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Students' Scientific Communications Session

BOOK OF ABSTRACTS

UNIVERSITY OF BUCHAREST
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Students' Scientific Communications Session

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Bachelor Level

Pomegranate wine obtaining process

Roxana-Andreea Băloiu, Alexandra-Mihaela Bădulescu,
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Fruit wines are quite appreciated by consumers probably due to the different sensory attributes, properties and a various scale of color, taste as well as alcohol content [1]. However, pomegranate wine is not so well explored at industrial level only a few research papers focus either on the production of this type of fruit wine, different analysis on the few commercially available pomegranate wines or utilizing the pomegranate residues as source of bio-active compounds. In this context a question that arises is how the obtaining process would be influenced by an industrial scale-up.

The purpose of this study is to prepare pomegranate wines in different amounts (0.5-3 L) from a commercial variety-Hicaz (from Turkey). The wines were further analyzed regarding their alcohol content, total soluble solids, sensory analysis, as well as spectrophotometric determination.

The experimental procedure consisted of an initial phase of cleaning, peeling and separating the seeds. The pomegranate juice was obtained after mixing the seeds using a blender and then solids were filtered off. The peels and the seeds were dried to constant mass and from which drying curves were depicted. The pomegranate wine must was prepared using the juice in water, sugar, wine yeast (*S. cerevisiae var. bayan*) and pectinase. Pomegranate wines were subjected to a primary fermentation (2.5 weeks) followed by a secondary fermentation period of about 2.5 weeks. During this process, CO_2 release was monitored and from this sugar consumption as well as ethanol production were determined.

After the fruit wine maturation, a sensory analysis was carried out and the prepared wines showed good commercial potential.

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Aspirin Analogues in the perspective of PET Valorization

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Polyethylene terephthalate (PET) is one of the most widely marketed aromatic polyesters with many applications in polymeric industry for plastic production in nowadays. The escalating PET waste has led to significant accumulation in Earth's ecosystems, stressing an urgent need for effective upcycling strategies [1]. In this context, an actual challenge is the valorization of PET waste. One of this alternatives involves the PET depolymerization leading to PET monomers, such as terephthalic acid (TPA) or bis(2-hydroxyethyl) terephtalate (BHET), as valuable precursors for chemical industry [2].

In this context, we propose the use of PET monomers for the synthesis of aspirin analogues in line of green chemistry concept. In our study, we designed a catalytic system for the synthesis of aspirin analogues starting from PET-derived precursors, respectively TPA or BHET, and salicylic acid (SA). The reactions were carried out in different solvents, specifically tetrahydrofuran (THF) and dimethyl carbonate (DMC). A systematic evaluation of the catalytic efficiency was performed by comparing conventional catalysts (sulfuric acid, ZIF-8, $Ca_{0,3}$@ZIF-8, $Cu_{0,3}$@ZIF-8, $Ca_{0,1}$@ZIF-8, $Cu_{0,1}$@ZIF-8, UIO-66, H-β-12,5-Des-Deal-MW, H-β-18,5-Des-Deal-MW, H-β-25-Des-Deal-MW, H-Mor-12,5-Des-Deal-MW) and biocatalysts (Novozyme 435, Lypase from *Aspergillus Niger*, Lypase R375, AN@ZIF-8, RO@ZIF-8, CR@UIO-66, CR@ZIF-8, CR2@ZIF-8). The resulting products were detected using high-Performance liquid chromatography with diode array detector (HPLC-DAD) as analysis method. The experimental results will be presented in detail during the presentation.

---

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Synthesis and structural insights into new organotin(IV) chalcogenides

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The research of organotin(IV) chalcogenides is relevant due to the antifouling [1], bactericide, algicide, and pesticide [2] properties of these compounds. They have the potential to serve as precursors for single-source materials used in the production of SnS and SnSe films [3].

We report on the synthesis of two new organotin(IV) chalcogenides. For both compounds, the dihalide $[2\text{-}(O{=}CH)C_6H_4]_2SnCl_2$ (**1**) was used as the starting material. The compounds $[\{2\text{-}(O{=}CH)C_6H_4\}_2SnS]_2$ (**2**) and $[\{2\text{-}(O{=}CH)C_6H_4\}_2SnSe]_2$ (**3**) were synthesized (Figure 1) and fully characterized by multinuclear (^1H, ^{13}C, ^{119}Sn) NMR spectroscopy and single crystal X-ray diffraction. The solid-state structures of compounds **2** and **3** revealed the formation of four-membered tin-chalcogen rings.

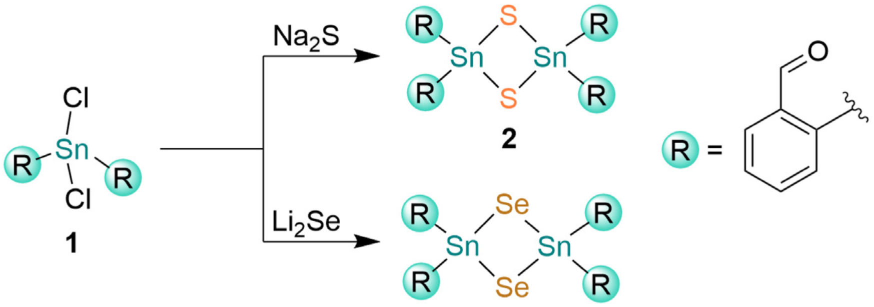

Figure 1. Synthesis of compounds **2** and **3**.

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Lignin modification with applicability as additive for improved bitumen production

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Lignin is one of the most abundant and widely distributed biopolymers on Earth, second only to cellulose. It is generated based on the cellulose extraction process from plant. Currently, it is treated as a residual by-product, with an annual amount of approximately 50–70 million tons [1]. Besides all these aspects, there is a strong desire to find an industrial-scale use for lignin to reduce waste quantities. On the other hand, asphalt contains bituminous materials that are largely petroleum-based. These materials are both expensive and polluting, or at the very least, unsustainable [2].

In this context, native and modified lignin were used as additives for bitumen. Lignin modification was performed via enzymatic catalysis using laccase (Laccase M120), following an oxidative polymerization approach. The incorporation of lignin led to the formation of lignin–bitumen composites. These materials were characterized by Fourier-transform infrared spectroscopy (FTIR) and gel permeation chromatography. FTIR analysis revealed structural changes in bitumen, while GPC provided information on molecular weight distribution.

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Toward the Synthesis of Nitrogen-Rich Macrocycles as Potential Artificial Ion Channels

<u>Rareș-Ștefan Căpușan</u>, Diana-Nicoleta Novac,
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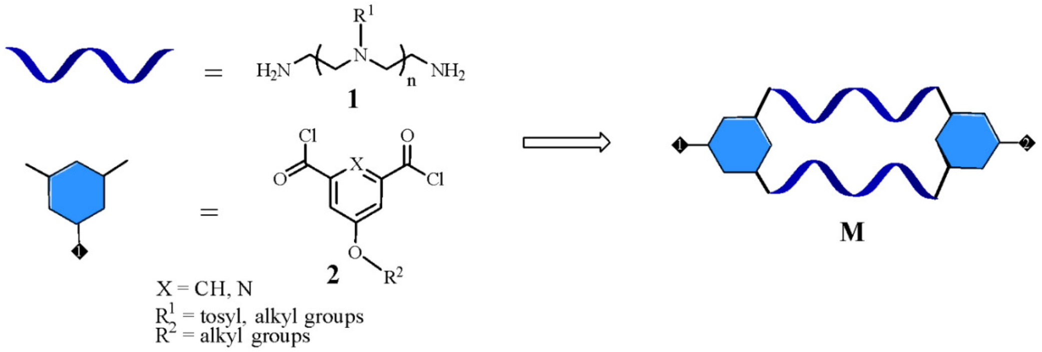
The transport of water and ions across biological and synthetic membranes is fundamental to many processes, ranging from cellular homeostasis to separation technologies [1]. Advances in supramolecular chemistry have enabled the rational design of transmembrane transporters [2]. For example, macrocycles, having pre-organized cavities were shown to facilitate transport by forming directional hydrogen-bonding interactions with guest species, while the lipophilic exterior ensures their incorporation into membranes [3].

Our aim is the synthesis of amide-based macrocycles **M** (Fig. 1) and the investigation of their potential use as artificial water or ion channels. As a first step, we focused on the preparation of the two main intermediates, the N-alkyltriamine derivatives **1** and the alkyl-substituted acid dichlorides **2** (Fig. 1). Their synthesis involves multistep sequences including O- and N-alkylation, protection and deprotection of primary amines, esterification, and ester hydrolysis. These intermediates are intended to serve as complementary building blocks for subsequent macrocyclization through amide-bond formation.



X = CH, N
R^1 = tosyl, alkyl groups
R^2 = alkyl groups

Figure 1. Structures of the intermediates **1-2** and design of the target macrocycles **M**.

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Efficient synthesis of multisubstituted α-Pyrones via Palladium-catalyzed cross-coupling reactions

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α-Pyrones serve as versatile scaffolds in organic, medicinal, and polymer chemistry [1], by virtue of their unique unsaturated lactone framework that mimics the reactivity of both conjugated dienes and aromatic systems. Their ubiquity in nature - ranging from fungi to higher animals - reflects a profound biological significance, manifested in diverse pharmacological properties such as antifungal, anti-inflammatory, and cytotoxic activities [1].

Driven by these attributes, we investigated the substrate scope of a palladium-catalyzed synthetic procedure reported by Grigalunas et al. [2], which enables the facile and versatile synthesis of multisubstituted α-pyrone derivatives. This multicomponent, one-pot approach involves a sequence of ketone α-arylation, α-alkenylation, followed by E/Z isomerization and lactonization. The obtained compounds have been characterized by spectroscopic methods, and their structural features suggest potential for further investigation of biological activity, given their similarity to naturally occurring bioactive α-pyrones.

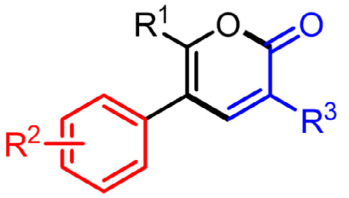

Figure 1. General structure of the synthesized compounds.

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Carbohydrazone-Based Precursors for the Synthesis of Functional Macrocycles

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Macrocyclic compounds bearing hydrogen-bonding motifs are attractive scaffolds forartificial water and ion transport across membranes [1,2]. In this context, carbohydrazone units provide reversible connectivity [3], multiple donor/acceptor sites, and structural adaptability, making them useful building blocks for functional macrocycles.

Herein, we present the synthesis of two series of 1,5-disubstituted carbohydrazones (Figure 1) functionalized with either phenolic groups (series **I**, Figure 1) or carboxylic acid groups (series **II**, Figure 1). The target compounds **I** and **II** were prepared by the reaction of 1,3-diaminourea with various hydroxybenzaldehydes for series **I**, or with keto acids for series **II**. The compounds were obtained in good to excellent yields and were isolated either as single E or Z isomers, or as mixtures of Z/E diastereomers, depending on the substrate. Their structures were confirmed by NMR spectroscopy and high-resolution mass spectrometry. In the next step, derivatives **I** and **II** will be used in macrocyclization reactions with compounds bearing complementary reactive groups to afford macrocycles of type **III**, designed as potential artificial water-channel candidates.

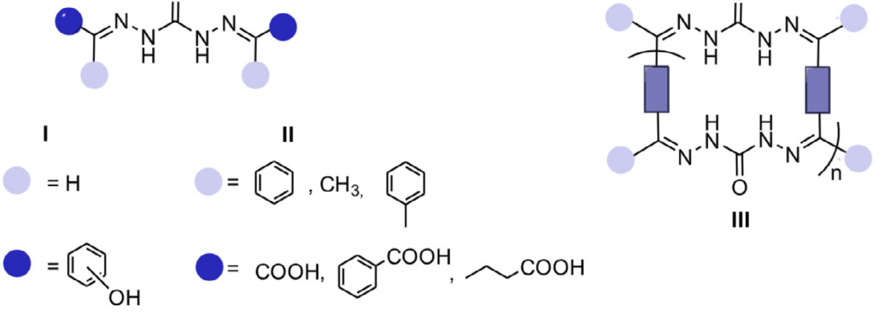

Figure 1. Structures of the target carbohydrazones **I**–**II** and macrocycles **III**.

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Coordination Complexes of 3d Metals with 3,5-Dimethylpyrazole

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Complexes containing 3,5-dimethylpyrazole represent an important class of coordination compounds that have been extensively studied due to their remarkable structural diversity and their similarity to certain biological active sites. The interest in these compounds is driven both by their unique structural and electronic properties, and by their potential applications in fields such as coordination chemistry, catalysis, and the modeling of biological systems [1].

The structural diversity of these complexes stems from the various coordination modes the ligand can adopt. This flexibility is due to the presence of two distinct nitrogen atoms within the molecule: a pyridinic nitrogen and a pyrrolic nitrogen. The specific coordination mode is highly influenced by the nature of the metal ion, as well as the specific synthesis conditions of the coordination compound [2].

The present work consists in the synthesis and characterization of one new Cu(II) complex combination, using the previously obtained starting material (copper acrylate, $Cu_2(acr)_2·2H_2O$). The characterization of the compound is based on elemental analysis, FTIR spectroscopy, UV-Vis-NIR spectroscopy. The compound $[Cu(L)_2(acr)_2]$ (L=3,5-dimethylpyrazole).

The complex will be tested for antimicrobial, antibacterial and antitumor activities.

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Fenton degradation of azo-dyes: a kinetic study on Bismarck Brown

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Water pollution is an ongoing global issue due to the negative effects on the environment and the contamination of potable water. The textile industry represents a major cause with dyes from wastewaters leaching into the soil. One such example is Bismarck Brown (BB), an azo-dye used in textile, leather, and paper industries.

This work aims to investigate the degradation kinetics of BB by Fenton reagent, which is commonly used in wastewater treatment due to its nonspecific oxidation activity and safety, as well as facile scaling up and low costs.

We determined the optimal ratios of the Fenton system by varying the hydrogen peroxide concentration. The 1st order, 2nd order, and a newly proposed biexponential model were used to model the experimental concentration–time curves. The obtained kinetic parameters were then correlated to the experimental conditions in order to assess their individual influence.

The results show that classical first and second order models do not adequately describe the kinetics of this reaction. The biexponential model gave better results, suggesting that the Fenton degradation of BB comprises two stages. The results also indicate an initial very fast degradation stage that we were not able to characterise given the experimental time resolution.

This study confirms the biexponential model outperforms the classical 1st and 2nd order kinetic models in describing the Fenton degradation of BB. The optimal hydrogen peroxide concentration and optimised ratio between the Fe^{2+} and H_2O_2 were determined. Future work will focus on the effect of the Fe^{2+} concentration and better understanding sthe degradation mechanism of this reaction.

The toxicity of Co^{2+}, Ni^{2+}, Cu^{2+} and Cd^{2+} heavy metals on Saccharomyces cerevisiae mutants

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Evolution has its own pace of problem solving by various methods, using natural selection which needs a great amount of time. Although humanity has the talent to create its own problems, eventually a solution is always on the way to make room for new issues to come.

Freshwater makes up about 2.5-3% of all water on Earth and from this amount only 1% is accessible due to its distribution in glaciers (~68%) and the groundwater (~30%). The negative side of this reality is not its relative quantity but humanity's decision making on the usage of it. A major portion of this freshwater is contaminated by various factors, most significant being heavy metals which are notoriously difficult to remove. This occurring issue is a topic that is discussed in detail for people to have an idea about the future role of yeast usage in bioremediation.

This largely used organism - *Saccharomyces cerevisiae* - serves as a model for studying molecular biology in eukaryotic life. With a well characterized genome and its fast life cycle suits it well for genetic and observational studies.

In this study, genetically modified yeasts were assessed for their ability to tolerate and immobilize heavy metals under metallic and oxidative stress conditions. Some mutants were engineered to express metal-binding functionalities on their cell surface, by acting like ligands, immobilizing them on their surface. We assessed cellular tolerance by monitoring population growth in the presence of toxic metal ions and quantified metal uptake at the cellular level. The results indicate that some mutants exhibit both tolerance and metal uptake, although significant variability was observed among strains. Some mutants demonstrated high resistance without metal accumulation, whereas others accumulated metals but showed reduced long-term viability. Comparative analysis allowed the identification of strains with optimal characteristics for use as biomaterials in heavy-metal bioremediation. Additionally, evidence suggests the existence of alternative metal–cell interactions, including intracellular sequestration and the reduction of metal ions to metallic nanoparticles.

These findings contribute to a better understanding of yeast-based bioremediation strategies and support the potential application of genetically engineered *S. cerevisiae* in fresh-water decontamination.

2,2′-Dipyridyl Disulfide as Ligand in Coordination Compounds: Synthesis and Structural Characterization

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This study explores the synthesis of coordination compounds based on 2,2’-dipyridyl disulfide, a ligand designed to mimic the disulfide pharmacophore of disulfiram while providing stable pyridine nitrogen donor sites for metal coordination. The ligand enables versatile coordination behavior toward Cu(II) and Co(II) centers, leading to the formation of self-assembled coordination architectures. The complexes were synthesized via a direct one-pot method under mild reaction conditions. The obtained compounds were characterized by Fourier-Transform Infrared Spectroscopy (FT-IR) and X-ray diffraction techniques. FT-IR analysis confirmed coordination through characteristic shifts associated with metal–nitrogen interactions, while X-ray diffraction provided detailed information regarding the crystalline phases, structural organization, and coordination environments of the resulting complexes.

Overall, this work highlights the coordination behavior of 2,2′-dipyridyl disulfide toward *3d* metal ions and contributes to the design of structurally well-defined coordination compounds with potential relevance in bioinorganic chemistry, medicinal inorganic chemistry, and anticancer research. In addition, the spectroscopic and crystallographic results suggest that the ligand promotes stable metal complex formation either through its bidentate coordination capability or through particular S–S bond transformations induced in the presence of metal complexes, depending on the reaction conditions employed. Such reactivity reflects the coordination versatility of diaryl and 2,2′-dipyridyl disulfide systems and their ability to generate diverse metal-organic architectures.

The study also demonstrates the potential of sulfur-containing pyridyl ligands in constructing transition-metal coordination systems with tunable structural properties. Such systems are of increasing interest due to their possible catalytic, redox, and biological applications. The incorporation of disulfide functionality may further influence the electronic and biochemical behavior of the complexes, particularly in relation to metal-mediated biological activity.

Hybrid Alginate–Carrageenan Biocomposites for Lipase Immobilization and Biocatalytic Reactions

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In the context of Green Chemistry and Sustainable development, biocatalysis has emerged as a crucial tool, offering high selectivity and mild reaction conditions. However, the industrial application of free enzymes is often hindered by their low stability and the high costs associated with their recovery [1].

The present study evaluates the immobilization strategy of lipases from *Aspergillus niger* and psychrophilic *Psychrobacter* from "Scărișoara" ice cave through entrapment in polymeric matrices. Two types of alginate-based matrices were evaluated: simple sodium alginate microspheres (AE system) and hybrid alginate-k-carrageenan microspheres (AKE system). The biocomposites were compared in terms of optimized biocatalytic efficiency and stability.

The structural integrity and morphology of the resulting microspheres were characterized using Environmental Scanning Electron Microscopy (ESEM) and high-resolution SEM. The enzymatic activity of biocomposites was assessed in hydrolysis of p-nitrophenyl butyrate (PNPB) and p-nitrophenyl palmitate (PNPP) substrates, over several catalytic cycles. Additionally, the obtained materials were tested in the biocatalytic reaction between bis(2-hydroxyethyl) terephthalate (BHET) or terephtalic acid (TPA) and Silibinin in different organic solvents.

The results showed that the hybrid alginate–carrageenan matrix provided better catalytic activity and mechanical resistance compared to the simple alginate support. This behavior is probably related to the optimized porosity of the hybrid network, which facilitates substrate diffusion while reducing enzyme leaching. The encapsulated enzymes led to good conversions toward the BHET–Silibinin material, especially in DMSO and THF, demonstrating good resistance to solvent-induced denaturation.

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New Coordination Polymers Based on Organotin(IV) Units and Dicarboxylate Spacers

<u>Cristian Andrei Dragnea</u>, Ariadna-Elena-Maria Beneș,
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Coordination polymers based on organotin(IV) units have attracted considerable attention due to their structural versatility, ability to generate architectures with different dimensionalities [1], as well as their potential applications in agriculture, industry, catalysis and biomedicine [2]. Recent studies have shown that the topology and dimensionality of organotin-based coordination networks are strongly influenced by both the organotin precursor and the geometry of the bridging ligands [3].

In this work, a series of new organotin(IV) coordination polymers containing n-tributyltin(IV) nodes and dicarboxylate spacers were synthesized under mild experimental conditions. The compounds were obtained by reacting $^{n}Bu_3SnCl$ with deprotonated dicarboxylic acids, such as adipic acid (H_2adp) and fumaric acid (H_2fum), followed by slow evaporation at room temperature for 25–40 days. This approach afforded colorless single crystals suitable for structural investigations.

The characterization of the new structures was carried out by single crystal and powder X-ray diffraction, as well as FTIR spectroscopy. Crystallographic investigations revealed that the structural organization of the resulting coordination polymers strongly depends on the nature of the dicarboxylate spacer. Variations in ligand rigidity, length and conformational flexibility generate different arrangements and extended network topologies, highlighting the important structure-directing role of the organic linker.

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Computational investigation of tetraborane(8) Lewis base adducts

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Boranes are simple boron hydrides with cluster-like structures that might fit into several structural types, such as *closo*, *nido* or *arachno*. Tetraborane(10) is an *arachno* borane with a butterfly structure with two boron atoms forming the body, bearing one terminal hydrogen atom and two boron atoms forming the wings, bearing two terminal hydrogen atoms. Four bridging hydrogens link the wing boron atoms with the body boron atoms, therefore the structure can be formulated as $B_4H_6(\mu\text{-}H)_4$[2].

By substituting two adjacent bridging hydrogen atoms in tetraborane(10) with a Lewis base, two isomers of B_4H_8L can be observed, namely the *endo* isomer with the ligand facing the cavity of the borane structure and the *exo* isomer with the ligand facing the convex side of the borane skeleton. *Axial* and *equatorial* isomers of B_4H_8L are obtained by redistributing the bridging hydrogen atoms.

Several compounds of this $B_4H_8{\cdot}L$ family were previously synthesized and characterized using diffraction techniques, structures being reported for L = CO, L = PF_3 and L = PF_2X where X is a halogen atom, other than fluorine.

A Density Functional Theory (DFT) analysis was performed using the PBE0 functional and the def2-TZVP basis set, using the GD3 empirical correction for dispersion forces. Computations were performed for $B_4H_8{\cdot}L$ systems, where L = CO, PF_3, PF_2X, PMe_3 and NMe_3.

The global minimum was found to be the *endo* isomer for L = CO, PF_3 and PF_2X, while for L = $PF_2(NMe_2)$, $PF(NMe_2)_2$, $P(NMe_2)_3$ and NMe_3 the most stable isomer was found to be the *exo* isomer. Computations were also performed for the $B_4H_8{\cdot}C_2H_4$ system which was found to have an *endo* cage-like structure.

Parallel synthesis of 1,3,4-oxadiazole-pyrene based fluorophores

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2,5-disubstituited-1,3,4-oxadiazoles congeners have emerged as powerful and interesting fluorescent motifs, owing to their (electro)luminescent properties and high chemical or thermal stability extremely valuable for fabrication of OLEDs [1]. The specific molecular architecture emphasizes the ability to function as acceptors unit in a Donor-Acceptor systems, therefore allowing modulation of emissive properties through different processes such as TADF or ESIPT [2].

The synthetic methodology for designing 2,5-disubstituted-1,3,4-oxadiazoles has evolved from classical reactions such as oxidative or dehydrative cyclization to more complex strategies involving cross-coupling reactions. Oxidative cyclization of N-acylhydrazones in presence of molecular iodine and potassium carbonate or hypervalent iodine reagents is very efficient for the oxadiazole ring closure, due to its reproducibility and high yield [3].

Herein, we describe the gram-scale synthesis of oxadiazole-pyrene fluorophores grafted with different functional groups and their structural characterization by NMR spectroscopy.

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Study on the Valorization of Various Conifer Vegetative Parts and the Influence of Conventional Fat Replacement on the Structural Behavior of a Dutch Waffle During the Technological Process Dynamics

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Dutch waffles (Stroopwafels) are highly appreciated pastry products due to their distinct sensory profile; however, their technological process involves a significant amount of saturated fats, essential for ensuring a tender texture and structural stability. The objective of this study is to improve the nutritional and functional profile of these waffles by partially or totally replacing conventional fats with structured lipid systems (sunflower oil-based oleogels) and fortifying them with bioactive compounds extracted from the vegetative parts of conifers: Silver Fir (Abies alba Mill.), Scots Pine (Pinus sylvestris L.), Norway Spruce (Picea abies L.), and European Larch (Larix decidua). These conifer vegetative parts are rich in phenolic compounds, which can provide the final product with high antioxidant activity and health-promoting properties. In this context, specific extraction methods were established, and the total phenolic content and antioxidant potential were quantified in the powders, the resulting doughs, and the final Dutch waffles. Furthermore, the influence of replacing traditional fat was analyzed in terms of texture, color, and viscosity parameters, as well as through fat content analysis.

Zn(II) complexes with tripodal imino/amino ligands

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Schiff condensation reactions are a highly efficient method for obtaining extended organic moieties in mild conditions. The substituents on the carbonyl and amino reactants can be widely varied with consistently high yields for the resulting imine.

In this study, we obtained tripodal Schiff base ligands from the pyridine carboxaldehydes and tris-(2-aminoethyl)amine. A series of Zn(II) complexes was synthesised using the imino and reduced amino ligands and characterised by single-crystal X-ray diffraction and NMR, FTIR, UV-visible spectroscopy. Single-crystal X-ray diffraction was employed in order to reveal the conformation of the ligand and the geometry of the central metal ion. Zn(II) ions adopt trigonal-bipyramidal geometries with variable axial ligands or octahedral geometry in the case of the imino ligand obtained from the 2-pyridine carboxaldehyde (Figure 1). We intended to study the influence of the axial co-ligand on the preferred conformation of the tripodal ligand using non-covalent interactions (hydrogen bonding, halogen-π interactions).

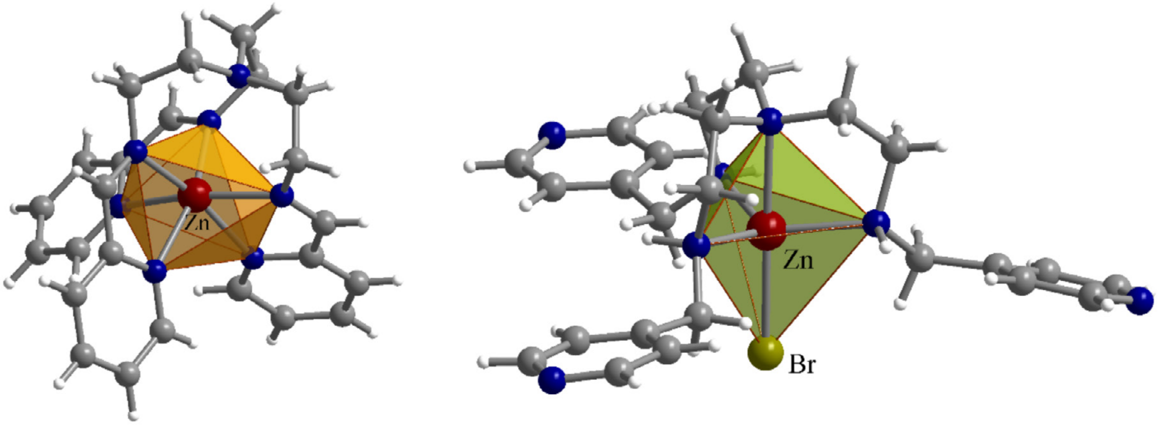

Figure 1. Crystal structures of two Zn(II) complexes obtained using imino and amino tripodal ligands

Oxidative Degradation Of Organic Compounds Over Mn/Ce Or Co/Ce-Type Layered Double Hydroxide Catalysts

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The removal of organic pollutants from wastewater remains a critical environmental challenge. Although many organic compounds do not affect aquatic life, antibiotics such as sulfanilamide (SA) significantly contribute to bacterial resistance, thereby complicating treatment. This research aims to investigate SA degradation in aqueous solutions using hydrogen peroxide (H_2O_2) as the oxidizing agent and manganese/cerium (Mn/Ce) or cobalt/cerium (Co/Ce) layered double hydroxide (LDH) as catalysts. It was assumed that these solids might have an enhanced activity due to a combined effect between the high oxygen storage capacity of Ce^{3+} and the redox properties of Mn^{2+} or Co^{2+} cations.

For this study, four catalysts Mn/Ce LDH (Mn6.4Ce, Mn4Ce, Mn3Ce with Mn/Ce ratios 6.4:1, 4:1, and 3:1) and Co/Ce LDH (Co4Ce; Co/Ce 4:1) were synthesized via co-precipitation at pH 10. The materials were subsequently characterized using XRD, DRIFT and DR-UV-Vis techniques. Degradation experiments of an aqueous solution of SA (0.1 mM) were conducted at room temperature and atmospheric pressure, either under conventional stirring or ultrasonication, at 64 molar ratio H_2O_2/SA. Mn6.4Ce and Co4Ce catalysts (1g/L) allowed reaching higher conversions of SA (e.g. 22-25%) at H_2O_2/SA=64, after 2 - 3 h under conventional stirring or 1 h under ultrasonication. The comparison of XRD patterns, DRIFT and DR-UV-Vis spectra before and after reaction showed that Mn6.4Ce was less affected than Co4Ce. The findings presented have significant implications for the characterization of the newly synthesized Mn/Ce and Co/Ce LDH catalysts, particularly regarding their impact on sulfanilamide mineralization, offering a promising new path for keeping our water supplies safe from pharmaceutical pollution.

Sea Buckthorn Berries – Valuable Source of Natural Flavonoids

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Hippophae rhamnoides (*Elaeagnaceae* fam., Sea buckthorn) berries are very nutrient-dense, containing nearly 200 bioactive compounds, including: vitamins (vitamin C, vitamin E), carotenoids (lycopene, β-carotene), carbohydrates (glucose, fructose), essential fatty acids (Omegas 3, 6, 9), phenolic acids (gallic acid, ferulic acid), flavonoids (isorhamnetin, quercetin, kaempferol), flavones, proanthocyanidins (prodelphinidin) and tannins, phytosterols, minerals (potassium, calcium, magnesium), fiber etc.

The total flavonoid content (FLC) and antioxidant activity (AA) of four ethanolic extracts from sea buckthorn fruits were determined.

The extracts in 96% ethanol were obtained by two classical methods (maceration, MAC, and continuous extraction with the Soxhlet extractor, SOX), but also by ultrasound-assisted extraction (UAE) and accelerated solvent extraction (ASE). FLC was determined using the method with aluminum chloride. To determine the AA, the ABTS (2,2`-azino-bis (3-ethylbenzothiazoline-6 sulfonic acid)) method was applied.

The linearity of the corresponding calibration curves for the applied spectrophotometric methods was good ($r^2 > 0.99$). FLC values ranged between 52.0 ± 1.4 and 63.3 ± 4.9 µg equivalents of (-)epicatechin (EE) /mL and between 171 ± 18 and 202 ± 5.1 µg equivalents of rutin (RE) /mL. AA values ranged between 16.3 ± 1.1 and 17.4 ± 0.35 µg/mL EE and between 42.8 ± 2.8 and 45.9 ± 2.1 µg/mL RE. The extract obtained by ASE showed a high FLC and the highest AA. From this concentrated extract, a fraction enriched in E and R was obtained by preparative HPLC.

The analyzed sea buckthorn berries had a high content of flavonoids, making them a valuable source of natural antioxidants.

Study on the Bioconversion of Fruits from the Wild Flora of Romania Rich in Biologically Active Compounds and the Influence of Conventional Fat Replacement on the Structural Behavior of Cookies During the Technological Process Dynamics

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Cookies are classified as sweet pastry products and are apreciated for their sensory properties, although they may contain high levels of conventional fats. The present study aimed to valorize wild fruits from the spontaneous flora of Romania, rich in biologically active compounds, and to reformulate cookies by replacing conventional fat with oleogels obtained from sunflower oil and glycerol monostearate. In addition, flour was partially substituted with powders obtained from Rosa canina, Crataegus monogyna, Prunus spinosa in order to improve the functional value of the final product. Within the study, the oleogels were obtained and characterized in terms of structure and texture, while the reformulated products were evaluated for their main physicochemical properties, moisture and ash content, color parameters, and textural profile. Furthermore, the total polyphenol content and antioxidant capacity were determined for the plant raw materials, the resulting powders, the doughs, and the cookie prototypes. The quality of the final products was also assessed by sensory analysis, in order to highlight the influence of the oleogel and fruit powders on product acceptability. The obtained results contribute to the development of reformulated cookies with enhanced functional potential and technological properties adapted to current requirements of the food industry.

Spectrometric Analysis of Ferulic Acid

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Ferulic acid, a phenolic acid known as a strong antioxidant, commonly found in medical plants, exibits remarkable physicochemical and biological properties, making it a subject of significant interest for pharmaceutical and therapeutic applications [1].

In this study, ferulic acid spectrophotometric behaviour was investigated at different pH values. The UV-Vis absorbtion spectra revealed a large maximum in the range 286 nm-348 nm which shifts in wavelength and intensity depending on pH values. Ferulic acid spectra family recorded in Britton-Robinson buffer solutions with different pH values and in NaOH media with different concentrations, presented an isosbestic point which enable the calculation of pKa =8.83. This value is in accordance with those reported in the literature for the deprotonation of the phenolic OH groups. Absorption was highest in 0.5M NaOH solution. The absorbance of ferulic acid solutions in 0.5 M NaOH medium varied linearly with the analyte concentration in the range 5.16×10^{-6} –7.73×10^{-5} M. Applying the optimized analysis conditions, ferulic acid was quantified in a commercial cosmetic product (Elemental Ferulic Acid). Recovery tests using calibration curve and standard addition methods, showed a good percentage values (108.26% and 102.36% for calibration curve and standard addition method, respectively). Ferulic acid was also investigated and determinated in presence of Curcumin. Recovery tests using the calibration curve method, absorption additivity and derivate spectrometry, showed a better recovery for derivate spectrometry (103.25%) compared to calibration curve (268.04%).

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Synthesis, structural characterization, and cytotoxic analysis on ***Saccharomyces cerevisiae*** of new copper (II) complexes with mixed ligands: acrylate anions and 5,6-dimethylbenzimidazole

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Synthesis and structural characterization of copper (II) complexes represent a major interest in contemporary coordination chemistry due to the high pharmacological potential derived from the synergy between the metal ion and organic ligands. Benzimidazole derivatives, specifically 5,6-dimethylbenzimidazole, are known for their ability to mimic essential biostructures and modulate enzymatic activity, providing metal centers with structural versatility that facilitates interaction with biological targets [1]. The use of copper, an essential element in cellular redox processes, allows the design of cytotoxic agents capable of inducing controlled oxidative stress, making these complexes promising candidates for developing new anti-fungal or antitumor therapies based on specific molecular mechanisms of action [2].

This work integrated coordination chemistry with cellular biology through the structural characterization and optimization of copper (II) acrylate complexes with 5,6-dimethylbenzimidazole. Beyond having obtained and structurally characterized three pure compounds, the research had evaluated their cytotoxicity using *Saccharomyces cerevisiae* as a model system. By utilizing specific oxidative stress-response mutants (ΔYAP1, ΔSKN7, ΔMSN2, ΔSOD1, ΔSOD2), I had aimed to delineate the intracellular interactions of the copper-ligand complexes and identify the biochemical pathways leading to programmed cell death. Furthermore, agarose gel electrophoresis had been employed to investigate DNA-binding affinity, providing insights into their potential genotoxicity and molecular targets.

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Thermal analysis as a controlled synthesis method for catalytic materials: the Cu-Zn-Al system targeting CO_2 valorization to methanol

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According to the 2025 statistics, human-induced CO_2 emissions exceeded 43 billion tons, a steep rise representing the double of 1970's [1]. This surge has a profound impact on global warming, climate change, and the frequency of extreme weather events. To address this, the concept of a circular carbon economy was introduced. Provided that H_2 is sourced from water electrolysis powered by the increasing amount of renewable electricity [2], this approach involves using CO_2 as a feedstock for large-scale catalytic hydrogenation processes to high-interest bulk chemicals:

CO_2→(Sabatier methanation)→CH_4
CO_2→(Reverse Water-Gas Shift)→CO→(Fischer-Tropsch)→C_xH_y fuels
CO_2→(catalytic selective reduction)→"green" CH_3OH

Sustainable CO_2 valorization to methanol is motivated by the roles of CH_3OH as chemical feedstock (to formaldehyde, acetic acid but most notably plastics by MTO-Methanol To Olefins), green energy carrier and also by the increasingly attractive economic feasibility of ICCU-Integrated Carbon Capture and Utilization processes [3]. An efficient catalytic system for CTM-CO_2 To Methanol is the $Cu/ZnO/Al_2O_3$ family of materials [4].

The present study aims to prepare such composite materials using inexpensive sources such as commercial thermally resistant paint (AlOil:Al + mineral oil), Cu and Zn acetates and stearic acid. The first step consists in the direct Cu- and Zn-stearates ($CuST_2$, $ZnST_2$) molten phase synthesis, followed by the preparation of the waxy precursor mixtures ($CuST_2$ -AlOil, $ZnST_2$ -AlOil, $CuST_2$ -$ZnST_2$ -AlOil). Controlled thermal decomposition in static air of specific amounts of waxy precursors (monitoring the weight loss/thermal effects) allow the precise synthesis of catalyst batches ready to be tested in the CO_2 to CH_3OH reduction.

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One-Pot Synthesis of Enzyme@ZIF-8 Biocatalysts: Structural and Catalytic Evaluation

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Metal-organic frameworks (MOFs) are porous materials with high surface area, tunable structure and good potential for enzyme immobilization. Among them, zeolitic imidazolate framework-8 (ZIF-8) is particularly attractive due to its mild synthesis conditions, suitable for one-pot synthesis and the good biocompatibility of Zn^{2+} ions with enzymes [1] . In this study, ZIF-8-based biocatalysts were prepared by entrapping different enzymes into ZIF-8 structure in a one-pot process,aiming to improve enzyme stability, recovery and reusability.

For the one-pot entrapment process, the linker, metal salt, and enzyme were mixed under optimized conditions. Three types of lipases, one peroxidase, one laccase, and mixtures of these enzymes were used to obtain enzyme@ZIF-8 biocomposites.

The obtained materials were characterized by IR spectroscopy (FTIR-ATR), powder X-ray diffraction (XRD) and thermogravimetric analysis (TGA-DSC) to confirm the formation of the ZIF-8 structure and to evaluate the incorporation of the enzyme. The catalytic activity was investigated using p-nitrophenyl butyrate as substrate for different lipases and ABTS for oxidoreductase and laccase. The enzyme@ZIF-8 systems were compared with the bare ZIF-8 material, and repeated reaction cycles were performed to assess their potential reuse. The results showed higher enzymatic activity for the immobilized lipases, while the immobilization efficiency and stability depended on the type of enzyme used.

Overall, ZIF-8 proved to be a promising matrix for enzyme entrapment, offering a good balance between structural protection and catalytic functionality under optimized conditions.

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Design of 1,10-phenanthroline derivatives for crystal engineering

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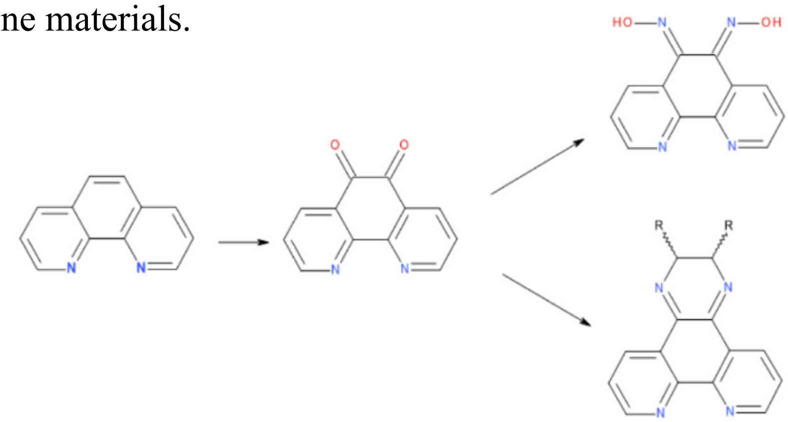
1,10-Phenanthroline derivatives are widely employed as molecular tectons in coordination chemistry and crystal engineering, owing to the combination of a rigid π-conjugated scaffold and a preorganized N,N′-chelating site. Beyond metal coordination, the extended aromatic surface of the phenanthroline core can contribute to solid-state organization through π–π stacking interactions, while suitable functionalization provides additional handles for tuning intermolecular contacts and crystal-packing preferences. In this context, carbonyl, oxime, and imine functionalities are of particular interest, as they can modulate the geometry, recognition sites, and supramolecular behavior of phenanthroline-based ligands.

In this study, 1,10-phenanthroline-5,6-dione was employed as a key precursor for the synthesis of 1,10-phenanthroline-5,6-dioxime and dihydropyrazine-functionalized derivatives. The targeted compounds were designed as phenanthroline-based tectons for crystal engineering, combining a rigid aromatic framework with coordination sites and functional groups able to support hydrogen bonding, metal binding, and π–π stacking. These features make them attractive candidates for supramolecular organization and the construction of crystalline materials.



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Comparative Study of Peptide Bond Formation for Synthesis of Membrane-Targeted Precursors for Imaging

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Electron microscopy stands as an invaluable tool across various disciplines, including materials science, cell biology, medicine or forensics duet to ability to resolve intricate details regarding the morphology, structural integrity, and precise dimensions of both biological cells and synthetic nanoparticles [1].

Advancements in electron microscopy have been shaped by the ongoing quest to selectively mark intracellular targets. The widely used immunogold staining faces technical limitations as OsO_4 often destroys antibody functionality during the fixation process. To address this, research was focused on developing alternative contrast agents that offer lower oxidative potential while maintaining high structural resolution [2]. One effective strategy for attaching transition metals involves functionalization of plasma membrane (i.e. functionalisation of choline) to facilitate conjugation of the transitions metal-ions directly to cellular membrane [3].

This work describes synthesis of a synthetic probe useful for Electron Microscopy visualization, designed to mitigate the oxidative degradation of antibody markers and bind transition-metal-ions. A comparative evaluation of the synthetic pathways was performed, focusing on peptide bond formation in both solution and solid support.

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Vibrational Spectroscopy Study of Calcium Phosphate Biomaterials for Human Tooth Analysis

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This study compares, the spectral signatures of natural dental minerals with those of synthetic calcium phosphate standards, namely hydroxyapatite (HAp) with different degrees of cristallinity, β-tricalcium phospate (β-TCP), and octacalcium phosphate (OCP). The aim of the work was to evaluate the complementary use of FTIR and Raman spectroscopy for the structural characterization of human tooth tissues and calcium phosphate biomaterials.

FTIR spectroscopy enabled the identification of the main functional groups characteristic of phosphate-based mineral phases, as well as, carbonate substitutions in the apatite lattice, evidenced by the adsorption bands around 1450 cm^{-1}. However, FTIR analysis proved insufficient for distinguishing variations in crystallinity levels and for highlighting subtle structural differences between enamel and dentin due to spectral overlap and band broadening.

Subsequent analysis using Raman microspectroscopy provided the necessary clarity, with the symmetric vibration band ν_1 PO_4^{3-} located near 960 cm^{-1} being used as the main indicator of mineral crystallinity. Results showed and ordered structure in enamel, similar to microcrystalline HAp, while dentine revealed a hybrid character, evidenced by the broadening of the ν1 phosphate band and the presence of collagen (Amides I and III). An important result obtained through Raman spectroscopy, which was undetected by FTIR due to spectral overlap, was the detection of the OCP precursor in dentin, indicated by the characteristic 1003 cm^{-1} band. The results demonstrate the higher sensitivity of Raman spectroscopy for identifying subtle structural variations and precursor mineral phases in biological hard tissues.

We acknowledge the support of the National Interest Infrastructure facility IOSIN—CETAL at INFLPR (for Raman measurements).

A thermal degradation forensic study of indigo-blue dyed cotton fabric samples

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Indigo is a blue dye originally extracted from the leaves of *Indigofera genus* plants several millennia ago. Its rare blue colour was once an exclusivist luxury distinction affordable only to the high class of the Roman or Greek societies. The industrial synthesis of indigo originates from the late 19th century Germany as an answer to the high interest for this vibrant blue. That historical period coincided with the introduction, by an American manufacturer, of wear-resistant rivet-reinforced utility jeans, tailored from an undyed white-cream "denim", a resilient textile fabric from Nimes, France. Altering the original color of the denim with synthetic indigo was an inexpensive way to improve the dirt-resistance aspect of the "blue jeans". Their popularity boosted tremendously, becoming now the undisputed most worn garment (jeans, jackets, vests, shirts, etc.), as well as an important fabric for forensic investigations.

The present study focused on investigating the resilience of indigo dyed onto cotton, specifically through thermal degradation of the fabric, an aspect which would potentially allow the forensic identification of burnt fabrics used in various fire settings (e.g. arson). For this, raw cotton was processed by pre-washing to remove waxes, followed by vat-dyeing using a fructose vat, drying, rinsing, and re-drying. It was observed that the dyed fabrics could be easily extracted via DMSO. These extracts, along with the extracts of the thermally-degraded samples, were analyzed via reversed-phase liquid chromatography using a diode array detector, to see whether Indigo was still observable. Further, the study also investigated the extracts to see whether, where indigo was no longer observable, cyanuric acid had formed.

Controlled thermal degradation experiments were performed while monitoring the mass loss and the amplitude of the thermal effects by using a thermobalance. Each textile sample was rolled and placed in an alumina crucible and subsequently heated with several programmed linear heating profiles in static air atmosphere. The thermal analysis investigation included series of raw, post-wash and indigo dyed cotton fabric samples.

Blue textile fiber dye extraction methods and their analysis via liquid chromatography with DAD detection in a forensic science context

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Textile fiber evidence plays a well-established role in forensic science, with dye composition representing one of the most discriminating characteristics for fiber comparisons. Blue cotton fibers present a particular analytical challenge due to their morphological uniformity and high prevalence in the general textile population. The current ASTM E2227-23 standard addresses forensic dye analysis through thin-layer chromatography, whose sensitivity and resolving power are insufficient for comprehensive profiling of blue dyes used for cotton.

This study evaluated three extraction systems: organic (DMSO), acidic (HCl 3M) and alkaline (NaOH 1.5%) applied to ten cotton textile samples by HPLC-DAD, assessing the potential to differentiate between extracts by following a barcode logic in which the chromatographic peak profile of each extract serves as its chemical fingerprint. No analytically significant signals were obtained from DMSO extracts. Extracts obtained with HCl 3M and NaOH 1.5% resulted in partial differentiation, but both destroyed the chromophores, yielding degradation products rather than identifiable dye molecules.

The findings identify the trade-off between extraction efficiency and chromophoric integrity as the central methodological obstacle and highlight a fundamental limitation of reversed-phase chromatography for this sample type. Together, these findings provide an empirical starting point for the development of optimized forensic HPLC-DAD methods for blue cotton fiber dye analysis.

Synthesis of Positively Charged 1,3,5- Triazines for DELs

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The rapid discovery of new cellular mechanisms of different diseases has led to a great number of possible proteins and enzymes that can be targeted using small molecular compounds [1]. A recent and convenient method for screening different varieties of compounds represented of DNA-encoded libraries (DELs), a combinatorial method consisting in simultaneously adding different substituents and a corresponding oligonucleotidic sequence to a scaffold. After the selection process, the obtained DNA sequence is read as a "barcode", and the corresponding small molecule is obtained [2]. 1,3,5-triazine moiety is very useful for developemnts of DELs due to the facile synthesis starting from cyanuric chloride and high regioselectivity of each step depending on the reaction conditions [3].

Therefore, in this work we present synthesis of a trisubstituted 1,3,5 trazine, containing one aromatic and positively charged substituent at physiological pH, that can serve as a model for creation of DELs targeting cellular targets that contain anionic sites that have affinity for aromatic moieties.

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A preliminary study of Surface-Enhanced Raman Scattering of silver nanoparticles dispersions on polymer surfaces

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Raman spectroscopy is a powerful non-destructive vibrational technique for molecular identification, yet its inherently weak scattering cross-section limits sensitivity at low analyte concentrations. Surface-Enhanced Raman Scattering (SERS) overcomes this limitation by placing target molecules near plasmonic metallic nanostructures, where localized surface plasmon resonance (LSPR) generates intense electromagnetic fields that amplify the Raman signal by several orders of magnitude. Silver nanoparticles (AgNPs) are among the most widely investigated SERS substrates due to their strong plasmon resonance in the visible range and large scattering cross-sections.

Two types of SERS substrates were evaluated: thin solid films formed by depositing AgNPs dispersions onto polypropylene (PP) surfaces, and liquid-phase colloidal mixtures prepared by combining AgNPs dispersions with a Rhodamine 6G (Rh6G).

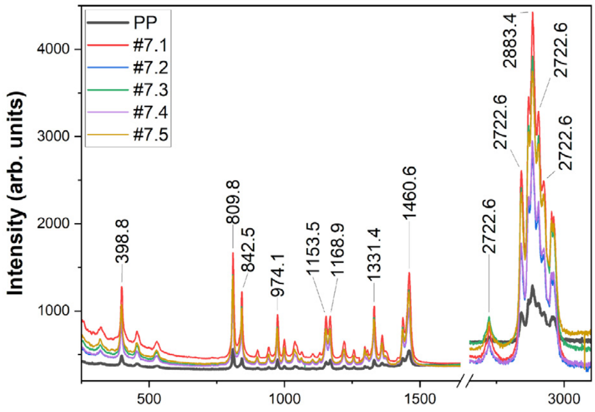

Figure 1. SERS effect on PP using AgNPs at 785 nm excitation laser wavelength

SERS enhancement was observed exclusively at 532 nm and 785 nm excitation. These findings highlight that both the nanoparticle size and the excitation wavelength must be carefully matched to achieve effective plasmonic hot-spot generation.

Valorization of PET Waste through Upcycling into MOF-Based Biocatalytic Materials

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Chemical valorization of poly(ethylene terephthalate) (PET) waste represents a promising strategy for the sustainable production of value-added materials. In this study, post-consumer PET was depolymerized by alkaline hydrolysis in a hydroalcoholic medium to recover terephthalic acid (TPA), a valuable precursor for the synthesis of metal–organic frameworks (MOFs). Different reaction parameters, including base concentration and ethanol content, were optimized, with particular attention given to the recycling and reuse of solvents and reactants in order to develop a more sustainable process while maintaining a quality of the recovered TPA comparable to pure commercial material.

The recovered TPA was subsequently used as an organic linker for the synthesis of zirconium-based UiO-66 MOFs. The obtained MOFs were further employed as supports for the immobilization of lipase from *Candida rugosa* by entrapment (Figure 1).

The recovered TPA, MOFs, and enzyme-containing biocomposites were characterized by FTIR-ATR spectroscopy, powder X-ray diffraction (XRD), thermogravimetric analysis (TGA–DSC), and HPLC analysis. The results demonstrated the successful recovery of terephthalic acid and the synthesis of UiO-66 materials with high yields through a sustainable process.

Moreover, the UiO-66@enzyme biocomposites demonstrated good catalytic activity, with the materials prepared from PET-derived TPA presenting even higher enzymatic activity compared to those obtained from commercial terephthalic acid.

Figure 1. Schematic Pathway of PET Upcycling into Biocomposites.

Synthesis and Structural Diversity of Organotin(IV) Compounds Derived from Terephthalate Ligands

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Organotin(IV) compounds represent an important class of organometallic systems due to their remarkable structural versatility and notable physicochemical and biological properties. The flexible coordination behavior of Sn(IV) centers, together with the bridging ability of multifunctional ligands, enables the formation of both discrete complexes and extended coordination architectures. In this study, a series of organotin(IV) compounds based on terephthalate derivatives were synthesized and structurally characterized.

The synthesized compounds were obtained using terephthalic acid and 2-aminoterephthalic acid as coordinating ligands. Depending on the reaction conditions and the presence of additional divergent diamine ligands, both discrete zero-dimensional (0D) complexes and one-dimensional (1D) coordination polymers were formed. The synthesized compounds were characterized by FT-IR spectroscopy, powder X-ray diffraction, and single-crystal X-ray diffraction. Structural analyses revealed the influence of the terephthalate and diamine linkers on the organization and dimensionality of the resulting architectures. The terephthalate derivatives act as bridging linkers between the Sn(IV) centers, leading to the formation of dinuclear units, while in the presence of diamine ligands, both types of linkers alternate within the coordination framework, generating extended 1D polymeric architectures.

The present study provides further insight into the structural chemistry of organotin(IV) coordination compounds and demonstrates the important role of terephthalate derivatives and divergent diamine ligands in directing the assembly of discrete and polymeric organometallic frameworks.

Hexanitrometalates. Structural and Thermal Analysis

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The hexanitrometalates represent an interesting class of coordination compounds in which a central metal ion is surrounded by six nitro (NO_2^-) ligands, typically forming octahedral complex anions of the general formula $[M(NO_2)_6]^{n-}$ (Fig.1a). Structurally, these complexes present a cubic crystal structure where nitro-nitrito isomerism [1] and lattice packing effects like the Jahn-Teller effect can influence their properties [2,3].

This study aims to expand the already existing poor library of hexanitrometalates by providing a deep dive into the structure and thermal behaviour of three series of hexanitrometalates, classified by their counter-ions (Fig.1b). The compounds were characterized by UV-VIS spectroscopy, Fourier transform infrared spectroscopy (FTIR), single-crystal (SCXRD) and powder X-ray diffraction (PXRD). Their thermal behavior was studied using Thermogravimetry/Differential scanning calorimetry (TG/DSC) up to 1000^{O}C in air. Variable temperature FTIR spectra up to 300^{O}C, indicate transformations related with a reversible nitro-nitrito isomerism. This research area lies at the intersection of coordination chemistry, solid-state chemistry and molecular magnetism, with ongoing interest in understanding metal–nitro bonding modes and electronic structure.

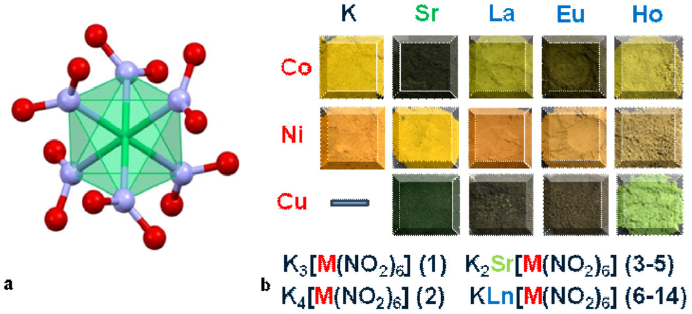

Fig. 1. Synopsis including: (a) Molecular structure for $[M(NO_2)_6]^{n-}$, showing Th symmetry. (b)The formula and colors for the synthesized compounds

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The Influence of Coordinated Anions on the Structure and Properties of Mn(III) Complexes with Schiff Bases

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Manganese(III) complexes with salen-type ligands (salen: N,N'-bis(salicylidene)ethylenediamine), represent a prominent class of coordination compounds, widely studied in coordination chemistry, molecular magnetism, and medicinal chemistry [1].

Research in this area focuses on how axial anions influence the electronic structure, magnetic anisotropy, and intermolecular exchange pathways [2]. Magnetically, Mn(III)salen complexes commonly exhibit high-spin d^4 configurations (S=2) and can form single-molecule magnets (SMM) [3] or magnetically coupled assemblies in polynuclear systems [4].

The aim of this work was to synthesize and characterize a new series of Mn(III) complexes with Schiff base ligands, in order to investigate the influence of different coordinated anions on their structure and properties. While $[Mn(salen)Br]_2$ **(1)** is a dimeric structure (Fig.1a), the other two compounds $[Mn(salen)(\mu\text{-}CH_3COO)]_n$ **(2)** (Fig.1b) and $[Mn(salen)(\mu\text{-}NO_2)]_n$ **(3)** (Fig.1c) are polymeric structures with only one {Mnsalen} complex unit repeating in the chain. All Mn(III) complexes were characterized by the UV-VIS and FTIR spectroscopy and crystallographic studies. The magnetic measurements and the electronic structure calculations are ongoing work.

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Spin States and Crystal Field Effects in New Fe(II) Complexes

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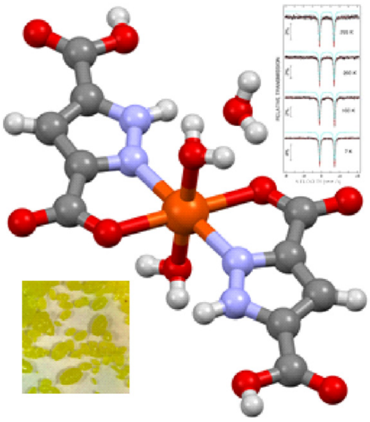
Five-membered aromatic heterocycles containing nitrogen atoms are a class of compounds, which afford different derivates of various field strengths. Among these derivatives, pyrazoles are by far the most accessible and act as versatile ligands in coordination compounds [1]. Iron complexes with pyrazole-based ligands represent an interesting research area within coordination chemistry and molecular magnetism, particularly due to their ability to exhibit spin-state variability. These systems typically involve Fe(II) centers coordinated in octahedral geometries, being highly sensitive to ligand field strength. The spin transition (ST) represent the switching of the metal ion spin state between a low spin (LS) and high spin (HS) configuration under the influence of an external stimulus. This process is highly cooperative, depending on the packing and being initiated by a vibration in the crystal lattice [2,3].



This work focuses on the synthesis and characterization of several new complexes. The compounds $[Fe^{II}L_2(H_2O)_2]$ (where L =4H-pyrazole-3,5-dicarboxylic acid for **1** or L = 4-nitro-pyrazole-3,5-dicarboxylic acid for **2**) are useful precursors. Since the water molecules can be replaced with different anions or complex ligands, the resulted compounds allow the study of the axial ligands influence on the Ligand Field. The compounds were characterized by Fourier Transform Infrared spectroscopy, electronic and Mössbauer spectroscopy and single-crystal X-ray diffraction. The structural analysis is completed by electronic structure calculations, in order to test the spin states of the studied systems.

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Section 2

Master
Level

Comparative structural study of collagen from animal sources by FTIR and FT-Raman spectroscopy techniques

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The present work evaluates the structural profile and conformational stability of 7 collagen samples extracted from various sources such as sturgeon, bovine, and rabbit and differently conditioned. Given the widespread use of these biomaterials in pharmaceutical and dermato-cosmetic formulations, a precise understanding of their molecular architecture is an essential step.

The characterization of the samples was mainly performed by Attenuated Total Reflection Fourier Transform Infrared spectroscopy (ATR-FTIR), and complemented by FT-Raman and micro-ATR-FTIR techniques for a detailed evaluation of structural homogeneity at the microscopic level. Data processing included the application of the Levenberg-Marquardt algorithm for the mathematical deconvolution of the amide regions, focusing on the Amide III band (1200–1300 cm^{-1}), a region highly sensitive to conformational changes in the triple helix.

The data obtained by FTIR spectroscopy confirm the preservation of the basic collagen architecture in all samples but highlight clear differences depending on the species and the type of physical conditioning (pearls/beads compared to flakes). Following the deconvolution of the Amide III band, the bovine collagen (pearl type) showed the highest stability of the triple-helix structure, with its profile being dominated by the 1233 cm^{-1} component (in a proportion of approximately 60%). In contrast, the marine-derived samples exhibited slightly shifted maxima (1228–1229 cm^{-1}) and a different profile of C–N vibrations, suggesting greater chain flexibility. At the same time, it was observed that the materials in the form of pearls present a much more compact molecular organization compared to the flake-type samples, where the fiber orientation appears more variable.

To complete this picture, the integration of Raman and Micro-FTIR data aims to confirm the conformational stability and evaluate the homogeneity of the samples. The correlation of these spectroscopic techniques allows for a fine differentiation of collagen types, providing extremely useful information for selecting the optimal source according to the specific requirements of the cosmetic and pharmaceutical industries.

The hydrodeoxygenation (HDO) of benzyl alcohol on noble metal-transition metal mixed oxides

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The catalytic hydrodeoxygenation (HDO) of oxygenated compounds derived from lignocellulosic biomass represents a key strategy for the production of sustainable fuels and valuable chemicals. In this study, benzyl alcohol was employed as a model compound to investigate the performance of transition and noble metal-based catalysts in the selective removal of oxygen, targeting toluene as the main product.

A series of mixed oxide catalysts were synthesized via co-precipitation, using layered double hydroxide (LDH) precursors, followed by calcination. Three different noble metals were investigated under comparable conditions: platinum (Pt), palladium (Pd), and ruthenium (Ru). They were used together with Mg, Fe and Cu nitrates to obtain mixed LDH precursors. All catalysts were prepared using the same synthesis protocol and subjected to identical characterization techniques and catalytic testing conditions to ensure a consistent comparison. The catalytic performance was evaluated in the hydrodeoxygenation of benzyl alcohol in a batch autoclave reactor at 230 °C under 5 atm hydrogen pressure. The reaction products were analyzed by gas chromatography, allowing the determination of conversion and selectivity. The main products identified were toluene, benzaldehyde, benzene, and benzyl benzoate.

Among the investigated systems, palladium-based catalysts exhibited the highest catalytic performance, achieving nearly complete conversion (up to ~99%) and high selectivity towards toluene (up to 87.3%). Platinum-based catalysts showed superior intrinsic selectivity at low metal loading but significantly lower conversion, limiting the overall yield. Preliminary catalytic results for ruthenium-based samples are in progress. The results highlight the strong influence of the nature of the noble metal on both activity and selectivity in the HDO reaction. Palladium catalysts provide the best balance between high conversion and selectivity, making them the most promising candidates for this efficient biomass valorization processes.

Electrochemical Biosensors Based on Self-Assembled Monolayers

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Ascorbic acid is essential for human health due to its antioxidant activity and its roles in collagen synthesis, immune support, tissue regeneration, and wound healing. Monitoring ascorbic acid levels in food products and biological samples is important for assessing nutritional status and preventing deficiencies [1]. Electrochemical methods provide highly sensitive detection of ascorbic acid, enabling quantification at low concentrations and making them suitable for pharmaceutical and food quality-control applications [2].

In this study, the complex dicarbonyl(η^5-cyclopentadienyl)(κN-maleimidato)ruthenium(II) was immobilized onto a peptide self-assembled monolayer (SAM)-coated gold electrode to improve the electrochemical detection of ascorbic acid under different pH conditions over a concentration range of 300 µM to 10 mM. Electrode surface functionalization is critical for enhancing biosensor performance. Peptide SAMs were used as immobilization platforms for the ruthenium complex, enabling efficient electron transfer and improved electrochemical detection. The presence of the ruthenium complex also increased the stability of the peptide SAM, leading to enhanced sensor reproducibility and stability. Maleimide derivatives selectively react with amino groups in proteins and peptides, forming stable covalent bonds that improve biosensor stability, reproducibility, and antifouling properties by reducing nonspecific adsorption [3].

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Modified Ex-LDH Mixed Oxide Catalysts for Methane Emissions Abatement

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Methane serves as a critical target for environmental catalysis, acting as a potent greenhouse gas with high global warming potential and as a primary pollutant in industrial emissions. Due to its high stability, methane also serves as a model molecule for evaluating the efficiency of VOC abatement. Layered Double Hydroxides (LDH) are a class of materials characterized by a unique brucite-like stacked structure that enables high metal dispersion, compositional versatility and high surface area. These materials act as an excellent platform for creating highly active and robust mixed oxides catalysts through the integration of various transition metal cations.

In the present work, the synthesis of Mg-Al and Ca-Al mixed metal oxides was realized through the co-precipitation and calcination of LDH precursors. During the co-precipitation stage, copper was successfully incorporated into the brucite layers as a partial substitute for the divalent Mg^{2+} and Ca^{2+} cations resulting in Cu(15%)MgAlO and Cu(15%)CaAlO heterostructures. The best performing catalyst of the series for methane combustion was further modified with various NaOH and HCl etching procedures to promote the formation of point defects, increase lattice oxygen mobility, and expose additional active catalytic sites.

The catalysts were characterised by several techniques including X-Ray diffraction, N_2 adsorption-desorption and temperature-programmed reduction that proved the presence of highly crystalline materials with small crystallite size. The modified catalysts presented conversions of methane at significantly lower temperatures compared to their unmodified counterparts and demonstrated superior stability over longer operational times.

Synthesis and magnetic properties of a family of dinuclear lanthanide complexes derived from 2-(phthalimidomethyl)-nitronyl-nitroxide

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Nitronyl-nitroxides have a rich coordination chemistry, allowing the synthesis of complexes with various spin topologies that show intriguing magnetic properties. While most radicals reported in the literature are obtained starting from the corresponding aldehydes [1], methods of grafting the nitronyl-nitroxide moiety onto a substrate have also been described [2], benefiting from simpler procedures and higher yields. This work focuses on the paramagnetic ligand obtained through the alkylation of phthalimide with 2-(chloromethyl)-nitronyl-nitroxide [1]. Its coordination versatility afforded two structural families of complexes (Figure 1): mononuclear transition metal (Ni^{II}, Co^{II}) complexes with two radical molecules bound to the metal ion, and dinuclear lanthanide (Pr^{III}, Nd^{III}, Eu^{III}, Gd^{III}) complexes with the radical moiety acting as a bridge. The structures of the ligand and complexes were solved by single crystal X-ray diffraction measurements. The magnetic properties of the second family have been investigated, revealing, in the case of the gadolinium complex, a ferromagnetic interaction (J_1 = 13.63 and J_2 = 0.21 cm^{-1}, $-J_{12}S_1S_2$ convention).

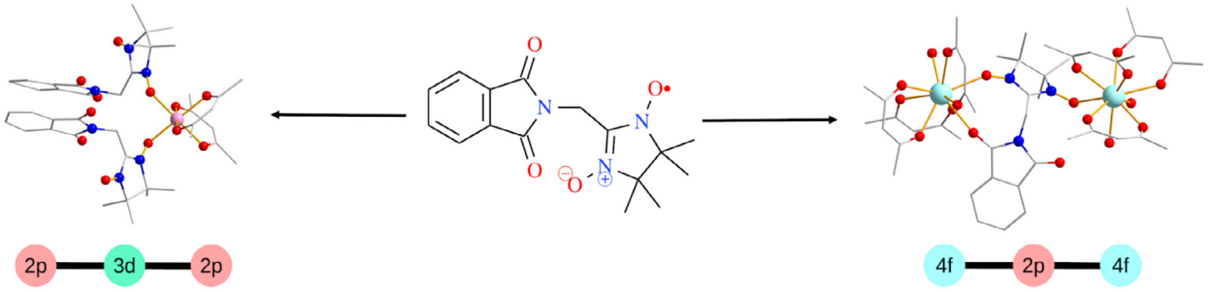

Figure 1. The structure of 2-(phthalimidomethyl)-nitronyl-nitroxide and its complexes.

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Heterodiradical ligands and their complexes

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The development of molecular magnetic materials has gained significant interest due to their potential applications in high-density data storage, quantum computing, and molecular spintronics [1]. Among strategies for designing such materials nitronyl nitroxide (NN) radicals have proven highly effective. Their coordination versatility allows strong magnetic coupling, and their functionalization enables bridging of multiple metal ions, leading to molecular assemblies with different spin topologies and dimensionalities [2].

Herein, we report the synthesis of a heterodiradical (**HL^1**) incorporating both NN and TEMPO radical moieties. The heterodiradical was further used as a paramagnetic ligand in the synthesis of three mononuclear Mn(II), Ni(II) and Tb(III) complexes, $[M(L^2H)(hfac)_3]$, respectively $[Tb(L^2H)(hfac)_3]$, using $[M(hfac)_3(H_2O)_2]$ and $[Tb(hfac)_3(H_2O)_2]$ precursors (where M = Mn, Ni). The previously reported heterodiradical (HL^1) was used as a ligand in the synthesis of a new trinuclear Tb(III) complex, $[Tb_3(L^1H)_2(hfac)_9]$ (Figure 1). Their structures were determined using X-ray diffraction measurements.

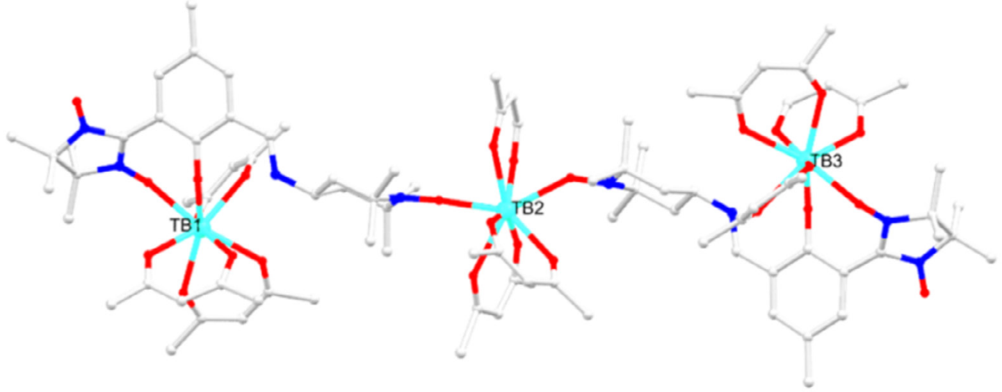

Figure 1. X-ray structure of the trinuclear complex $[Tb_3(L^1H)_2(hfac)_9]$ obtained from the ligand HL^1. Fluorine and hydrogen atoms have been omitted for clarity.

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Synthesis of copper-chelating azides for biochemical applications

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Owing to their ability to undergo copper(I)-catalyzed [3+2] cycloaddition reaction (CuAAC or "Click" reaction), azides have become versatile building blocks for synthesis of 1,2,3-triazole cores under mild and biocompatible conditions [1]. Copper-chelating azides are very valuable in CuAAC chemistry because they stabilize Cu(I) species, suppress disproportionation, thereby enhancing reaction rate under mild conditions. Moreover, copper-chelating azides combine chemical stability with bioorthogonality, enabling their selective incorporation into complex biological systems for efficient bioconjugation and labeling [2,3].

Herein, we describe synthesis and spectral characterization of several copper-chelating azides aimed for various "click" reaction-based biomedical applications. The reported compounds were purified and structural characterized.

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The Fenton reaction – an environmentally friendly alternative for antibiotic decontamination in wastewaters

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This study aims to develop and optimise an efficient and environmentally friendly alternative for antibiotic decontamination in hospital wastewaters using the Fenton reaction. This method consists in the formation of highly reactive HO• radicals in the reaction between H_2O_2 and Fe_2SO_4 in acidic medium. Moxifloxacin (MOX) was chosen as a class representative given the large quantities detected in hospital wastewaters [1] and the lack of studies regarding degradation of this particular compound. Continuous exposure to fluoroquinolones has been associated with antibiotic resistance [2].

First step was to determinate the optimal reagent ratio for maximum degradation efficiency by measuring the decrease in absorbance at 295 nm in batch reactions. The same data was collected using a special rapid mix accessory, that can register the sudden drop in absorbance in the first 10 seconds of the reaction. This data was then used in kinetic modelling. The maximum degradation efficiency was obtained for an initial molar ratio $MOX/Fe_2SO_4/H_2O_2$ of 1/2/500; at higher Fe_2SO_4 and H_2O_2 concentrations the reaction is inhibited. The oxidation process can be described by two consecutive first order reactions; the first one, exhibiting a higher rate represents the interaction between MOX and HO• radicals. The reaction was then carried out in a complex matrix simulating the components present in hospital wastewater. The greatest impact on degradation efficiency was observed for NaCl, with an increase of more than 50%. Samples were collected at different times during the degradation process and analysed by HPLC-MS technique to identify the degradation products obtained.

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Voltammetric Investigation of Nitrazepam

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Nitrazepam (NZP) is a benzodiazepine (BZD) drug used as a hypnotic, tranquilizer and anticonvulsant [1], often prescribed in anxiety and insomnia, due to its long duration of action [2]. Plasma determination of NZP is essential for monitoring the treatment, especially in elderly and epileptic patients [1]. Since BZDs, including NZP; are frequently used as date-rape drugs there has been a need to develop reliable and rapid methods for their detection [3].

BZDs are electroactive because they contain the >C=N group that can be reduced. Moreover, NZP contains an electro-reducible -NO_2 group. Therefore, we investigated its voltametric behaviour at a pencil-graphite disposable electrode (PGE) using cyclic voltammetry (CV). This study emphasized a complex electro-activity demonstrated by the presence of pH-dependent signals due to the reduction of the -NO_2 group. An irreversible reduction peak was observed at more negative potentials, which was used for further studies, as well as a pair of peaks at less cathodic potentials. Differential pulse voltammetry (DPV) was employed for NZP quantification in optimized conditions (HB type PGE, phosphate-buffer solution pH 7.50). A linear dependence between the cathodic peak current and NZP concentration was observed in the range $2.45 \times 10^{-6} - 9.75 \times 10^{-5}$ M. The limits of detection and quantification were 1.13×10^{-6} M, 3.76×10^{-6} M NZP, respectively.

The practical applicability of the DPV at HB_PGE method was tested by NZP quantitative determination from pharmaceutical tablets and spiked soft drinks. The recoveries ranged from 95.64 to 109.64%.

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Section 3

PhD
Level

Promising EC-SERS substrate based on silver nanoparticles for sensing applications

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Surface-enhanced Raman scattering (SERS) is a powerful tool that can be coupled with electrochemistry (EC-SERS) to provide, in addition to ultrasensitive detection, mechanistic insights into complex processes, whether biochemical or electrochemical [1]. Cost-effective EC-SERS substrates were obtained from screen-printed electrodes via drop-casting or in-situ nanoparticle generation, but reproducibility remains challenging [2,3].

To achieve reproducible, sensitive, and stable EC-SERS devices, we report the development of substrates prepared by layer-by-layer deposition of chitosan and silver nanoparticles on screen-printed carbon electrodes. SERS performance was assessed with 4-mercaptobenzoic acid, and the results showed suitable reproducibility, with RSDs of 1.91% and 9.98% for the intensities of characteristic Raman bands at 1061 cm^{-1} and 1577 cm^{-1} , respectively. Evaluation of the substrate's performance for EC-SERS was based on the fungicide thiram, as a model compound, by measuring the SERS signal during amperometry and voltammetry experiments.

This study represents a promising start toward the development of novel devices for EC-SERS-based sensing applications.

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Rational Design and Structural Investigation of Zn(II) Complexes with Polydentate Schiff Base Ligands

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The development of polydentate imino and amino ligands has played a key role in advancing the chemistry of Zn(II) coordination complexes. Derived from N-(1-naphthyl)ethylenediamine and various phenolic aldehydes, these ligands possess multiple coordination sites that enable diverse coordination modes and allow fine-tuning of the resulting physicochemical properties.

In the present work, a series of new Schiff base ligands was synthesized using N-(1-naphthyl)ethylenediamine and different phenolic aldehydes. Both the resulting imino compounds and their reduced amino derivatives were employed, either individually or together with additional chelating ligands, to obtain mono- and polynuclear Zn(II) complexes. Structural characterization of the ligands and complexes was carried out by single-crystal X-ray diffraction, highlighting the versatility of the imino and amino frameworks as well as the variety of coordination geometries and arrangements adopted by the complexes. Figure 1 illustrates the general synthetic strategy used for preparing Zn(II) complexes based on these ligand systems.

In addition, the optical behavior of the synthesized ligands and complexes in the solid state was investigated using several spectroscopic techniques. Particular attention was given to their luminescence properties, as the extended π-conjugated systems of the ligands can promote enhanced fluorescence emission.

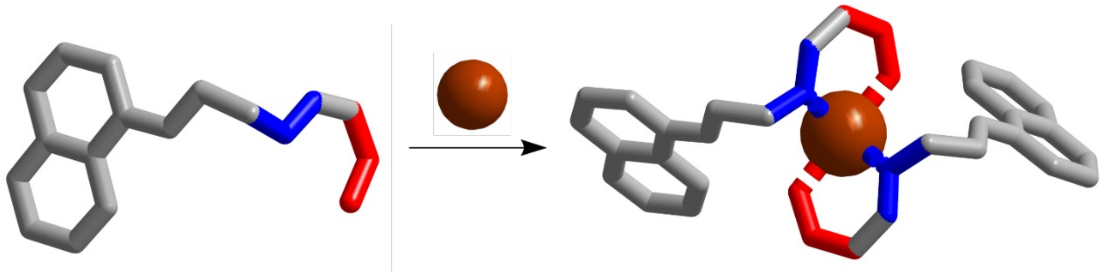

Figure 1. Schematic synthesis of 3d complexes using Schiff base ligands.

Spectroscopic characterization and electrochemical detection of PFAS contaminants using biologically synthesized gold nanoparticle-modified sensors

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Biologically synthesized nanomaterials offer green, cost-effective alternatives to traditional chemical sensors for environmental monitoring. The specific functional groups present in biological extracts serve as surface-reducing and stabilizing agents. These groups optimize the nanoparticle surface chemistry for target contaminant interaction. This study presents a sensitive detection platform for per- and polyfluoroalkyl substances (PFAS) utilizing gold nanoparticles (AuNPs) fabricated via plant-extract green synthesis.

To validate the sensor mechanism, UV-Vis spectroscopy was utilized to track the optical response and binding affinity between the green-synthesized AuNPs and PFAS. For quantitative screening, the nanoparticles were drop-casted onto commercially available screen-printed sensors. This diagnostic platform achieved a limit of detection (LOD) of 0.64 nM for perfluorooctane sulfonate (PFOS). This performance demonstrates the system's capacity for rapid, trace-level screening of persistent "forever chemicals" in threatened water supplies.

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Luminescent heteroleptic dinuclear copper(I) complexes: synthesis and characterization

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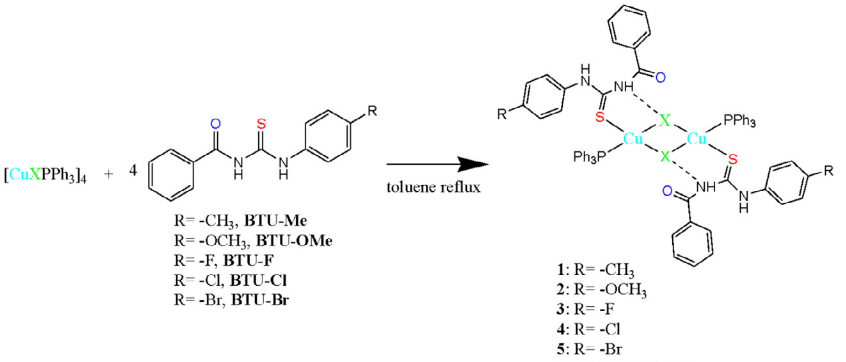
This study reports the synthesis and characterization of twelve new dinuclear copper(I) complexes combining phosphine (PPh_3) and different N-benzoyl thiourea (BTU) ligands, prepared via halogen-bridged precursors ($[CuXPPh_3]_4$, X = Cl, Br, I), as shown in the following scheme:



Scheme 1. Synthesis of copper (I) complexes discussed in this work.

Structural analyses (NMR, IR, X-ray diffraction) confirmed S-monodentate BTU coordination and distorted tetrahedral geometries, with notable emission properties in the solid state (λ_{em} = 544–588 nm) arising from mixed MLCT/LC transitions. Key complexes exhibited thermally activated delayed fluorescence (TADF) with lifetimes of 1.51–21.47 µs and quantum yields up to 2.39% (compound **4b**).

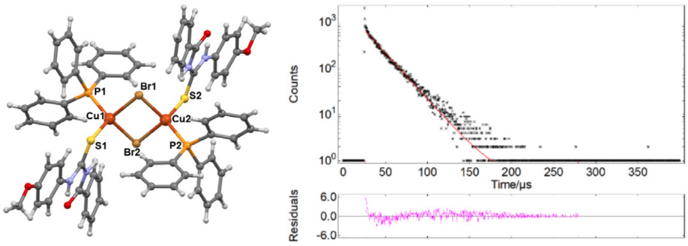


Figure 1. The asymmetric unit for **2b** with atom numbering scheme (left) and lifetime decay curve of compound **4b** (right)

These results highlight the potential of these cost-effective, luminescent Cu(I) systems for optoelectronic applications, particularly as alternatives to noble-metal-based emitters in OLEDs.

Tuning the chiroptical properties of coordination compounds using enantiopure ligands with various types of chirality

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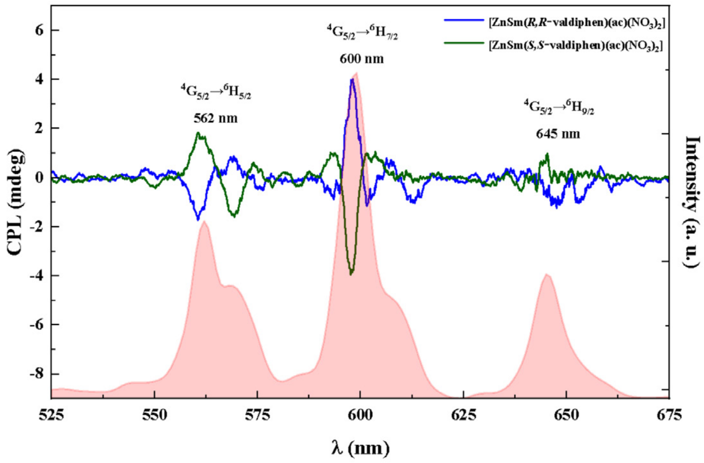
The chiroptical properties of Ln(III) coordination systems originate from parity-forbidden 4f–4f transitions with significant magnetic dipole character, the magnitude of g_{lum} being governed by the ratio of magnetic to electric dipole moments [1]. The structural modularity of coordination compounds enables efficient transfer of chiral information by employing ligands with point, axial or helical chirality within the coordination sphere. Together with the narrow emission bands of lanthanides, these features enable such systems promising for optoelectronic applications [2]. Herein, we report optically active 3d–4f coordination compounds based on enantiopure ligands, targeting controlled chirality interplay. Diamagnetic Zn(II) centers preserve 4f luminescence and facilitate ligand to Ln(III) chirality transfer, yielding circularly polarized luminescence, as demonstrated by a Zn(II)–Sm(III) enantiomeric pair (Figure 1).



[ZnSm(valdiphen)(ac)$(NO_3)_2$].

Figure 1. The CPL spectra of the enantiomeric pair (R,R) and (S,S).

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Designing a Biosensor for Herbicide Detection Using *Coccomyxa sp.* LT4 Thylakoids Isolated from Scărișoara Ice Cave

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Assessing water quality is essential for protecting both public health and aquatic ecosystems, as well as preventing habitat degradation [1]. Since harmful compounds such as pesticides are continuously released into aquatic environments and conventional water-quality assessment methods are labor-intensive and time-consuming, there is an increasing need for simple and rapid analytical tools capable of monitoring water contamination [2].

The aim of this study was to develop an electrochemical biosensor for the detection of photosynthesis-inhibiting herbicides using a paper membrane impregnated with thylakoids isolated from *Coccomyxa* sp. LT4 microalgae. The membrane was deposited onto a screen-printed carbon nanotube electrode, and the amperometric assay conditions were optimized.

The developed biosensor successfully detected diuron in real seawater samples at concentrations as low as 125 ppb. In addition, the sensor generated a conclusive response within 300 s. These findings demonstrate the potential of this electrochemical biosensor, following further optimization, as a novel, rapid, environmentally friendly, and low-cost analytical tool for water-quality assessment.

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