far show that the compounds investigated have promising cytotoxic properties, but further experiments are needed to clarify better their antitumor potential.

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ULVAN EXTRACTED FROM ULVA LACTUCA SEAWEEDS USED FOR GREEN SYNTHESIS OF Au NANOPARTICLES

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Ulva lactuca, a green macroalga, is recognized as a valuable source of bioactive compounds, including polysaccharides, pigments, and polyphenols. Its renewable nature enhances its potential for various applications, making it a promising resource for industrial exploration [1]. The main polysaccharide obtained from *Ulva lactuca*, ulvan, is composed of rhamnose, xylose, iduronic acid, and glucuronic acid [2]. This polysaccharide exhibits antioxidant, antimicrobial, antiviral, antihyperlipidemic, antitumor, and anti-inflammatory properties, making it a potential candidate for biomedical applications [3]. Consequently, *Ulva lactuca* polysaccharides may be further used in the development of biocompatible composite materials with various applications, including drug delivery, wound dressing, and tissue engineering.

The polysaccharides were extracted in water from *Ulva lactuca*, harvested from Romania's Black Sea coast under high autogenous pressure. The extract was characterized by FT-IR spectroscopy, differential scanning calorimetry and thermogravimetric analysis, wide angle X-ray diffraction (XRD), and scanning electron microscopy coupled with energy dispersive X-ray (SEM-EDX) analysis. The amount of carbohydrates was determined using anthrone method, sulfated groups content was evaluated through barium chloride - gelatin method, and uronic acids were quantified using orcinol method. The protein content was also assessed. The *Ulva lactuca* extract had high amounts of carbohydrates and uronic acids (61.6 % and 29.5 %, respectively).

The *Ulva lactuca* extract was used as stabilizer for a green synthesis of gold colloidal nanoparticles (NPs). The resulting AuNPs were characterized by UV-vis spectroscopy, dynamic light scattering, XRD, and scanning electron microscopy.

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MAGNESIUM-BASED METAL ORGANIC FRAMEWORKS SYNTHESIZED THROUGH ALTERNATIVE METHODS. SYNTHESIS AND CHARACTERIZATION

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Alternative synthesis methods [1], such as: microwave assisted synthesis, sonochemical synthesis and mecanochemical synthesis replaced the classic synthesis of metal organic frameworks that uses heat and requires longer reaction time. All these methods have many advantages, for example: the time and the speed of the reactions are shortened, are greener, economical, and there is less waste in the case of the mecanochemical synthesis.

The aim of this study is to synthesize and characterize magnesium-based metal organic frameworks using the alternative methods considering the 12 principles of green chemistry, and then the obtain materials to be used for different applications. The Mg-based metal organic frameworks were synthesized from the reaction between etidronic acid (HEDP) as the organic linker, and magnesium nitrate hexahydrate as the inorganic node, at different ratios and pH, using water as solvent and under various conditions, such as: hydrothermal [2], ultrasound and microwave assisted synthesis. The obtained compounds (MgHEDP) were further characterized by X-ray Diffraction (XRD), Thermogravimetric Analysis (TGA), Fourier Transformed Infrared Spectroscopy (FTIR) and Elemental Analysis (EA). From the FTIR it was observed that the P-OH bond corresponding peak was not present due to P-O-Mg bond formation, confirming that the MgHEDP materials were obtained. The best yield, 55%, was acquired in the case of MgHEDP at the ratio 1:1 (metal:acid) under hydrothermal conditions.

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SOL-GEL HYBRID FILMS CONTAINING BN–C NANOSTRUCTURES: DEPOSITION AND FUNCTIONAL CHARACTERIZATION

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Hybrid materials obtained by the sol-gel method represent a versatile class of functional coatings, with broad applications in fields such as anticorrosive protection, optoelectronics, sensing, self-cleaning surfaces, and materials for energy storage and conversion. The functionalization of these hybrid layers through the incorporation of nanomaterials has become an intensively researched topic, due to its potential to enhance the physicochemical properties of the coatings. In this context, boron nitride (BN) nanoflakes and their carbon-based derivatives (B–C–BN) have proven to be highly effective additives, owing to their excellent chemical stability, hydrophobic character, and remarkable dielectric properties [1–3].

This work presents the synthesis and characterization of hybrid sol-gel coatings, obtained from precursors tetraethyl orthosilicate (TEOS) with either cyclohexylmethyldimethoxysilane (CHMDS) or dimethoxydimethylsilane (DMDMS), in variable proportions (TEOS : CHMDS / DMDMS = 2:0.2–2 v/v), and doped with microspheres composed of boron nitride-carbon nanoflakes, in concentrations ranging from 1-10% relative to the total volume of the sol-gel solution. Hydrolysis and condensation were catalyzed by 0.01 M HCl, at 25 °C for 24 hours. The coatings were deposited onto glass substrates by dip-coating, followed by thermal treatment at 120 °C to consolidate the silica network and anchor the microspheres within the host matrix.

The morphology of the coatings was analyzed using scanning electron microscopy (SEM) to reveal surface structure, phase dispersion, and potential defects. The chemical structure was characterized by Fourier-transform infrared spectroscopy (FTIR), while the structural and optical properties influenced by composition were evaluated through thermogravimetric analysis (TGA), contact angle measurements, and UV-Vis spectroscopy. The results confirm the feasibility of the sol-gel method for producing complex hybrid films, with hierarchical microstructures and tunable properties depending on chemical composition and post-deposition treatments. Due to their uniform microstructure, thermal stability, and adjustable optical behavior, sol-gel hybrid coatings functionalized with boron nitride-carbon microspheres are suitable for applications such as optical sensors, anti-reflective optical filters, UV-protective layers.

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AGRO-INDUSTRIAL WASTES AS PROMISING MATRICES FOR ENZYME IMMOBILIZATION: A SUSTAINABLE ALTERNATIVE FOR PRODUCING BIOACTIVE FLAVONOLS

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Flavonols, a major subclass of flavonoids, have recently gained attention for their diverse bioactivities, including antioxidant, neuroprotective, cardioprotective, anti-aging, and cytotoxic effects [1-3]. Glycosylation of flavonols represents one of the most promising strategies to enhance water solubility, leading to improved bioavailability and medicinal potential [4–5]. Glycoside production via UDP-glycosyltransferases (UGTs) offers notable benefits such as greater specificity, elimination of toxic chemicals, and more efficient, cost-effective processes [6–7]. Immobilisation of UGTs on agro-industrial lignocellulosic biomass offers an attractive and low-cost alternative with improved operational stability and reusability of the biocatalyst, thereby preventing protein leaching and lowering industrial production expenses.

Rice husk and groundnut husk are waste products of food processing which provide cheap engineering materials as well as help to waste management. In this study the investigation was carried out on the morphology, composition and thermal degradation characteristics of the rice and groundnut husk with a view to explore their suitability as matrices for UDP-glycosyltransferases immobilization.

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BI COMPUTING: INTERACTIVE B-FACTOR ANALYSIS FOR PROTEIN–LIGAND COMPLEXES IN COMPUTATIONAL CHEMISTRY

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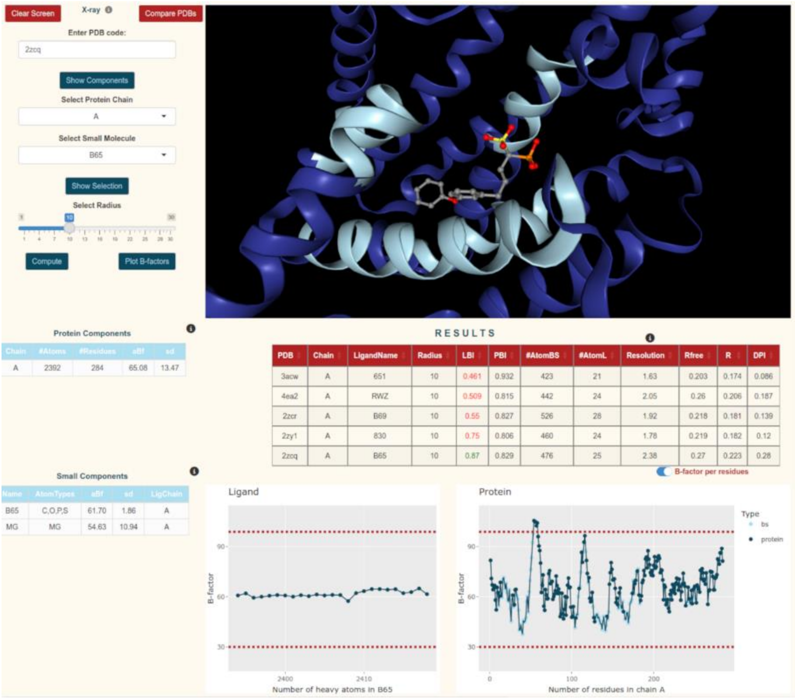
The Ligand Binding Index (LBI) is a valuable computational metric for evaluating protein-ligand interactions based on crystallographic B-factors. [1, 2] To facilitate its widespread adoption in computational chemistry and chemoinformatics, we present the BI Computing Tool, an open-access web application (https://chembioinf.ro/tool-bi-computing.html) developed using R and the Shiny framework. [3] This tool enables the calculation of LBI and Protein Binding Index (PBI) metrics from PDB entries, offering real-time visualization of protein-ligand structures via NGLViewerR and graphical analysis of B-factor distributions. The interface allows users to select specific chains, define binding site radii, compare multiple PDB entries, and assess structural quality parameters such as R-values and Diffraction Precision Index (DPI). By integrating these features, the BI Computing Tool not only aids in identifying high-quality protein-ligand complexes but also enhances structure-based workflows for computational chemists and structural biologists. The tool's ability to incorporate structural dynamics through LBI analysis offers new perspectives for rational drug design and protein engineering, bridging the gap between crystallographic data and dynamic molecular behavior. This study demonstrates the potential of user-friendly, web-based tools in advancing structure-based computational approaches in drug discovery and chemoinformatics.



Enter PDB code: 2zcq

Select Protein Chain: A

Select Small Molecule: B65

Protein Components

Chain	#Atoms	#Residues	aBf	sd
A	2392	284	65.08	13.47

Small Components

Name	AtomTypes	aBf	sd	LigChain
B65	C,O,P,S	61.70	1.86	A
MG	MG	54.63	10.94	A

RESULTS

PDB	Chain	LigandName	Radius	LBI	PBI	#AtomBS	#AtomL	Resolution	Rfree	R	DPI
3acw	A	651	10	0.461	0.932	423	21	1.63	0.203	0.174	0.086
4ea2	A	RWZ	10	0.509	0.815	442	24	2.05	0.26	0.206	0.187
2zcr	A	B69	10	0.55	0.827	526	28	1.92	0.218	0.181	0.139
2zy1	A	830	10	0.75	0.806	460	24	1.78	0.219	0.182	0.12
2zcq	A	B65	10	0.87	0.829	476	25	2.38	0.27	0.223	0.28

Figure 1. Overview of the BI Computing Tool showing user options for evaluating protein–ligand interactions based on crystallographic data

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A COMPARATIVE ANALYSIS OF MOLECULAR PROPERTIES IN AGROCHEMICALS AND DRUGS

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The development of new drugs and agrochemicals represents two of the most significant endeavors in applied chemistry, yet the principles governing their design often operate in distinct scientific spheres. Understanding the similarities and differences in their physicochemical properties is crucial for enhancing molecular design, improving safety profiles, and exploring potential cross-domain applications. [1] This study presents a large-scale comparative chemoinformatic analysis to quantitatively delineate the chemical space occupied by agrochemicals and drugs. Data extracted from PubChem [2] and DrugCentral [3] resulted in a comprehensive set of small-molecules. Several well-known molecular descriptors critical for bioactivity and bioavailability were computed and used to compare drugs targeting human and non-human proteins with agrochemicals. We describe similarities and differences between the physicochemical profiles of these compounds. Our results define the chemical space of bioactive compounds, where new molecules, safer, more effective agrochemicals with reduced environmental impact as well as novel therapeutic candidates can be found.

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IMPROVING THE ACCESSIBILITY OF QUANTITATIVE ESTIMATE OF PESTICIDE-LIKENESS (QEP) SCORING THROUGH ALTERNATIVE METHODS FOR ESTIMATING THE PARTITION COEFFICIENT (LogP)

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Agrochemicals are vital to modern agriculture, but their development must strike a careful balance between biological efficacy and environmental safety. During early-stage screening, physicochemical descriptors are used to prioritize candidate compounds based on predicted performance. One key descriptor is the partition coefficient (logP), which influences bioavailability, mobility, and environmental persistence. Computed logP is a critical input in the Quantitative Estimate of Pesticide-likeness (QEP) [1], a scoring system that integrates multiple molecular descriptors to assess the agrochemical potential of compounds.

However, the original QEP model was calibrated using Chemaxon CxLogP [2], a proprietary software requiring a license, which limits its accessibility. To address this barrier, we investigated how different logP estimation methods (computed with the freely available RDKit [3] or CDK toolkit) [4], i.e., SlogP, Mannhold logP and XLogP, compare with CxLogP, and consequently affect QEP scores. Our analysis used a dataset of 100 highly active compounds selected from over 3,000 agrochemicals tagged in PubChem [5] database.

The results highlight the variability in QEP scores depending on the logP method used and recommend viable alternatives to CxLogP. This work makes the QEP scoring framework more accessible, facilitating faster and broader prioritization of candidate compounds in early agrochemical design.

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PYTHON-BASED WORKFLOW FOR CLUSTERING AND SELECTING NATURAL COMPOUNDS USING SIMILARITY COEFFICIENTS

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The identification and selection of natural compounds with potential antiviral activity represent a significant challenge in the discovery of new effective and safe therapies. This study proposes a Python-based [1] workflow for analyzing and clustering natural compounds, starting from an initial set of known antiviral drugs. Utilizing molecular similarity coefficients [2,3,4] such as Tanimoto, alongside Euclidean and Manhattan distances, compounds are grouped into homogeneous classes, facilitating the selection of the most representative candidates for further investigation. The workflow automates hierarchical clustering and identification of relevant compounds, providing a rapid and flexible method for analyzing natural compounds with potential antiviral activity. Top-ranked natural compounds were subsequently characterized in terms of their pharmacokinetic profiles, drug-likeness (including Lipinski's and Veber's rules), and Absorption, Distribution, Metabolism, Excretion, and Toxicity (ADMET) properties, as well as bioavailability scores and synthetic accessibility.[5] This approach aids early stages of computer-aided molecular design, accelerating the development of potential novel antiviral agents derived from natural products.

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STRUCTURALLY DESIGNED CHLORONITROBENZOIC DERIVATIVES AS PROMISING ANTIBACTERIAL AND ANTI-BIOFILM AGENTS

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The growing prevalence of multidrug-resistant bacteria creates an urgent demand for innovative antimicrobial strategies, including the development of new compounds that act through alternative mechanisms beyond conventional antibiotic. [1] Chloronitrobenzoic acid derivatives represent a versatile chemical scaffold with promising biological potential. [2] In this study, two new derivatives were designed and synthesized to improve antimicrobial efficacy. The compounds were fully structurally characterized, including single-crystal X-ray diffraction (SCXRD) analysis. Their antibacterial activity was tested against a range of Gram-positive and Gram-negative bacterial strains, covering both standard laboratory strains and clinically relevant multidrug-resistant isolates. The evaluation included minimum inhibitory concentration (MIC) measurements, bacterial viability assays, and biofilm inhibition tests to comprehensively assess their antimicrobial potential.

The synthesized compounds demonstrated antibacterial activity both in gram-positive and gram-negative strains, particularly against *Staphylococcus aureus*, including methicillin-resistant strains (MRSA). They effectively reduced bacterial growth and showed a dose-dependent ability to disrupt biofilm formation, with resistant isolates being especially susceptible. These results support the potential of chloronitrobenzoic acid derivatives as promising candidates for the development of next-generation antimicrobial agents.

Acknowledgements
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INTERACTIONS OF SMALL MOLECULES WITH BLOOD PROTEINS

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The two major blood proteins, serum albumin and hemoglobin (Hb), both interact with a variety of small molecules. Albumin's multiple ligand binding pockets are well characterized due to its physiological role in transporting endogenous molecules, and its propensity to also bind exogenous ligands such as therapeutic agents. On the other hand, small molecule binding to Hb has mostly been described in terms of the ability to either coordinate to the iron, or bind to the polypeptide and trigger oxidative changes at the heme active site (such as autooxidation to metHb or the formation of ferryl Hb), or modulate the affinity for molecular oxygen. Recent evidence indicates that beyond Hb's classical ligand sites (the heme iron and the central 2,3-BPG cavity), additional unconventional small-molecule binding sites exist on its surface. [1] These non-canonical sites, though less characterized, may directly modulate Hb's redox reactivity and oxygen affinity. [2,3] Here, we present an integrative approach to identify and characterize such non-canonical binding pockets on Hb, using serum albumin as a reference. We combine molecular docking to predict potential ligand-binding pockets and paramagnetic ^{1}H-NMR spectroscopy to monitor binding induced spectral changes.

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A COMPARATIVE STUDY OF MCM-48 MEZOPOROUS MOLECULAR SIEVE OBTAINED BY DIFFERENT SYNTHESIS METHODS

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The present work is focused on characterization, investigation and the comparison of MCM-48 mesoporous molecular sieves obtained by two synthesis directions. MCM-48 with cubic Ia3d structure was synthesized at room temperature using the cationic surfactant hexadecyltrimethylammonium bromide (CTAB) as a template agent and tetraethylorthosilicate (TEOS) as a silica source. On the other way the same composition for MCM-48 mesoporous material was place in an autoclave under static conditions for 24 respectively 48 h at 150 °C. After that the resulted MCM-48 material was cooled down at room temperature. The prepared samples were filtrated and rinsed with deionized water and ethanol, and dried at room temperature overnight. The resulted samples were annealed at 540 °C for 6 h applying a ramp rate for heating 2 °C/min to remove the CTAB from the composite material. Some of the specific surface areas of the investigated mesoporous molecular sieves are presented in Table 1.

Table1. Textural properties of MCM-48 molecular sieves.

No.	Sample	Specific surface area (m^2/g)	Pore volume BJH_{Des} (cc/g)	Average pore diameter BJH_{Des} (nm)
1.	MCM-48	1466.09	0.802	3.48
2.	MCM-48 A24h	871.89	0.629	2.94
3.	MCM-48 A48h	1100.52	0.931	2.97

The synthesized materials were further characterized by different investigation methods: X-ray diffraction (XRD), Brunauer–Emmett–Teller (BET) surface area, pore size distribution (PSD), scanning electron microscope (SEM), Fourier transform infrared (FT-IR) and thermal investigation.

Since the discovered of MCM-48 mesoporous molecular sieves, substantial studies have been done on both their preparation and applications directions. [1] It found that can be used as efficient catalyst carrier's adsorbents [2], and cutting-edge drug delivery systems. These materials have high thermal stability, specific pore volume up to 1.2 $cm^3\ g^{-1}$, surface areas between 1000–1500 $m^2\ g^{-1}$, a narrow pore-size distribution, and "non-cytotoxic" properties. [3]

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CUBIC MESOPOROUS SILICAS FOR CO_2 CAPTURE: STRUCTURE AND THERMAL BEHAVIOR

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Mesoporous molecular sieves (MMSs) with cubic structures, such as KIT-5 (Fm3m), KIT-6 (Ia3d), MCM-48 (Ia3d), and SBA-16 (Im3m) possess three-dimensional pore networks that facilitate efficient gas diffusion and adsorption-desorption processes. [1] KIT-6 and MCM-48 have highly interconnected 3D mesoporous networks, whereas KIT-5 and SBA-16 have limited 3D connectivity between spherical cages (Figure 1).

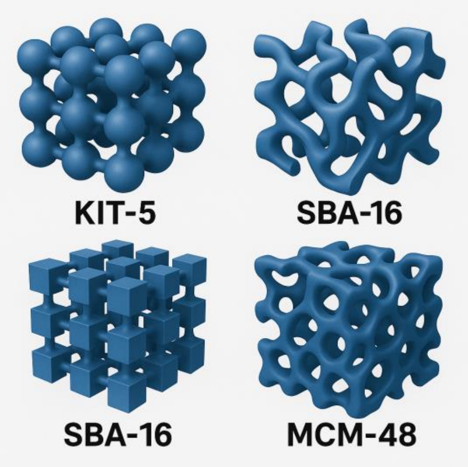

Figure 1. Mesoporous molecular sieves.

To increase the CO_2 adsorption capacity of mesoporous silica materials, silanization can be applied. This process introduces functional groups that have stronger interactions with CO_2 molecules.

In this study, these materials were synthesized via templated sol–gel processes and structurally characterized using X-ray diffraction (XRD), nitrogen sorption (BET), and transmission electron microscopy (TEM), confirming their distinct cubic mesophases and interconnected pore systems. Their performance in CO_2 adsorption was evaluated through thermal analysis techniques, including thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC).

The analysis revealed that the 3D pore connectivity and surface area significantly influence CO_2 uptake and thermal stability. KIT-6 and MCM-48, demonstrated the highest adsorption capacity and thermal regeneration potential with their bicontinuous channel networks. These results underscore the crucial role of mesostructural architecture in governing adsorption behavior, positioning cubic mesoporous silicas as strong candidates for cyclic CO_2 capture technologies in thermally dynamic systems.

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SYNTHESIS AND CHARACTERIZATION OF FUNCTIONALIZED ME/KIT-6 TYPE MESOPOROUS SIEVES

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The Me/KIT-6 materials with a metal loading of 30 wt% (Ni, Ce and Zn) were prepared using the impregnation method. An adequate amount of $Ni(NO_3)_2 \cdot 6H_2O$, $Ce(NO_3)_3 \cdot 6H_2O$ and $Zn\ (NO_3)_2 \cdot 6H_2O$ (Merck, Darmstadt, Germany) was dissolved in 0.6 mL deionized water. The KIT-6 support was then added in the solution, and the mixture was stirred for 2.0 h. Next, the formed slurry was further filtered to obtain dried powder samples, and the obtained powder samples were dried at 80 ºC overnight. Finally, the powder samples were calcined at 250 ºC for 4.0 h.

The mesoporous silica KIT-6 was synthesized and functionalized with 3-aminopropyltriethoxysilane by grafting at 110 ºC. The obtained materials were characterized by thermogravimetric analysis (TGA) in air and nitrogen atmospheres, Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), and nitrogen adsorption–desorption measurements.

ENHANCING DOCKING ACCURACY: THE LIGAND B-FACTOR INDEX (LBI) AS A PREDICTIVE METRIC

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Docking, a structure-based cheminformatics tool, is widely utilized in early drug discovery. It leverages the three-dimensional structure of a protein target to predict protein-ligand binding interactions, estimate corresponding binding affinities, and perform virtual screenings to identify new active compounds.

This study introduces the Ligand B-Factor Index (LBI), a novel metric for prioritizing protein-ligand complexes in docking, a crucial step in drug discovery. LBI quantifies the relative atomic flexibility between a ligand and its binding site, defined as the ratio of their median B-factors.

Using the CASF-2016 benchmark, LBI demonstrated a moderate correlation with experimental binding affinities, outperforming several traditional docking scoring functions.

This easily computable metric offers a valuable tool for enhancing the reliability and efficiency of structure-based cheminformatics workflows.

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A NOVEL CYCLODEXTRIN-BASED OXIDATIVE IMPURITY IN INDUSTRIAL MANUFACTURING AND FURTHER INVESTIGATIONS IN OXIDATIVE TRANSFORMATIONS

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Sugammadex (Bridion®), the first cyclodextrin-based active pharmaceutical ingredient (API), was developed through rational drug design and exhibits a well-defined mechanism of action. [1,2] Due to its unique structure, Sugammadex is typically produced as a single isomer. However, the complexity of its synthesis and purification processes has led to the identification of various impurities, which are increasingly important as generic production scales up after patent expiration.

In this study, we describe the first synthesis and comprehensive structural analysis of a novel impurity, mono-(6-sulfinic acid)-Sugammadex, which forms via oxidative transformation of the thiol-containing side chain.[3] This impurity is particularly significant, because sulphur-containing groups are sensitive to oxidation during manufacturing.

Multi-step synthetic strategies were applied, starting from γ-CD to generate the impurity. This involved bromination- and sulfonylation-based transformations, substitution with 3-mercaptopropionic acid, followed by oxidation. The impurity was characterized in detail using high-resolution mass spectrometry (HRMS), 1D and 2D NMR spectroscopy (including HSQC, COSY, HMBC), and HPLC-DAD-MS.

Furthermore, our investigation was extended to study the further formation of the sulfinic acid moiety through another synthetic and oxidative transformation, which involved applying various reaction conditions, oxidizing agent, and bases along with the preparation of another key intermedier, namely mono-6-butylmercapto-γ-CD.

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