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BOOK OF ABSTRACTS

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ORGANOMETALLIC SPECIES OF HEAVY PNICTOGEN (ANTIMONY, BISMUTH)–C–H BOND ACTIVATION AND REACTIVITY. RECENT RESULTS

Gabriel DUNEŞ[a], Alpar PÖLLNITZ[a], Yann SARAZIN[a,b], Cristian SILVESTRU[a]

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C-H bond activation using heavy organopnictogen(III) species is a topic of seminal interest in the modern organometallic research.[1, 2] Organobismuth(III) bis(phenolate)s and the unusual Bi-oxyaryl species $[2,6\text{-}(Me_2NCH_2)_2C_6H_3]Bi(C_6H_2\text{-}^tBu_2\text{-}3,5\text{-}O\text{-}4)$ (**1**) raised particular interest. [3, 4] By contrast, the chemistry of the lighter metalloid, antimony(III), is comparatively less developed. Here we report on recent results in the synthesis, characterization and reactivity of organopnictogen(III) (Sb, Bi) bis(phenolate)s and related thio derivatives, $ArPn(EAr')_2$ (E = O,S) [5,6] where the Ar groups attached to the metal atom are aromatic ligands with two pendant arms, *i.e.* $2,6\text{-}(R_2NCH_2)_2C_6H_3$ (R = Me, ^{i}Pr) or $2,6\text{-}\{E'(CH_2CH_2)_2NCH_2\}_2C_6H_3$ (E′ = NMe, O). The reactions of $ArPnCl_2$ with $[2,6\text{-}^tBu_2\text{-}C_6H_3O]K$ were investigated and special attention was given to the synthesis, structure and reactivity of $[2,6\text{-}(Me_2NCH_2)_2C_6H_3]Sb(C_6H_2\text{-}^tBu_2\text{-}3,5\text{-}O\text{-}4)$ (**2**), an organoantimony(III)-oxyaryl species obtained upon C_{sp2}– H bond activation in a phenolate ligand. The mechanism leading to the formation of **2** is highly sensitive to steric considerations as probed experimentally and by DFT calculations. All data agree with a process involving charged species, rather than free radicals as previously considered for congeneric bismuth species. The nucleophilic behaviour of the oxyaryl ligand in **2** was illustrated in derivatisation reactions, *e.g.* insertion of CS_2 in the Sb– $C_{oxyaryl}$ bond which generates $[2,6\text{-}(Me_2NCH_2)_2C_6H_3]Sb(S_2C\text{-}C_6H_2\text{-}^tBu_2\text{-}3,5\text{-}O\text{-}4)$ (**3**).

Financial support from National University Research Council (CNCSIS, Romania; Research Project No. PN-III-P4-ID-PCE-2020-2651) is highly acknowledged.

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METAL-BASED ANTICANCER DRUGS FOR SELECTIVE TUMOUR-TARGETING

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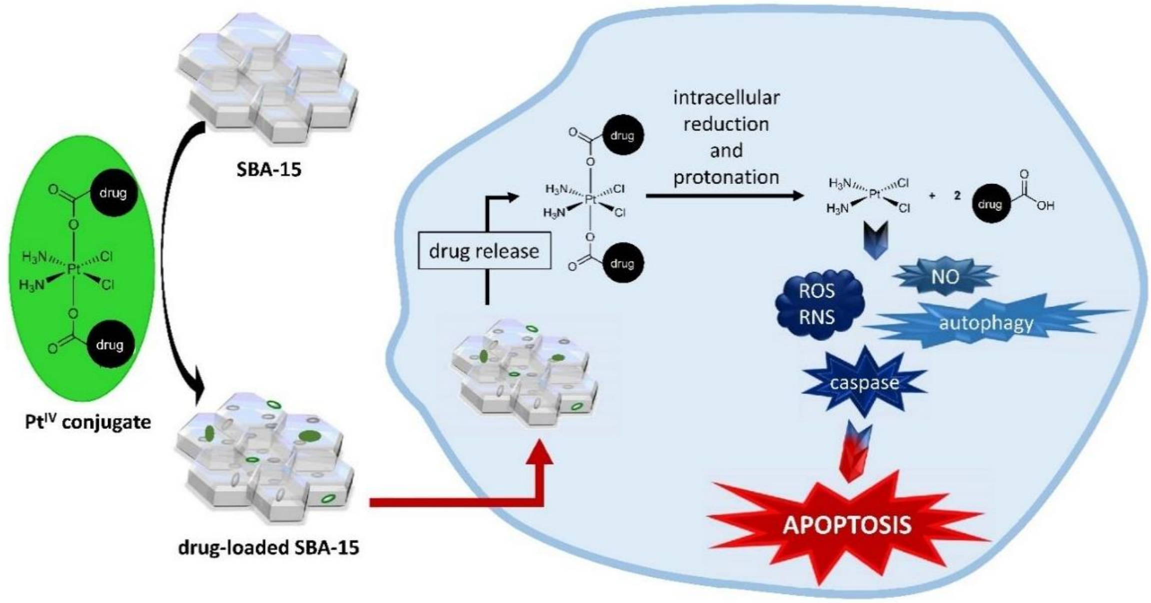
Cancer is among the leading causes of death worldwide. Chemotherapy, one of the most common treatments, is often accompanied by significant side effects, and tumour resistance to certain chemotherapeutic drugs is another major problem. Therefore, the search for new antitumour agents and new therapy methods is important.

The Hey-Hawkins group designs metal-based chemotherapeutic agents which, when combined with biologically active compounds or drugs already used in cancer therapy, have a higher selectivity and activity towards tumour cells (hybrid compounds, dual therapy). [1] Furthermore, in collaboration [2] these drug conjugates were loaded into mesoporous silica SBA-15 with the aim to utilise the passive enhanced permeability and retention (EPR) effect of nanoparticles for accumulation in tumour tissues.



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NEW SYNTHETIC APPROACH TO A LIBRARY OF FURANICS FROM D-FRUCTOSE

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Since 5-(hydroxymethyl)furfural (HMF) has been labelled as the "sleeping giant" of the bio-based platform-chemical realm, numerous investigations have been devoted to the exploitation of this versatile molecule and its endless chemical transformations into novel monomers for producing bio-based polymers. However, beyond 2,5-furandicarboxylic acid (2,5-FDCA), little attention has been devoted to key aspects that deserve being addressed before bringing forward other HMF-derivatives into the bio-based plastic market, i.e., procedures, scaling-up of the syntheses, products' purification, physical-thermal properties, and above all green metrics (sustainability/greenness of procedures).

In our research group we are interested in investigating the synthesis and the subsequent upgrade of HMF into a variety of value-added derivatives, such as chemicals, fine chemicals, materials, bio-based polymers and fuels. In this prospect it is essential to develop simple (multi) gram scale synthetic approaches addressing both isolation and purification of these compounds. In recent years we have investigated gram scale syntheses of HMF, [1] 5-bis(hydroxymethyl)furan (BHMF), 2,5-bis[(alkoxycarbonyl)oxymethyl]furan (BAMF), [2] 2,5-bis[(alkoxycarbonyl)oxymethyl] furan (BCMF) [3], 2,5-furandicarboxylic acid dimethyl ester (FDME) [4] and 5,5 '(oxy-bis(methylene)bis-2-furfural (OBMF) and its derivatives. [5] This presentation will focus on the synthetic procedures of most of the abovementioned compounds employing commercially available catalysts, green solvents, mild reaction conditions and the products were isolated as pure via simple purification procedures. Besides in some cases the related green metrics will be presented.

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HYBRID LANTHANIDE-FLAVONOID CHEMISTRY IN ANTICANCER THERAPEUTICS

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Lanthanides have over the years emerged as versatile metal ions promoting chemistries with a diverse spectrum of organic substrates, leading to metal-organic materials of distinctly differentiated physicochemical profile compared to those of first and second row transition metal ions. Progressively, their physicochemical profile was studied in biological environments, revealing anti-inflammatory, antimicrobial, antioxidant, and antitumor activities. As a result, the derived lanthanide materials emerged as viable candidates in drug therapeutics. [**1, 2**] Diseases, like cancer and diabetes, have come under scrutiny with respect to the chemotherapeutic regiments appropriate for each type of specific phenotype and tissue aberrant symptomatology. In that respect, a plethora of organic drugs have been developed, aspiring to treat the associated medical conditions, albeit to a certain extent and with various and often serious side-effects. To that end, metallodrugs came into play as alternative drugs, with a significant number of them currently being in use as diagnostics and therapeutics. Thus, lanthanides emerged as viable metallodrug candidates due to their physicochemical properties as a result of their position in the Periodic Table. Concurrently, natural products, including polyphenols and flavonoids, have been known for their ability to combat oxidative stress acting as competent antioxidants. Collectively, the combination of rare earth metals and such naturally occurring binding agents, i.e. flavonoids, presented a well-formulated pathway toward development of metallodrugs in contemporary theranostics. In an effort to pursue new metallodrugs comprised of lanthanides and naturally-occurring antioxidants, synthetic efforts were launched in our Lab to target ternary systems involving a) lanthanide ions (e.g. La(III), Nd(III), and Eu(III)), and b) flavonoids, such as chrysin, and the N,N'-aromatic chelator (phen). The systematic effort led to the isolation of pure crystalline materials, comprised of mononuclear assemblies of variable composition in their lanthanide and flavonoid components. The derived materials were meticulously characterized physiochemically, accompanied by BVS and Hirshfeld surface analysis. Furthermore, their binding capabilities with important plasma proteins were investigated by examining their interactions with a specific global molecular carrier, such as BSA (**Fig. 1**). [**3**] The studies included UV-Visible, spectroscopy, luminescence spectroscopy, and circular dichroism analysis. Elucidation of their structural, electronic, and magnetic properties pointed out the salient features of the individual species with structural attributes linked to their chemical and in vitro biological profile. The latter profile was studied in different cell lines, in comparison to physiological tissue cultures, thereby denoting the importance of the appropriate target tissue when it comes to cancer phenotypes. The collective body of information on binary-ternary lanthanide-flavonoid chemistry reveals the importance of well-defined approaches leading to well-defined materials, with the latter possessing biologically competent profiles in both diagnostic and therapeutic applications. Consequently, this interdisciplinary work emphasizes the role of molecular engineering in the development of hybrid lanthanide metallodrugs in future cancer therapeutics.

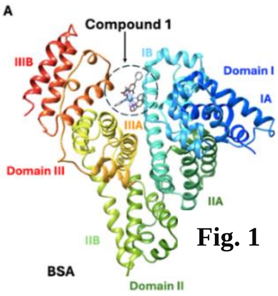

Fig. 1

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BINDING OF BIOMEDICALLY RELEVANT AGENTS TO HEMOGLOBIN AND RELATED PROTEINS

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We propose the interactions of hemoglobin (Hb) with small molecules to fall into 5 categories. [1] Type 1 involves direct interaction with the heme. Within this category, Type 1a involves coordination to the iron (e.g., O, NO, CN, nitrite, sulfide, peroxides), Type 1b involves small molecules that interact with the iron-bound ligand (e.g., nitric oxide interacting with the iron bound O_2 molecule), Type 1c involves small molecules/ions that covalently attach to the porphyrin (e.g., sulfide, generating sulfheme), and Type 1d includes ligands binding at the solvent-exposed edge of the heme. Type 2 includes physiological allosteric effectors binding at the center of the Hb tetramer. Type 3 involves hydrophobic pockets within the protein, probed with inert gases such as xenon. Type 4 involves binding at locations other than the heme or the central intersubunit cavity. Within Type 4, Type 4a involves sites that affect heme reactivity and can act as entry points for electrons towards the rest of the protein, with final targets including redox-active aminoacids (α Trp14, β Trp15, β Trp37, Cys93, Y145, Y35, Y24, Y42, Y130, Y140). [2-6] Type 4b involves no redox-active aminoacids. Type 5 involves small molecules that interact with each other outside Hb, but still affect Hb indirectly, for instance leading to apparent autocatalytic processes (e.g., superoxide, from Hb's autooxidation reaction). We explore here the Type 4 interactions with biomedically relevant ligands in Hb as well as, for comparison, serum albumin, using docking calculations as well as experiments.

Funding from the Romanian Ministry of Education and Research (project PNRR-III-C2-2023-18-CF76) is gratefully acknowledged.

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FROM FORM TO FUNCTION: NEW APPROACH IN STRUCTURAL CHARACTERIZATION OF PHARMACEUTICAL COMPOUNDS

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For drugs delivered in crystalline form, the physical properties of the active pharmaceutical ingredient (API) are strongly depending on the crystal form, having the potential to impact bioperformance, particularly for low-solubility compounds, where the rate-limiting-step in drug uptake may be the dissolution, often controlled in the final API crystallization step. Therefore, well-controlled crystallization of the API is a vitally important operation due to the uncertainty in the crystal forms that will appear, and because of the many challenges associated with scaling-up crystallizations from laboratory to manufacturing scale.

The goal of this lecture is to highlight the complexity of the problem, while providing perspective regarding the challenges, gaps in knowledge or capabilities, and opportunities for improvement in the development of pharmaceutical crystallization processes. In this perspective, crystal structure determination is fundamental for understanding the substance's function, as well as for controlling the material performance throughout the entire drug development process.

Additionally, this lecture exemplifies the basic principles of solid forms screening and several analytical techniques, using febuxostat as model compound. Febuxostat has been selected as model compound because its significant propensity to form salts and co-crystals [1, 2] and because exhibits more than forty polymorphs and solvates already reported [3].

The significance of combining crystal structure knowledge with theoretical methods in understanding complex polymorphic systems is also demonstrated. Furthermore, the emerging potential of Electron Diffraction to provide crystal structures of pharmaceutical nanocrystals will be explored in the context of febuxostat polymorphism [4, 5].

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SYNTHETIC APPROACHES OF PHOTO-SENSITIVE AZO-BASED SWITCHING PROBES

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Molecules that are able to display multiple states due to reversible change of structure under light irradiation are usually called photoswitches. Azobenzene derivatives are the most representative examples of photoswitches which developed a lot during the past ten years, in order to overcome drawbacks of the parent azobenzene, such as incomplete conversion between the two *E-Z* isomers or short half-life of the least stable isomer. Replacing a phenyl with a heterocycle molecule yielded heteroarylazo compounds as a totally new alternative, providing a very large number of possibilities to explore their structures, properties and mechanisms of actions.
This talk refers to design and synthesis of novel (hetero)arylazo compounds involving various azole moieties (i.e. 1,3,4-oxadiazole, 1,3,4-thiadiazole, pyrazole), including compounds that combine multiple switching units (*i.e.* azo and N-acylhydrazone groups) as well as investigation of the main parameters displayed by the resulted compounds to describe their photoswitch ability.

This work was supported by grants from the Romanian Ministry of Education and Research, CNCS - UEFISCDI, project number PN-III-P1-1.1-TE-2019-1003, and PN-III-P2-2.1-PED-2021-2529 within PNCDI III, as well as PNRR/2022/C9/MCID/I8, project number CF 760056/23.05.2023, code 235/29.11.2022.

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GREEN CHEMISTRY INSPIRED SYNTHESIS OF BIOLOGICALLY ACTIVE COMPOUNDS: MULTICOMPONENT REACTIONS, MICROWAVE AND FLOW CHEMISTRY

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Multicomponent reactions (MCRs) emerged in the past decades, and continuously attract great attention as one of the most useful and efficient tools for the synthesis of versatile biologically active compounds. [1, 2] Products are usually formed in a single step from simple starting materials in highly atom efficient reactions. The possibility of applying diverse reagents makes them ideal for creating new molecular libraries. Moreover, in most cases, the principles of green chemistry also prevail to save time and energy. Combining these features with microwave (MW) and/or with flow chemistry provides new methods for the rapid and efficient synthesis of heterocyclic compounds. [2]

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. [3]

One of the main goals of our research was to develop MC methods for the synthesis of various *N*- and *O*-heterocycles containing phosphonate or phosphine oxide moiety (Figure 1). Most of the reactions were carried out under MW heating, where the reaction time was significantly reduced, and the use of solvent and catalyst can be avoided. Several derivatives synthesized showed good or promising anticancer and/or antibacterial activity.

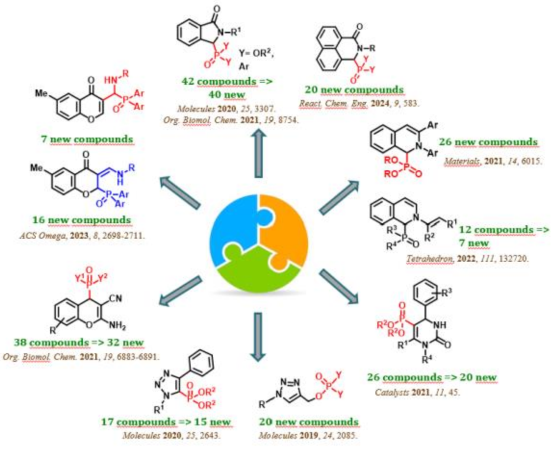

Figure 1. *N*- and *O*-heterocycles containing phosphonate or phosphine oxide moiety.

Another aim of our group is to develop continuous flow methods for the synthesis of bioactive compounds. Therefore, we have elaborated the first flow synthesis of capsaicine derivatives based on three reaction steps. The flow method developed is a greener, safer, faster and more atom-efficient process than the batch approaches described. Furthermore, using self-developed 3D printed flow reactors, we have demonstrated an alternative and cheaper way of flow chemistry. [4]

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OXIDOVANADIUM COMPOUNDS WITH BIOMEDICAL APPLICATIONS

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The remarkable chemical and biological properties of vanadium compounds have attracted the attention of researchers, sparking extensive investigations into their chemistry, biochemistry, and potential medicinal applications [1]. Over the last 20-25 years, the field of vanadium chemistry has experienced exponential growth, particularly in the quest for their therapeutic applications [2]. Vanadium being a biologically relevant element, it is not surprising that numerous vanadium-based therapeutic agents have been proposed for the treatment of several types of diseases, such as diabetes [3], cancer [4], and diseases caused by parasites and bacteria [5].

This presentation will focus on the synthesis and characterization of a family of oxidovanadium(V) complexes with Schiff base ligands and the assessment of their potential biomedical application as insulin-mimetic or antitumor agents [6,7]. The compounds synthesized from vanadyl sulfate, DL-amino acids, and salicylaldehyde or *o*-vanillin were characterized, in solid state and solution, using UV-Vis, IR, CD, single-crystal and powder XRD techniques, revealing optical activity and structural stability. The potential antidiabetic and antitumor activities of the obtained compounds were investigated. Some of the synthesized compounds display cytocompatibility at biologically relevant concentrations, exert antidiabetic potential and insulin-mimetic activities by inhibiting the α-amylase and protein tyrosine phosphatase activity, and a long-term increase of insulin receptor phosphorylation compared to the insulin hormone [6], while other compounds show antitumor properties against the human hepatocarcinoma (HepG2) cell line [7]. Lately, our efforts have focused on obtaining insights into their beneficial effects on health and modes of action, as well as understanding the structural characteristics of these oxidovanadium(V) compounds that is responsible for their biomedical applications and is crucial for advancing their therapeutic potential and could pave the way for novel treatments in diabetes and cancer.

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CELL MODELS OF SKIN IN BIOMEDICINE: ADVANTAGES, LIMITATIONS AND OPPORTUNITIES

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The skin is the largest organ in the human body and plays a crucial role in our overall health and well-being. It is the body's first line of defense against bacteria and viruses, performs important immunological functions, supports the exchange of fluids, salts and gases, helps to regulate the body temperature, the skin is extremely sensitive and recognizes even the gentlest touch, as well and the pain.

Cell model systems of the skin are necessary for testing the biological/pharmacological activity of various medical and cosmetic products, the antitumor effect of compounds, the cytocompatibility of wound dressings, as well as for studying normal and pathological processes in it such as regeneration, healing, aging and carcinogenesis.

The advantages and limitations of different cellular skin models will be discussed with the opportunities they provide in different areas of biomedicine and material science.

HOW TO MATCH THEORY WITH AN EXPERIMENT - A KEY FEATURE OF UNDERSTANDING INTERPHASE

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Understanding adsorption mechanisms as well as catalytic processes is of key importance for the creation of more efficient, long-lasting, and cheaper (electro)catalysts and/or adsorbents. Density Functional Theory (DFT) is a quantum mechanical method used to investigate the electronic structure of many-body systems, particularly atoms, molecules, and condensed phases. DFT is widely used in materials science due to its balance between accuracy and computational efficiency. The application of quantum mechanical tools, particularly Density Functional Theory (DFT), facilitates the examination of numerous systems and the identification of optimal candidates for further experimental measurements. This approach substantially conserves time and laboratory resources.

Desirable adsorbents are materials that effectively capture and hold molecules from gases or liquids onto their surfaces, characterized by high surface area, selectivity, and capacity. They are crucial in various applications such as gas separation, water purification, and environmental remediation. The development of adsorbents with desirable pore sizes and surface functionalities enhances their performance by allowing selective adsorption of specific contaminants or target molecules.

On the other hand, electrocatalysts are critical components in various energy conversion technologies, such as fuel cells and electrolysers, where they enhance the performance of reactions like oxygen reduction and hydrogen evolution. Highly active, stable, and cost-effective electrocatalysts are essential for the advancement of sustainable energy systems. Recent research focuses on the design and synthesis of novel nanostructured electrocatalysts with optimized electronic properties and surface morphologies to maximize catalytic activity and durability.

Quantum chemical methods enable the modeling of the adsorbent's geometry and the adsorbent/adsorbate bond length. Furthermore, these methods facilitate the calculation of adsorption energies, thereby allowing the identification of active sites for the adsorption of organic dye or pesticide molecules. The results obtained from these calculations are integrated with experimental data, such as XRD and IR/Raman spectroscopy, to enhance their reliability, especially for zeolites and soil-derived minerals. In the realm of electrocatalysis, alloys or bimetals containing cobalt or nickel are investigated as potential alternatives to the highly efficient Rh and Pt electrocatalysts. Density Functional Theory (DFT) is employed to calculate adsorption energies and the center of the d-band, which is associated with catalytic centers on the surface, with these theoretical results being correlated with electrochemical measurements for validation.

In summary, the integration of experimental techniques and DFT calculations provides a robust and comprehensive approach, combining the strengths of both methodologies to advance scientific understanding and technological development.

A TORCH TO SHED LIGHT ON THE DARK KINOME: THE DISCOVERY OF PI3K-C2β HIGHLY SELECTIVE INHIBITORS

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Phosphoinositide 3-kinase (PI3K) is a family of lipid kinases involved in several cellular signaling pathways and it is of high biomedical interest not only for cancer treatment, but also for non-oncologic diseases such as asthma, COPD, and thrombosis. [1] Interestingly, great efforts to develop PI3K inhibitors have been predominantly focused on class I, resulting in drug compounds reaching the market. [2] In stark contrast, only recently isoform specific class II PI3K inhibitors have been reported. [3] This is highly surprising given the recent strong links to human diseases and crucial biological roles of PI3K class II isoforms, in terms of vesicular trafficking, cytokinesis, primary cilia function and cell signaling. [4, 5] Hence, the identification of a highly selective class II phosphoinositide-3-kinases is pivotal to untangle the future role as potential drug discovery targets. Here, we present the development of active and selective PI3K-C2β inhibitors. Our efforts towards the identification of a distinct chemical scaffold that selectively inhibits PI3K-C2β started by analyzing the biochemical profile of AZ-3458, which is a sub-nanomolar drug-like PI3Kγ inhibitor with an off-target activity on the isoform C2β. Through SAR studies, we have rationalized the structural determinants for PI3K-C2β activity and selectivity, achieving a decisive selectivity switch and thereby abolishing class I PI3K activity. The medicinal chemistry program culminated in the creation of three lead compounds with nanomolar activity on PI3K-C2β and no off-target effect on a panel of 117 kinases (including all homologous lipid kinases, except PI3K-C2γ). Cellular proof-of-concept studies to demonstrate their viability to probe specific PI3K-C2β functions are ongoing, but initial results indicate that these selective and non-cytotoxic inhibitors are able to recapitulate cellular phenotypes, mirroring genetic PI3K-C2β knockdowns. [6] Our investigation discloses the first potent isoform specific PI3K-C2β inhibitors and defines key structural determinants necessary not only for affinity towards PI3K-C2β, but also for the specificity within the lipid kinase family. These probes will facilitate the elucidation of the role of PI3K-C2β in cell signaling and physiology and are valuable starting points for the development of PI3K-C2β targeting drugs.

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CELL-PENETRATING PEPTIDES AS ANTIMICROBIALS

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Cell-penetrating peptides (CPPs) are a captivating group of peptides known for their effective ability to traverse cellular membranes. The exceptional ability of CPPs makes them indispensable tools for investigating membrane structure and function in scientific research. Not only do their variety help in comprehending biological processes, but it also makes them attractive contenders for many therapeutic uses. Cationic cell-penetrating peptides (CPPs) provide novel approaches to tackle existing obstacles in medicine, such as targeted drug delivery and overcoming cellular barriers, by enabling the transportation of diverse molecular payloads, including medicines, nucleic acids, and other therapeutic agents. The ongoing study on CPPs is revealing their significant promise in advancing both fundamental biological investigations and therapeutic applications. [1,2,3,4] Antimicrobial peptides (AMPs) are characterized by diverse structural features, such as amphipathic structures and specific amino acid residues, which enable selective interactions with various membranes. Their mechanisms of action involve disrupting lipid bilayers through different pathways, depending on the peptide's properties and the membrane's composition. These versatile capabilities make AMPs crucial for both innate immunity and the development of new antimicrobial therapies. [1] We present the development of ten newly designed CPPs/AMPs, obtained by using solid phased peptide synthesis an an automated synthesizer. They present low toxicity to normal human cells and high antimicrobial activity against bacterial strains tested (*Escherichia coli*, *Pseudomonas aeruginosa*, *Salmonella typhimurium*, *Staphylococcus aureus*, *Bacillus subtilis* subsp. *spizizenii*). Investigating CPPs (cell-penetrating peptides) with antimicrobial properties demonstrates promise for developing novel therapeutic approaches to combat infections, cancer, and obstacles in drug administration. [1,2,3,4,5,6].

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COMPARATIVE PRETREATMENT APPROACHES FOR BIOETHANOL PRODUCTION FROM AGRO-INDUSTRIAL BY-PRODUCTS BY SIMULTANEOUS SACCHARIFICATION AND FERMENTATION (SSF)

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The use of fossil fuels has led to an increase in greenhouse gas emissions, the main cause of global warming with a negative impact on the planet. In addition, the rapid depletion of fossil fuels requires the identification of alternative and renewable energy sources such as biofuels. [1] Second-generation biofuels obtained from lignocellulosic biomass, such as food and forest by-products, show considerable potential and should be further developed for the sustainable decarbonization of transport and the energy sector. [2]

The aim of the present study was to assess the effect of different pretreatment methods including microwave-assisted organo-solvolysis, chemical and biological pretreatment methods for efficient delignification of biomass and subsequent the fermentation to bioethanol in SSF mode. The effectiveness of the pretreatment methods used was highlighted by determining the lignocellulosic composition, as well as the morphological and structural characterization, before and after pretreatment. Cellulase obtained from *Trichodrema Reesei* and *ß-glucosidase* were used as hydrolytic enzymes and the fermentation of simple sugars to ethanol was carried out with *Saccharomyces Cerevisiae*. The control of the fermentation process was carried out by monitoring reducing sugars and total sugars by UV-Vis spectrophotometric methods or by measuring °BRIX, while the alcohol content of the fermentation broth was determined using a digital laboratory equipment for measuring alcoholic strength by volume.

Preliminary data obtained for the transformation of lignocellulosic biomass into bioethanol through the process of SSF indicated the achievement of an alcohol content between 11.0 g/L for grape pomace and 14.0 g/L for conifer bark after delignification, indicating that by delignification with sodium chlorite a greater amount of ethanol was obtained, but at the same time the process is unfriendly to the environment. Depending on the pretreatment method, the ethanol content of the fermentation broth obtained from apple pomace ranged between 10.40-13.41 g/L, with 70% yield of bioethanol when enzymatic pretreatment was used. Laboratory research will continue in order to improve the yield of obtaining cellulosic bioethanol by optimizing the operational parameters of the SSF process (amount of biomass, inoculum, hydrolytic enzymes and specific yeasts, nutrients, temperature, pH).

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PREPARATION OF CU$_2$O MICROSPHERES AND ITS APPLICATION FOR STRUCTURAL COLOR ON POLYESTER FABRIC

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Cu_2O microsphere is a promising material for constructing photonic crystals and for generating structural colors due to its high refractive index. [1] In this work, Cu_2O microspheres were synthesized by a two-step reduction method at room temperature, and the sizes of Cu_2O microspheres were adjusted by changing the molar ratio of citrate to Cu^{2+}. And then a dispersion containing Cu_2O microspheres, poly(butyl acrylate) were prepared and applied onto polyester fabric by spraying technology. At last, the structural colored fabrics were developed. The Cu_2O microsphere was evaluated in terms of morphology, monodispersity and XRD; the stability of the Cu_2O microsphere dispersion was investigated; and the effect of concentration of Cu_2O microsphere, concentration of adhesive, size of Cu_2O microsphere on structural color were discussed. The results demonstrated that the Cu_2O microspheres had good monodispersity, generated different structural colors based on different sizes, and the structural colored fabrics had good color fastness to bending and friction.

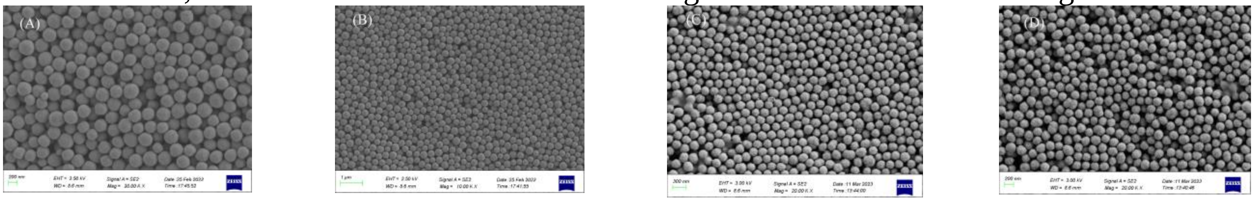

Fig. 1. Morphology of Cu_2O microsphere with different size (a) 275 nm (b) 240 nm (c) 210 nm (d) 190 nm

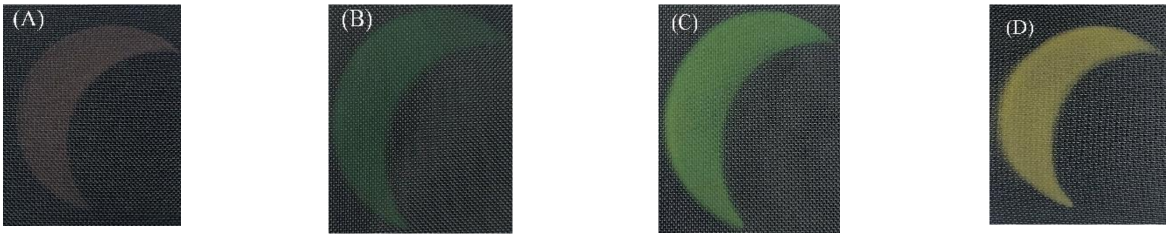

Fig. 2. Structural color from Cu_2O microsphere with different sizes (a)190 nm (b)210 nm (c)240 nm (d)275 nm

Figure 3. The structural color of fabrics with different Cu_2O microsphere concentration
(a) 0.5 wt.%; (b) 1.0 wt.%; (c) 3.0 wt.%; (d) 5.0 wt.%

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DRUGCENTRAL: A PUBLIC DIGITAL DATABASE OF APPROVED DRUGS SUPPORTING DRUG DISCOVERY AND REPURPOSING

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DrugCentral is an open-access, comprehensive online database designed to support the global scientific community by offering up-to-date information on drug ingredients, including their chemical properties, biological activities, pharmacologic actions (such as mechanism-of-action targets), therapeutic uses, adverse effects, and pharmaceutical formulations. The database currently encompasses data for approximately 5,000 approved drugs, including those used in veterinary medicine. In addition to approved drug information, DrugCentral includes data on off-label uses and drug combinations, further enhancing its utility. Key features include: mechanism-of-action data for around 2,000 drugs, over 19,000 drug-target activity values, approximately 12,000 drug indications and 2,500 off-label uses, and pharmacokinetic profiles for around 1,000 drugs [1]. The database also offers a detailed analysis of adverse drug events, broken down by gender and age using data from the FAERS reports. Moreover, DrugCentral provides a ranking system for drug repurposing opportunities, informed by the market status and patent rights of FDA-approved drugs [2], [3]. With over 142,000 FDA-approved drug products in its repository, DrugCentral serves as a pivotal resource for drug discovery, pharmacological research, clinical decision-making, and the exploration of drug repurposing opportunities.

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SPECTROSCOPIC DETECTION OF DRUGS USING METALLOPORPHYRINS AS SENSITIVE MATERIAL AN OVERVIEW

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The spectroscopic detection of various analytes has gained tremendous momentum in recent years, due to the simple, fast and economic aspects of this technique.

Of utmost importance is the quantification of minute quantities of drugs in the blood serum or in the urine of human patients, as toxic side effects could lead to health damages. [1]

A brief overview of sensitive Mn(III)-, Zn(II)-, Co(II)-, Pt(II)-metalloporphyrins, synthetically designed to act as selective compounds for the detection of β-carotene [2], ascorbic acid [3] or drugs such as, among others, diclofenac [4] or procaine [5] is presented.

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ADSORPTION PERFORMANCE OF IONIC LIQUID FUNCTIONALIZED MOFs IN THE REMOVAL PROCESS OF ORGANIC POLLUTANTS FROM AQUEOUS SOLUTIONS

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Water is a limited resource essential to human well-being and can be renewed if managed properly. Persistent organic pollutants represent the most hazardous substances, characterized by chemical properties such as high toxicity, chemical stability and bioaccumulative potential that can significantly affect human health and the environment. Among the available treatment technologies, adsorption processes using solid adsorbents show potential as one of the most effective methods for the treatment and elimination of organic pollutants in wastewater treatment.

The most important element in an adsorption process is represented by the adsorbent material. MOFs exhibit a variety of supramolecular framework architectures, properties which make them suitable to be used as adsorbent materials. Moreover, if they are impregnated with ionic liquids is opened a new concept that could afford access to design and reengineering a type of advanced composite material with versatile functionalities and extraordinary properties.

Therefore, the paper presents studies regarding the functionalization of different MOFs with various ionic liquids to obtain efficient and selective adsorbent materials for OPs (phenol, phenol derivatives, tetracycline) removal from aqueous solutions.

In all the cases the adsorption capacity increases with the increasing contact time, increasing temperature and increasing equilibrium concentration of OP. The presence of ionic liquid significantly improves the efficiency of MOFs in the removal process of OP from aqueous solutions. The adsorption kinetics were better described by the pseudo-second-order kinetic model compared to the pseudo-first-order kinetic model. The experimental data showed a good fit with the Langmuir isotherm.

The combination of the ILs with the MOF combines the properties of MOFs with the advantages of the ionic liquids, being used very small amount of ILs which lead to a decreasing of the capital and operating costs and make it easy to scale up. Using the ILs for the MOFs modification increases the efficiency and selectivity of the obtained adsorbent materials.

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Mg_3Al-LDH/IONIC LIQUID/CHITOSAN – HYBRID MATERIALS FOR PALLADIUM RECOVERY

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Palladium is a rare metal widely used in industry and beyond because of its properties. As primary reserves are continually depleting, palladium's applications are manifold, and the price of the metal is fluctuating upwards, its recovery from by-products and scrap becomes imperative. The recovery processes are manifold: smelting, chlorination, dissolution in acids, co-precipitation, ion exchange, adsorption, etc. Special attention is paid to adsorption, being one of the most promising methods due to its simplicity and high efficiency, attributes that determine the widespread use of this recovery method.

As a result, the present work studied the possibility of recovering palladium ions from aqueous waste solutions by adsorption on hybrid materials, Mg_3Al-LDH/ionic liquids/chitosan, demonstrating that all the raw materials used to obtain the adsorbates have proven their effectiveness.

To synthesize the double layered hydroxide, Mg3Al, the low supersaturation coprecipitation method was used. The same method was used to obtain the compound functionalized with 10% ionic liquid, except that the nitrate mixture was added to the ionic liquid solution dissolved in acetone by dripping. The mechanical resistance of the obtained adsorbates (Mg_3Al and Mg_3Al-IL) was increased by dispersing them in a solution of chitosan dissolved in 1% acetic acid, obtaining the hybrid materials: Chitosan/ Mg_3Al, Chitosan/ Mg_3Al-IL, Chitosan/ Mg_3Al/IL. The hybrid materials were characterized by X-ray diffraction, Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM) coupled with energy dispersive X-ray (EDX) detector.

The XRD spectrum of the Mg_3Al sample, obtained by co-precipitation at low supersaturation, suggests a good compatibility of chitosan with LDH, leading to the formation of porous networks.

For all studied materials and for all initial palladium concentrations, the adsorption capacity of the studied materials increases with increasing contact time up to 60 min, after which it remains practically constant.

To clarify the adsorption mechanism of palladium on the studied materials, three kinetic models were used: pseudo-first-order kinetic model, pseudo-second-order kinetic model and intraparticle diffusion model (Weber-Morris), the pseudo-second-order kinetic model being the one that best confirmed the experimental data, the value of the correlation coefficients R^2 being approximately 1, regardless of the working temperature.

To study the nature of the adsorption process of palladium on the studied materials, the thermodynamic parameters: enthalpy, entropy, Gibbs free energy, activation energy were calculated, the results confirming that the reactions are spontaneous, endothermic, and the adsorption process of palladium on the studied materials corresponds to chemosorption.

Langmuir, Freundlich, Temkin and Redlich-Peterson isotherms were used to identify the mechanism of the process and to evaluate theoretically the adsorption capacity at equilibrium, and it was found that the Langmuir isotherm best describes the adsorption process of palladium on the synthesized materials.

REMOVAL OF PHENOL FROM METAL ORGANIC FRAMEWORK IMPREGNATED WITH IONIC LIQUID. ELECTROCHEMICAL ASSAY

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Many researchers have been attempting to regenerate and reuse different types of adsorbents in the past few years. [1] Metal-organic frameworks (MOFs), a type of compounds made up of metal ions or clusters coupled to organic ligands to form one-, two-, or three-dimensional structures, are an appropriate adsorbent for hazardous organic chemicals from water. Electrochemical oxidation (EO) of potentially hazardous organic substances is a promising remediation technique. [1,2]

Industrial effluents contain phenols (PH), which are dangerous and have problems with bioaccumulation even at low quantities. Phenolic compounds are present in effluents produced by chemical businesses and the food industry. Several alternative approaches (solvent extraction, enzymatic treatment, or heat treatment in an oxidizing atmosphere) have been proposed for the recovery or annihilation of phenols. [2]

The electrochemical method relies on the production of hydroxyl radicals (also known as active chlorine, or •OH) in situ. [2,3] The phenoxy radical produced during the electrooxidation process can react with other phenol molecules to form a dimeric radical or mix with other species already present in the solution to produce products. Through electrochemical oxidation, MOF-type adsorbents impregnated with ionic liquids—which are used to extract phenol from wastewater—can also be renewed. In a solution containing 3% NaCl, the electrochemical performance of commercial graphite electrodes was examined. [4]

The electrolyte's PH content had an impact on the immediate EO; a lower concentration and a delayed release of PH seemed to hasten the synthesis of BQ. Following an hour and half duration, PH electrooxidation (EOPH) attained an efficiency of close to 37% from Cu-PA and around 40% from Cu-PA-IL, respectively. This work demonstrates the possibility of recovering spent adsorbent and electrooxidizing desorbed PH simultaneously.

This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-III-P4-PCE-2021-0089, within PNCDI III and partially from the "Coriolan Dragulescu" Institute of Chemistry Timisoara, Romania, Program 2.

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NEW SYNTETIC STRATEGY FOR THE SYNTHESIS OF HETEROCYCLIC COMPOUNDS MEDIATED BY HYPERVALENT IODINE AGENTS

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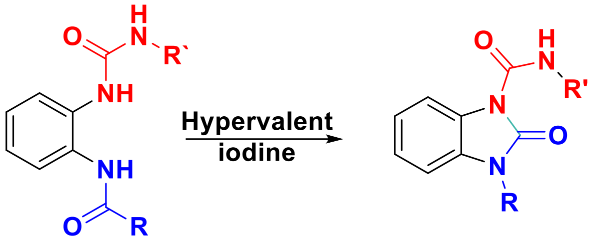
Iodine compounds in higher oxidation states, known as "hypervalent iodine compounds", have developed as some of the most versatile and environmentally safe oxidative reagents in organic chemistry. [1] Among their vast applications is the formation of new carbon (heteroatom) -heteroatom bonds, such as C-N, N-N or C-S in numerous heterocycles. [2] However, till now they haven't been explored as oxidative mediators of the cyclization step, with the formation of a C-N bond in the synthesis of benzimidazol-2-ones, so by investigating this reaction we implemented a new synthetic methodology for these compounds.

Our work consists in the synthesis of new benzimidazol-2-one derivatives, through an intramolecular oxidative cyclization mediated by a hypervalent iodine agent, using an amido-urea substrate as a starting material (Figure 1). The key step for the preparation of the target compounds was carried out in the presence of a pentavalent iodine agent (Dess-Martin periodinan), but also a trivalent iodine agent (PIDA). Derivatives of benzimidazol-2-one [3] have been shown to have biological activity and thus the newly synthesized heterocyclic systems have relevant potential applicability in the pharmacological field. All compounds were purified and characterized by NMR spectroscopy, HRMS spectrometry and X-ray crystallography to confirm their identity.



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ION MOBILITY TANDEM MASS SPECTROMETRY: A NOVEL METHOD IN GLYCOLIPIDOMICS OF HUMAN BIOPSIES

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Gangliosides (GGs), sialylated glycosphingolipids, represent a class of *O*-glycoconjugates consisting of a mono- to polysialylated oligosaccharide chain of variable length attached to a ceramide moiety of different composition with respect to the types of sphingoid base and fatty acid residues. Being enriched in specialized microdomains, GGs interact with signal transducers, mediate carbohydrate-dependent cell adhesion, induce cell activation, motility and growth and participate in cell–cell interactions, modulating or triggering various biological events [1].

The central nervous system (CNS) encompasses the highest content of GGs; neuronal membranes contain several times higher concentrations of GGs than the extraneural cell types. For these reasons, GGs are valuable indicators in the early diagnosis of CNS pathologies, being in the focus of our research as potential biomarkers and/or therapeutic targets [2]. An efficient separation and a detailed structural characterization of GGs represent essential prerequisites for elucidating specific function of each particular structure and to use it, accordingly, as a therapeutic agent in treatment of diseases and/or as a specific diagnostic marker [3,4].

In this context, we report here on the development of a novel, high performance nanoelectrospray ionization (nanoESI) ion mobility separation (IMS) mass spectrometry (MS) and tandem MS (MS/MS) by collision-induced dissociation (CID) approach for glycolipidomics of CNS GGs. The methodology was systematically implemented for: i) screening and structural characterization of GGs expressed in different normal adult and fetal brain regions such as the frontal lobe, hippocampus, and cerebellum; ii) GG biomarker discovery in malignant primary (melanoma, glioblastoma multiforme) and secondary (lung adenocarcinoma) tumors and iii) GG profiling in human cerebrospinal fluid. IMS MS represents also a novel concept in structural analysis of GG biomarkers, due to its unique ability to separate isomers, isobars and conformers. The conducted studies have shown that the modified expression together with the observed upregulation of certain glycolipids in human patient biopsies as compared to healthy controls, have the potential to serve for disease diagnosis. Moreover, the discovery for the first time of species altered by CH_3COO^- raises a series of issues regarding the cholinergic activity of GGs. IMS CID MS/MS provided new insights into the GG composition and structure in the studied matrices, since it was able to unambigously identify the isomers from a series of possible candidates and provide their detailed structure. The results demonstrate that IMS MS is a powerful and highly efficient technique able to unequivocally detect and characterize complex glycolipids with potential biomarker role and discover new structures.

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Ag(I) and Cu(II) COORDINATION COMPOUNDS AS MULTIFUNCTIONAL ADDITIVES FOR NANOCELLULOSE-BASED MATERIALS

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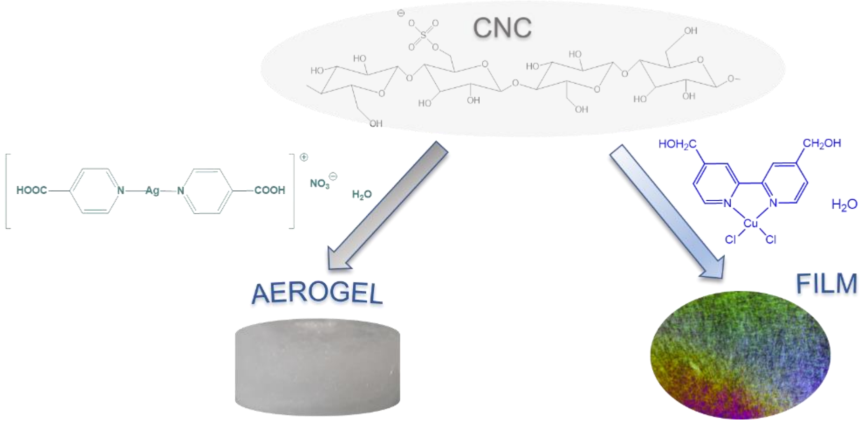
The finite availability of petroleum-based materials and the escalating effects of climate change highlight the need for a transition to renewable materials and eco-friendly practices. Nanocellulose (NC) materials, including cellulose nanocrystals (CNC) and cellulose nanofibers (CNF), offer sustainable alternatives to fossil fuel-based materials. The extraordinary properties of nanocellulose, such as its lightweight and high strength, make NC materials (films, hydrogels, aerogels) appealing candidates for a wide range of applications, including food packaging, thermal insulation, and gas absorption [1]. However, to fully harness the practical potential of these materials, it is crucial to address their primary limitations: poor water resistance and susceptibility to microbial attack [2, 3].

The innovative use of Ag(I) and Cu(II) coordination compounds as multifunctional additives for nanocellulose is presented herein. By specifically designing water-soluble complexes with ligands that can cross-link NC, the water resistance and mechanical properties of NC can be significantly enhanced. Furthermore, the incorporation of the metal centers imparts additional functionalities to the NC materials, broadening their application scope. For instance, the use of Ag(I) complexes, such as $[(ina)_2Ag]NO_3$ (*ina* = isonicotinic acid) can impart antibacterial properties to CNC aerogels. Alternatively, the incorporation of Cu(II) complexes can make CNC films effective for electromagnetic interference (EMI) shielding.

Here, a water-soluble Ag(I) coordination compound, $[(ina)_2Ag]NO_3$, is used as a multifunctional additive for the preparation of CNC suspensions and aerogels. Additionally, hybrid CNC colloids and films have been obtained by combination with a water-soluble Cu(II) complex, $[(bpy\text{-}OH)CuCl_2]$ (*bpy-OH* = 4,4'-bis(hydroxymethyl)-2,2'-bipyridine). An in-depth investigation of the hybrid materials, compared to reference materials containing only CNC, revealed the significant role of the inorganic compounds in modifying CNC properties.



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HYBRID SILICA ADSORBENTS FOR CAPTURING PHARMACEUTICALLY ACTIVE COMPOUNDS FROM WATER

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Bioaccumulation of pharmaceutically active compounds (PAC) in food chains and water bodies poses a serious threat to human health due to their toxicity and non-biodegradability. Among them, antibiotic residuals occupy a special concern for the ecosystem as they are found to be the reason for the generation of bacterial-resistant genes [1]. Removing these compounds from aqueous media through adsorption has attracted significant attention recently [2]. This study aimed to develop, characterize and apply silica-based xerogels as adsorbents for capturing PAC from water. For this purpose, hydrophilic silica-based adsorbents have been prepared via a single-step sol-gel method under ambient conditions. A classical silica tetraalkoxysilane was used as the main silica precursor during the synthesis. Adding organic functionalities such as methyl, amino, epoxy, vinyl, and methacrylate to the silica backbone was also investigated as a process parameter. Modifying the silica backbone with organic functionalities (methyl, amino, epoxy, vinyl, and methacrylate) had a significant effect on the silica structure and also on the adsorptive performance.

The adsorptive performance of the synthesized materials was tested on some representative classes of antibiotics (fluoroquinolone and ornidazole). These studies were carried out by batch sorption experiments tuning several parameters such as initial drug concentration, adsorbent dosage, contact time, and the solution pH to determine optimal operating conditions. Results of the adsorption experiments confirmed the high uptake of antibiotics (>50 mg/g) in low contact time (<30 min) with endurable cyclic performance (over 5 cycles). Imparted organic functionalities enhanced the adsorption ability of these materials even more due to the improved chemical interactions. The obtained results indicated that hybrid functional amorphous silica materials can be successfully used as adsorbents for the remediation of pharmaceutical effluents from aqueous media.

This study was financially supported by Ege University Scientific Research Project Coordination Unit under contract number of 23943.

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ORGANOCHALCOGEN COMPOUNDS AND THEIR METAL COMPLEXES. SYNTHESIS, STRUCTURE AND POTENTIAL APPLICATIONS

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Organoselenium compounds continue to attract a significant interest as valuable candidates in medicinal chemistry, catalysis and organic synthesis, or as key species for optoelectronic devices. [1,2,3] A special attention was paid during last years to derivatives bearing organic groups with nitrogen or oxygen donor atoms, showing an increased thermal and hydrolytic stability and enhanced specific properties.

Our recent studies were focused on new classes of diorganodichalcogenides or homo- and heteroleptic diorganochalcogen(II) compounds bearing organic groups with N or O donor atoms, as well as on their main group or late *d* metal complexes.

We report here about compounds of type R_2Se_2 and R^1R^2E (E = S, Se), where R^1, R^2 = 2-$XC_6H_4CH_2$ (X = Br, Me), 2-$(R_2NCH_2)C_6H_4$ [R = Me, Et; R_2 = $(CH_2CH_2)_2O$], CH_2CH_2pz (pz = pyrazole), CH_2Phtz (Phtz = phenylthiazole), as well as upon several pyridine based derivatives bearing pendant arms with donor atoms. Their coordination behavior towards main group (Sn, Sb) and late d metals (Cu, Ag, Au, Zn, Cd) is discussed. Selected compounds were investigated for their biological properties, *e.g.* antiproliferative or antioxidant activity, as appropriate. Optical properties of selected metal complexes and of the corresponding free ligands are also presented.

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COMPUTATIONAL AND APPLIED BIOCATALYSIS FOR THE SUSTAINABLE SYNTHESIS OF BIO-BASED OLIGOESTERS

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The interest in polymers derived from renewable sources has amplified as demonstrated by the large number of recent patents and publications. The material and polymer sectors are facing the challenge of integrating the sustainability of both processes and products, including their management after disposal [1,2]. To minimize the effects of their dispersal in open environments due to specific applications (cosmetics and fishing nets, food packaging) stringent eco-design criteria focused on biodegradability and ecotoxicity are required. Biocatalysis can boost such innovation, leveraging on enzymes that overcome the limitations of conventional chemical strategies by catalyzing, under highly selective and mild conditions, the targeted modification, synthesis or degradation of polymers and, most importantly, biobased polymers. Hydrolases, such as lipases and cutinases, were successfully used for *in vitro* polycondensation of bio-based diacids and polyols, leading to biodegradable polyesters with controlled structures. In parallel the capacity of several cutinases and lipases to degrade polyesters was evaluated by several groups [3,4]. The possibility to correlate structural features of a polymer with the catalytic properties of an enzyme would allow the rational design of environmentally safe new tailor-made biodegradable polymers.

Our approach integrates experimental and computational methods, analyzing short oligomers to rapidly screen for sustainable alternatives, particularly bio-based ones. This integrated study sheds light on the relationship between chemical structure and properties, including biodegradability in marine environments and eco-toxicity. Experimental results suggest that while aromatic monomers tend to accumulate, slight biodegradation occurs under certain conditions, indicating ecosystem adaptation to chemical pollutants [5,6].

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 101029444 (RenEcoPol), from ICSC – Centro Nazionale di Ricerca in High Performance Computing, Big Data and Quantum Computing, funded by European Union – NextGenerationEU - PNRR, Missione 4 Componente 2 Investimento 1.4 Grant number CN00000013.

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GREEN ALTERNATIVES FOR THE SYNTHESIS OF METAL–ORGANIC FRAMEWORKS

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The amount of research articles examining phosphorus-based metal-organic networks indicates that these kinds of materials have attracted a lot of attention [1-3]. Comparing carboxylic and phosphonic metal organic networks, phosphonic acids, through the three oxygen atoms attached to the phosphorus atom, increase the potential of the compounds to form new structures. Changing the synthesis parameters, for example pH, allows the deprotonation of phosphonic acids in successive stages. Thus, obtaining new adsorbent materials, metal organic networks (MOFs) modified with ionic liquids (ILs) in very small quantities, combines their properties and also favors the reduction of capital and operating costs and respectively facilitates the expansion of this technology on a large scale. It is well known that both IL and MOFs are versatile materials and present an encouraging potential for wide applications [4-6]. The variation of synthesis methods is very important by using the advantages brought by each method, both on the reaction product and on the environment [7-9]. Metal-organic networks (MOF) were synthesized starting from etidronic acid (HEDP), phosphonoacetic acid (PA), N,N-bis-phosphonomethylglycine (GLY) with the following monovalent metals M(I): silver, divalent M(II): cobalt, nickel, zinc, copper, manganese, calcium and trivalent metals M(III): cerium and lanthanum. Hydrothermal synthesis methods were used in different working conditions: hydrothermal synthesis at room temperature, in a water bath, in an autoclave. Accordingly, syntheses were also made under microwave, ultrasound assisted conditions and mechanochemical syntheses. The reaction parameters were optimized by varying: pH in the range 1-8; temperature between 25-180°C; the reaction time was varied between 2h -72h, the ultrasonic amplitude and the ratio between the reactants. The IL@MOF composites were made in 2 ways by co-synthesis and post-impregnation using N-methyl-N,N,N-trialchylammonium chloride (Aliq. 336); 1-butyl-3-methylimidazolium trifluoromethanesulfonate [BMIM][OTF], 1-butyl-3-methylimidazolium nitrate [BMIM][NO3], 1-butyl-3-methylimidazolium chloride [BMIM][Cl] and 1-hexyl-3-methylimidazolium [HMIM][Cl]. The synthesized compounds were analyzed and characterized by FT-IR, X-ray diffraction, TGA, SEM, EDX.

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CUTTING-EDGE MOLECULAR INSIGHTS FOR SUSTAINABLE SYNTHESIS OF HIGHLY SOLUBLE PRODRUGS VIA TARGETED BIOCATALYTIC ESTERIFICATION

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Enzymes have revolutionized chemistry by seamlessly blending molecular precision with environmental care. This innovative approach has facilitated the development of sustainable methods for producing fine chemicals, offering a greener alternative to traditional synthesis by replacing harmful solvents with eco-friendly, regio- and stereospecific biocatalysts.

Herein, we highlight the biocatalyzed synthesis of highly soluble prodrugs of several compounds with significant market impact, including ursodeoxycholic acid[1], used in the treatment of gallstones; ibuprofen[2], one of the most widely used anti-inflammatory drugs; and various cinnamic acid derivatives, such as ferulic and caffeic acids. To address these challenges, we studied the molecular mechanisms of regio- and stereo-selective esterification through molecular docking studies, which elucidated the interactions between the lipases and the substrates. Nine different cinnamic acid derivatives, celebrated for their antioxidant and anti-inflammatory properties, were studied[3]. Through both molecular docking and experimental evidence, we demonstrated that hydroxyl groups on the aromatic ring can significantly limit the conversion to corresponding esters. Moreover, the degree of unsaturation of the derivative influences the favorable poses in the active site of the lipase, resulting in conversions exceeding 95% under optimal conditions (10 g/L of lipase, 90°C, molar ratio of 3:1 acid/alcohol, 72 hours). These advancements not only highlight the superior efficacy of prodrugs over traditional compounds but also reflect the commitment to sustainability and the circular economy. This journey illustrates a harmonious integration of chemical innovation and environmental responsibility, heralding a future where chemistry continues to advance in alignment with sustainability and health protection.

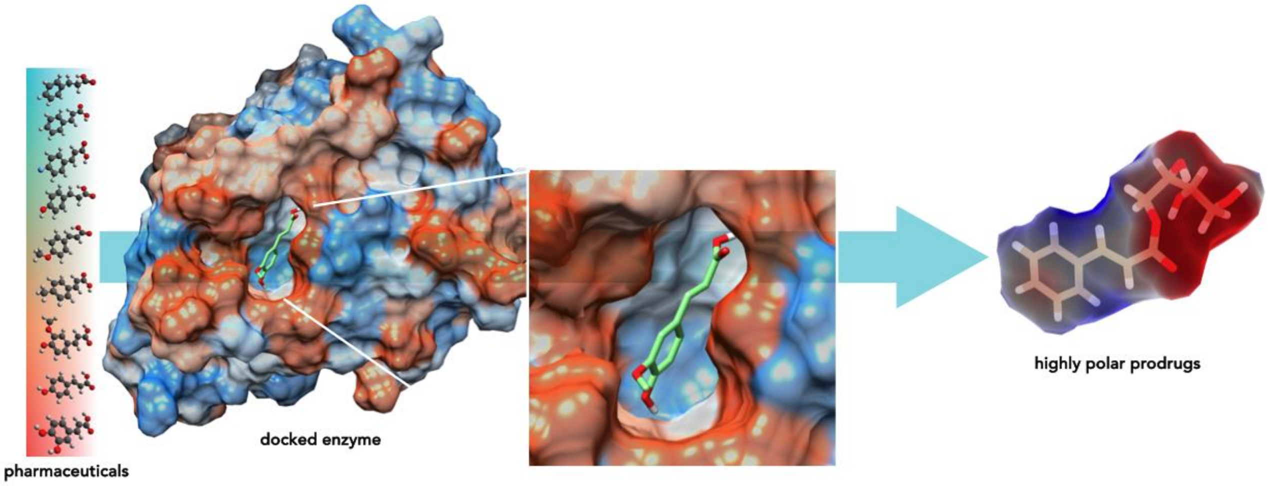

Figure 1: Docking and experimental optimization of enzymatic processes for the green synthesis of enhanced biobased prodrugs.

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THE SYNTHESIS OF NOVEL POLYESTERAMIDES THROUGH BIOCATALYTIC METHODS FROM ε-CAPROLACTAM AND HYDROXY ACIDS

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In the quest for new polymeric materials, a biocatalytic approach represents an exciting opportunity to develop innovative polymers of the polyesteramide class [1]. The sustainability of biocatalysis circumvents problems associated with classical chemical catalysis, such as residual toxicity and the high energy demand of elevated temperatures [2]. Another important element of this research direction is the incorporation of various monomers to customize the properties of these polymers [3]. Strategies such as integrating different units of hydroxy acid into the polymeric chain or leveraging the diverse morphologies arising from ε-caprolactam are progressive approaches in the synthesis of polyesteramides [2]. Given that hydroxy acids and ε-caprolactam can be produced by converting a wide range of renewable biomass resources, they serve as suitable building blocks for biobased polyesteramides, providing an alternative to fossil-based polymeric materials [4].

Four novel polyesteramides were successfully synthesized enzymatically using ε-caprolactam and a selection of different saturated hydroxy acids, namely L-malic acid, 3-hydroxybutyric acid, 12-hydroxystearic acid and 16-hydroxyhexadecanoic acid, respectively, all derived from fatty acids or their metabolites. Utilizing a green and sustainable method, the synthesis of short chain polyesteramides was achieved, which may find applications in biomedical nanomaterials and cosmetics, such as nanosized drug carrier formulations. The effects of several reaction parameters were explored, including reaction temperature, the molar ratio of monomers, the reaction medium, and the time course of the reaction. Characterization of the reaction products was conducted through various methods, including SEC chromatography, MALDI-TOF MS, FT-IR spectroscopy, as well as NMR. The properties of these enzymatically synthesized polyesteramides can be precisely adjusted for specific applications based on the required characteristics. The most effective results were achieved by employing 16-hydroxyhexadecanoic acid in a 2:1 molar excess to ε-caprolactam at 80°C, resulting in a product with a copolymer content of 75% and an average molecular weight greater than 3000 Da. Biodegradation assessment showed that 45% of malic acid-based polyesteramide was degraded within 21 days. Hence, this methodology introduced ε-caprolactam alongside a hydroxy acid as a co-monomer for the first time in the lipase-catalyzed synthesis of both linear and cyclic polyesteramides.

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COMPARATIVE STUDY OF METAL CONCENTRATION DETERMINATION IN ALBUMEN OF HEN EGGS ORIGINATING FROM INDUSTRIAL POULTRY FARMS, BACKYARD AND FREE-RANGE HENS USING ICP-OES TECHNIQUE

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There have been multiple types of research focusing on the relationship between feed ingredients and metal content in the egg white due to their role in human nutrition. The aim of the present study is to determine the metal concentration in hens' eggs and, in particular, to compare the metal concentration in egg albumen originating from industrial poultry farms with that of backyard and free-range hens.
All samples were collected in Romania from five separate counties and 10 different farms, over a period of two weeks and, as a result, a total of 50 were collected, 10 from each housing system (batteries/cages, litter/soil, free-range, organic and backyard). The measurements of the metals were taken by Inductively Coupled Plasma Optical Emission Spectrometry (ICP-OES), with a wide range of elements reported. For the essential elements, we measured Cr, Cu, Fe, Mn and Zn; Al, Cd, Ni and Pb for the heavy metals and, in addition, we measured B, Ba, Sr, Ca and Mg.
The present study revealed that the metals in eggs from free-range hens are richer in essential elements with mean concentrations as follows: 1.528 mg/kg for Fe, 3.278 mg/kg for Zn, 0.058 mg/kg for Mn and 1.362 mg/kg for Cu.
We concluded that the egg quality is closely connected with the housing system and nutrition. Furthermore, the results demonstrate that eggs from backyard housing are no better than those from free-range hens in terms of essential metal composition. The heavy and non-essential metal contents, present in the albumen of all the examined eggs, were much lower than the maximum allowed concentration and, therefore, egg consumption does not pose any risk to human health.

RESEARCH ON THE USE OF WALNUT SHELLS-DERIVED BIOCHAR FOR THE ADSORPTION OF PESTICIDES FROM AQUEOUS MEDIA

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Modern agriculture heavily relies on pesticides. Nevertheless, inefficient application, pesticides resistance, as well as the environmental conditions can decrease their efficiency, conducting to pesticides transfer into surface waters and soil, adversely affecting the physicochemical properties, flora and fauna, or enzymes activity. If different pesticides interact, a combined toxicity may result, affecting the biodiversity. Moreover, pesticides exposure can result in both acute and chronic effects on human health. Biochar, due to its high specific surface area and porosity, offers numerous adsorption sites, proving its use in agriculture or environment. Added to water or soil, biochar can absorb or degrade pesticides from contaminated sites. This study provides a laboratory model of pesticides removal from aqueous media. The biochar was previously synthesized from walnut shells by pyrolysis at 550 °C, followed by a treatment with 1M $FeCl_3$, re-calcination at 550 °C, and functionalization of the magnetic biochar with cetyltrimethylammonium bromide [1]. For comparison, a char was prepared using commercial activated carbon according to the same scheme. For the pesticide's adsorption tests, a 0.1 mg/L solution containing 20 pesticides was prepared using an organochlorine pesticides mixture (LGC Standards). Sampling was achieved after 5, 8 and 24 hours and a GC-ECD analysis was performed for identification and quantification before and after adsorption. Total organic carbon (TOC) and chemical oxygen demand (COD) were determined using HACH cuvette test TOC (differential method) 60-735 mg/L C and cuvette test COD 0-1000 mg/L O_2. The adsorbents were investigated by FTIR before and after adsorption. It was observed that, after 5 hours most of the pesticide's concentrations sharply decreased, trend kept after 8 hours (some of pesticides being under limit of detection-LOD of 10 µg/L), after 24 hours all pesticides being under LOD. Comparing, when commercial activated carbon was used, no significant decrease of pesticides concentration was observed after 5 or 8 hours, the adsorption process starting after this period, the concentration of all pesticides being under LOD at the end of experiment. Although after 24 hours the concentrations were undetected/under LOD in both adsorption models, it was noted that, in the case of using magnetic biochar obtained from waste, the necessary adsorption time decreased, this influencing also the adsorption rate. The results were confirmed by TOC and COD analysis, in the case of biochar all values being under the ones when commercial activated carbon was used. Various pesticide`s functional groups were identified within the FTIR spectra, confirming their immobilisation. The study can represent a starting point in using agriculture wastes for obtaining added-value products in order to reduce pollution induced by pesticides usage, in the context of environmental protection and circular economy, targeting the concept of "*zero waste*".

Part of this complex research was conducted under Sectorial Plan-ADER 2026, Project ADER 6.3.7 – "*Applicability measures regarding the investigation of the organochlorine and organophosphorus contaminants distribution on the soil-plant-vegetable/fruit-finished product chain, following different types of soils in various areas*" financed by the Ministry of Agriculture and Rural Development – Romania; the other part was conducted under NUCLEU Program—Financing Contract 20N/05.01.2023, project PN 23150402-"*Laboratory experiments valorisation in the development of technologies for the production of biofuels from agro-industrial waste*", financed by Romanian Ministry of Research, Innovation and Digitalization.

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COMPUTATIONAL DESIGN OF SELECTIVE JAK1 INHIBITORS FOR PSORIASIS

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Autoimmune diseases like psoriasis are increasingly prevalent, especially among young individuals, and pose a significant medical challenge due to their complex nature and the urgent need for effective therapies to enhance patients' quality of life. Current treatments for psoriasis often target specific proteins involved in these pathological processes, such as TNF-α, IL-17, IL-33, and PDEs. A more recent approach involves targeting Janus kinases (JAKs), particularly JAK1, due to their role in cytokine signaling. Although JAK1 inhibitors have shown significant efficacy in alleviating psoriasis symptoms, they can also cause undesirable side effects, such as immune suppression and increased infection risk. To address this, developing more selective JAK1 inhibitors that minimize interaction with JAK2 is a promising strategy to enhance the safety of JAK-targeted therapies. This study aims to identify selective JAK1 inhibitors using computational chemistry and cheminformatics methods. We evaluated the interactions between the studied compounds and JAK1 and JAK2 kinases, which share significant sequence similarity (>85%). This similarity complicates the development of selective inhibitors necessary to avoid adverse effects. The study incorporated protein flexibility into molecular docking simulations, utilizing multiple static frameworks to represent the full conformational space of JAK1 kinase. Compounds with high affinity for JAK1 and minimal interaction with JAK2 were selected for further experimental testing, potentially leading to safer and more effective therapies for psoriasis.

FABRICATION OF CHITOSAN/POLYVINYL ALCOHOL/GLYCEROL NANOFIBROUS MEMBRANE AND ITS PROFERMANCE

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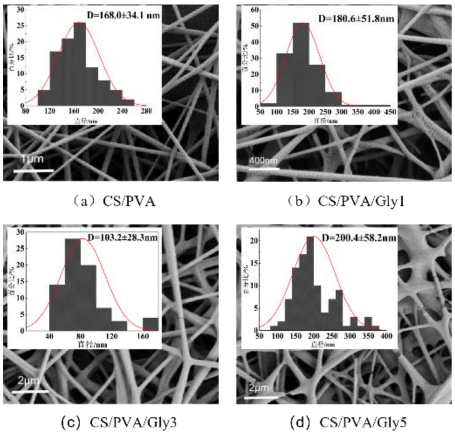
Chitosan is a natural biopolymer derived from chitin and has been taken as promising material for biomedical applications. Therefore, the chitosan nanofibrous membranes have attracting much attention in recent year. However, it has some disadvantages in mechanical property and water stability [1]. In this work, a mixture of chitosan (CS), polyvinyl alcohol (PVA) and glycerol (GLY) has been prepared, and then its nanofibrous membrane was prepared by electrospinning. The CS/ PVA/GLY nanofibrous membrane was evaluated in terms of morphology, microstructure, thermal property, hydrophilicity, water stability, mechanical property and anti-bacteria property. The results showed that GL improved the hydrophilicity, water stability, and mechanical property of CS/ PVA/GLY nanofibrous membrane. Besides, the CS/ PVA/GLY nanofibrous membrane demonstrated a good anti-bacteria property to Escherichia coli and Staphylococcus aureus, corresponding to anti-bacteria rate of 94.39% and 89.65%.



(a) CS/PVA (b) CS/PVA/Gly1 (c) CS/PVA/Gly3 (d) CS/PVA/Gly5

Figure 1. Morphology of nanofibrous membranes

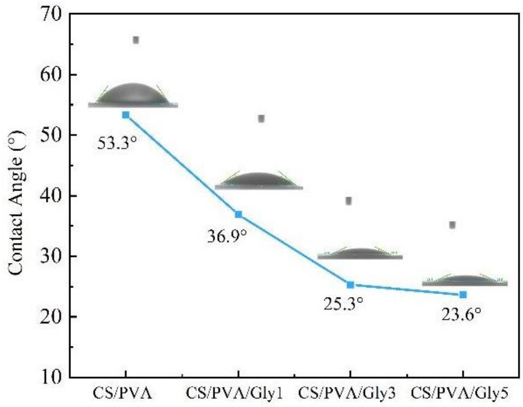


Figure 2. Hydrophilicity of nanofibrous membranes

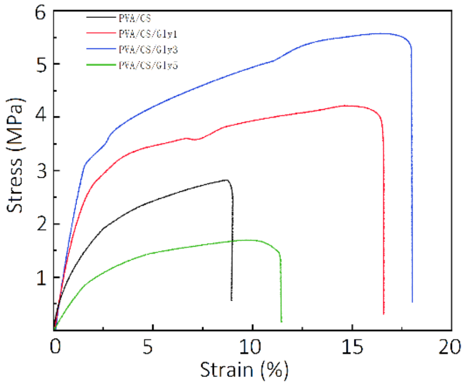
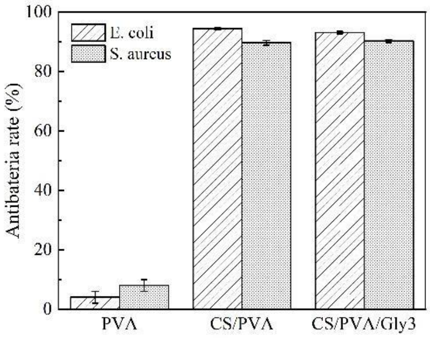


Figure 3. Tensile property of nanofibrous membrane



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SYNTHESIS AND CHARACTERIZATION OF NOVEL POTENTIAL THERAPEUTICAL COMPOUNDS BASED ON 5-BROMO-2-THIOPHENE CARBOXYLIC ACID SCAFFOLD

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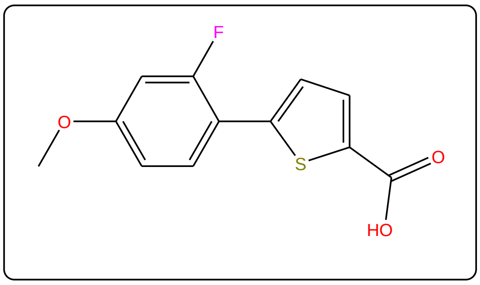
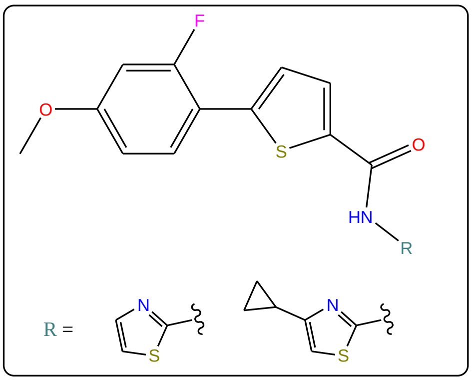
Aiming for high efficiency and selectivity with low toxicity and very few side effects in cancer treatment is almost an impossible task and sounds much more of a dream than a reality [1]. Cancer poses a real threat and the only certain aspect of it is that it is a silent killer and there is not much of a treatment available to face such a tremendous challenge [2]. Cancer is not a single disease but rather a group of diseases that act upon cell's proliferation mechanisms, inducing a chaotic and uncontrollable multiplication of cells [3]. Developing a treatment for a disease requires, by any means, precise knowledge about the root cause of the disease, which, currently showed up on the stage as many possible triggering pathways for cancer [4]. Pharmaceutical companies and many research facilities around the world are trying, every single day, to come up with a wonder compound that can at least decrease the probability of death caused by cancer if not to cure it [4]. Here we present the synthesis and characterization of a novel series of compounds (Scheme 1) and (Scheme 2) which will be tested for potential selective cytotoxic activity against cancer cell lines. Structural aspects regarding these compounds resides in the design of a thiophene scaffold substituted on positions 2,5. In position 2 it has an amide group with different types of substituents found in many candidates showing promising activity as anticancer agents as well as a 3-fluoroanisole substituent in position 5. Structural characterization as well as purity of the synthesized target compounds was carried out using 1D and 2D-NMR spectroscopy.



Scheme 1. Chemical structure of 5-(2-fluoro-4-methoxyphenyl) thiophene-2-carboxylic acid



Scheme 2. Chemical structure of 5-(2-fluoro-4-methoxyphenyl) thiophene-2-carboxamide compounds

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DETECTION OF LIDOCAINE BY OPTICAL METHOD USING AS SENSITIVE COMPOUND A Co(II)-AZAPORPHYRIN

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Lidocaine hydrochloride is one of the most used local anesthetics in dentistry due to its important properties as fast relief, excellent anesthetic effects, and minimal allergenicity [1]; offers cerebral protection in post-surgery when patients often suffer from postoperative neuropsychological impairment, as a high-risk perioperative brain injury [2]. Certain levels of lidocaine (8 to 14 µg/mL) can induce convulsions and loss of consciousness and starting from 26 µg/mL it can even lead to cardiac arrest [3]. In order to detect lidocaine, we propose an economical, fast, and precise UV-Vis method, using a metalated porphyrin, namely Co(II)-2,7,12,17-tetra-tert-butyl-5,10,15,20-tetraaza-21H,23H-porphine (Co-TBAP), that can act as sensitive material.

The detection of lidocaine by this spectroscopic method can be accurate in the concentration domain $1.95 \times 10^{-5} – 1.38 \times 10^{-4}$ M, without interference of other species present in blood serum. The limit of detection is 6.724×10^{-6} M. The lidocaine concentration domain detectable by this method fits with the limits in blood and serum [4].

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ION MOBILITY MASS SPECTROMETRY REVEALS THE HIGH COMPLEXITY OF ANENCEPHALY ASSOCIATED GLYCOSPHINGOLIPIDS

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Anencephaly is the most frequent lethal congenital malformation of the central nervous system, that results from defective closure of the neural tube, during fetal development [1]. This condition involves the total or partial absence of the cranium, cerebrum, cerebellum and basal ganglia [2]. Anencephaly can lead to death before or after birth, often within a week [1]. Typically, it can be detected by ultrasound screening, in the first trimester of pregnancy [3], but over the years, various methods based on the identification of molecular markers have been developed to facilitate earlier diagnosis. Since the level of glycosphingolipids, especially of the sialylated glycoforms known as gangliosides, is higher in the central nervous system than in the extraneural tissue, they play a crucial role at the brain level in health and disease. Most recently, anencephaly-associated gangliosides have been investigated by a variety of techniques, mostly by mass spectrometry, alone or coupled with separation methods. However, currently ion mobility mass spectrometry is one of the most powerful analytical systems for mapping and structural characterization of central nervous system gangliosides, due to its capacity to separate even low abundant ions depending on their mass, charge, shape, number of sialic acid residues, glycan chain and ceramide composition.

In this context, here we have optimized and introduced nanoESI IMS MS and collision-induced dissociation (CID) tandem MS (MS/MS) in negative ion mode, under identical conditions for each sample, to investigate the ganglioside expression in human anencephaly. The three native ganglioside mixtures explored in our study were extracted from histopathologically defined residual cerebrum from anencephalic fetuses in the 28th, 35th and 37th gestational weeks (g.w.) and compared with each other and with a normal fetal frontal lobe ganglioside mixture. Using IMS MS a total of 343 distinct species of anencephaly-associated gangliosides were detected. The largest number of species was observed in the 37 g.w. sample (223), followed by 35 g.w. (197) and 28 g.w. (162), suggesting that during brain development the number of species increases even in the residual cerebrum affected by anencephaly. IMS MS method revealed significant differences in ganglioside expression between the three samples and between anencephalic remnant and normal fetal tissue. IMS MS allowed the identification of 2.2 times more anencephaly-associated species compared to any previously used method, including fucosylated, acetylated, CH_3COO^-- and *O*-GalNAc-modified structures. The fragmentation analysis by CID MS/MS enabled the isomer discrimination and a detailed structural characterization of species with potential biomarker role.

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PHYSICO-CHEMICAL PROPRIETIES OF POROUS SILICA SYNTHETIZED USING IONIC LIQUIDS FOR HYDROGEN STORAGE APPLICATION

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Mesoporous silica particles were synthesized by the sol-gel method, starting from different ratio of tetramethoxysilane (TMOS) and trimethoxymethylsilane (MTMS). The 1-Butyl-1-methylpyriolidinium tetrafluoroborate [(BMPy)(BF4)], an ionic liquid, was added to the silica precursor in water solution, as co-solvent and as directing agent [1].

All produced samples were analyzed with Scanning Electron Microscope (SEM), Energy Dispersive X-ray spectroscopy (EDX), and Fourier-transform infrared spectroscopy (FTIR) to have the morphological and the chemical characterization [2]. Subsequently, porosimeter analyses were carried out with nitrogen at 77K up the relative pressure p/p°=1. Using the Brunauer–Emmett–Teller (BET) and Barrett-Joyner-Halenda (BJH) model, the specific surface area, pore distribution, and total pore volume were respectively calculated [3].

In addition, to physical-chemical characterizations, preliminary tests were carried out on the use of materials produced for the adsorption of hydrogen. Hydrogen isotherms were acquired at the temperature of liquid nitrogen and low pressure up to 1 bar. The nanostructures synthesized showed interesting performance in terms of gas adsorbed.

The purpose of research was to understand how the concentrations and method of extraction of the direct agent influence the surface and structure of the samples produced, correlated to the gas adsorption.

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MCM48 MESOPOROUS MOLECULAR SIEVES: SYNTHESIS, CHARACTERIZATION AND CO_2 ADSORPTION-DESORPTION INVESTIGATIONS

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The adsorption-desorption of CO_2 and the influence of temperature for CO_2 adsorption on MCM48 mesoporous molecular sieves by using temperature programmed desorption – TPD method was investigated. MCM48 with cubic Ia3d structure was synthesized using the cationic surfactant hexadecyltrimethylammonium bromide (CTAB) as a template agent and tetraethylorthosilicate (TEOS) as a silica source. The resulted material was first functionalized with (3-glycidyloxypropyl)trimethoxysilane (KH560); further, two types of amination reagents were used: ethylene diamine (N2) and diethylene triamine (N3).

These mesoporous silica-based materials, have been developed as efficient catalyst carriers, adsorbents, and cutting-edge drug delivery systems [1]. This is because of their very considerable thermal stabilities, porous morphologies, huge surface areas, and highly reactive surfaces in contact with the silanol groups [2, 3].

The modified amino-functionalized materials were further characterized by different investigation methods: X-ray diffraction (XRD) at low angles, infrared spectroscopy (FT-IR) and nitrogen adsorption–desorption experiments at 77 K.

Table 1. Textural properties of investigated mesoporous molecular sieves.

No.	Sample	Specific surface area (m^2/g)	Pore volume BJH_{Des}(cc/g)	Avarage pore diameter BJH_{Des}(nm)
1.	MCM48	1466	0.803	3.49
2.	MCM48-KH560	626	0.296	3.92

In case of MCM48 KH560 N3 were obtained very promising result for CO_2 adsorption at 30 °C: adsorption capacity of 3.17 mmol CO_2/g SiO_2, and an efficiency of amino groups of 0.58 mmol CO_2/mmol NH_2. In case of adsorption–desorption cycles the results shows that the performance of the MCM48 KH560 N2 and MCM48 KH560 N3 adsorbents is relatively stable, presenting a low decrease in the adsorption capacity. The results reported in this paper for the investigated amino-functionalized molecular sieves as absorbents for CO_2 can be considered as promising.

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MOLECULAR DYNAMICS STUDIES FOR MODELING AHAS – HERBICIDE BINDING PROCESS

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Molecular dynamics (MD) simulations are a tool designed to help explore and understand "macromolecular structure-to-function relationships". [1] MD simulations investigate the dynamic evolution of the systems over time, giving us insight about fluctuation, flexibility and stability of the systems, as well as about the interaction between the molecules of a complex. In this work MD was applied for the study of herbicide - enzyme acetohydroxyacid synthase (AHAS) complexes, which are involved in herbicide resistance issues. It is known that AHAS enzyme is a top target for developing of many herbicides, but in the recent years the intensive use of these herbicides led to the emergence of resistance of weeds. It has been observed that certain point mutations predispose to the appearance of resistance. In this context, the W574L, one of the most prevalent mutation, in some cases the only one necessary to confer resistance [2], was taken into consideration to be further investigated by in silico methods, such as: homology modeling, molecular docking and MD simulations. The proteins obtained by homology modeling for the AHAS enzyme were subjected to molecular docking along with a series of herbicides that induce resistance. MD simulations were performed on the best poses obtained by docking, in the NPT ensemble at temperature of 300 K and 1 bar pressure over 200 ns, and allowed us to draw the following conclusions. Residues R377 and K256 work like key anchors of herbicides in AHAS binding site. For the susceptible variant the stabilization of the ligand in the binding site was much stronger than in the case of the resistant variant. These results allow a deeper understanding of the mode of action of herbicides on the susceptible/resistant AHAS enzyme belonging to invasive plants.

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INFLUENCE OF THE HYDROGEN PEROXIDE PRESENCE ON THE PHOTODEGRADATION EFFICIENCY OF DYES USING COPPER(II) COORDINATION POLYMER

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The rapid expansion of cities and the development of the textile industry in recent decades have caused serious water pollution problems. In recent years, various methods have been tested for the treatment of colored wastewater. Among these photodegradation, an advanced oxidation process has been successfully applied for the degradation of chemicals, e.g. dyes, from industrial effluents [1]. Recently, coordination polymers have attracted increased interest, due to their effective application in the sustainable treatment of wastewater [2, 3]. Therefore, as a continuation of our work [4] in the present study the photodegradation efficiency of two azo dyes from single and binary system, using a copper(II) coordination polymer was investigated. $^{1}_{\infty}[Cu_3L_2(N_3)]CH_3COO$ was applied as catalyst and Acid Orange 7 (AO7) and Methyl Orange (MO) were selected as water pollutants. The influence of the hydrogen peroxide presence, reaction time, and dye concentration on the photodegradation efficiency of AO7 and MO was investigated. The use of H_2O_2 for the degradation of colored pollutants is useful as an auxiliary oxidant, due to the formation of additional highly reactive hydroxyl radicals [5]. The obtained results with and without H_2O_2 under visible light irradiation, highlights the fact that the removal efficiency of AO7 and MO increased slightly in the presence of hydrogen peroxide. For the binary solution, lower degradation efficiencies were obtained compared to the single solutions due to the fact that the dyes in the binary solution compete for the active centers on the coordination polymer surface, available for adsorption and degradation. From the point of view of the individual dyes in the binary system, yields higher than 72% were obtained for both dyes using the studied coordination polymer. When H_2O_2 was added, similar to single dye solutions, the degradation efficiency of both dyes in the binary system increased to over 81%.

Overall, taking into account that the addition of hydrogen peroxide into the system slightly increased dye degradation by 6.70% for AO7 and 24.30% for MO along with the additional costs and possible pollution involved we considered that is more feasible to continue further studies in the absence of H_2O_2.

The photodegradation efficiency decreases and the necessary time for the degradation process increases with increasing concentration of the dye solutions.

The excellent stability of the copper(II) coordination polymer after the photodegradation process of dyes from both simple and binary solutions was demonstrated by the consistency of the initial and final structure of the complex.

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THE USE OF CHROMATOGRAPHIC METHODS FOR MONITORING FERMENTATION PROCESSES WITH OBTAINING BIOFUELS

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Due to the scarcity of fossil fuels and the high demand for energy associated with environmental risks, the attention of the population has turned to finding alternative sources of green energy, such as biofuels [1]. Biotechnological transformation of lignocellulosic biomass in to biofuels (bioethanol, biohydrogen, biomethane, hythane) by saccharification of the pretreated lignocellulose, followed by fermentation of the resulted sugars by microorganisms represent a promising technology which can promotes a sustainable development and contributes to circular bioeconomy development [2]. The resulting fermentation broth is a complex mixture which require continuous monitorization in terms of carbohydrate composition, by-products and inhibitors in order to optimize the quality of the resulting biofuels.

This study aims to develop some chromatographic methods for the control of the fermentation processes aiming to obtain biofuels, particularly bioethanol. Thus, high performance liquid chromatographic methods were developed for carbohydrate composition (xylose, arabinose, fructose, glucose, galactose and sucrose) by HPLC-CAD, organic acids (formic, acetic, propionic and butyric acids) and inhibitors (furfural and 5-HMF) by HPLC-DAD. Chromatographic conditions (stationary phase and mobile phase, gradient elution, separation temperature) were optimized in order to obtain efficient separation of the compounds. The calibration curves were made based on successive solutions made from stock solutions, covering a calibration range between 25-500 µg/mL for each sugar compound, 0.25-2.5 mg/mL for organic acids and 0.025-0.25 mg/ml for furfural and 5-HMF. In order to determine the alcohol content of the fermentation broth (ethanol, propanol, isopropanol and isobutanol) a GC-FID method was optimized using TG-WAXMS column (60 m x 0.32 mm x 0.25 µm) with a temperature gradient from 40ºC to 200ºC and with N_2 for elution of the sample through the column with 30ml/min. The calibration range was between 0.5-5 mg/mL for propanol, isopropanol and isobutanol and between 2.5-25 mg/mL for ethanol. Good linearities were obtained for all the analyzed compounds.

The proposed chromatographic methods for monitoring the fermentation broth proved to be adequate and the validation parameters of the methods fulfilled satisfactory criteria. The methods were successfully used to control the fermentation process of lignocellulosic biomass to obtain bioethanol.

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THE ROLE OF DIFFERENT STRESSORS IN ALTERING PLANT PHYSIOLOGY AND SECONDARY METABOLITES

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Plants are subjected to a variety of stressors, including abiotic factors such as drought, extreme temperatures, and salinity, as well as biotic factors like pests, pathogens, and herbivores. To cope with these stressors, plants employ various defense strategies that are categorized as direct or indirect. Direct defense strategies involve the production of physical barriers like thorns and trichomes, and chemical defenses such as synthesizing toxic compounds or enzymes that deter herbivores and pathogens. Indirect defense strategies include attracting the natural enemies of herbivores or pathogens, for example, by releasing volatile organic compounds that attract predatory insects feeding on the herbivores attacking the plant. In this study, we investigated the influence of different abiotic and biotic stressors on plants from the *Galium* and *Helichrysum* genera to understand how these plants respond to various stresses. Plants were grown from seeds in growth chambers and subjected to different abiotic stresses (temperature, drought, flooding) and biotic stresses (pests, pathogens, herbivores). Secondary metabolites were analyzed using the HPLC method, while photosynthetic parameters were measured using a gas exchange system. Our results revealed that environmental stress conditions significantly altered photosynthetic parameters, volatile organic compound emissions, chlorophyll content, and total polyphenol concentrations in these plants. Additionally, secondary metabolite concentrations varied for plants grown in different locations. Overall, our study demonstrates that *Galium* and *Helichrysum* plants exhibit significant changes in physiological and biochemical parameters in response to abiotic and biotic stressors, with notable effects on photosynthetic parameters, volatile organic compound emissions, chlorophyll content, and total polyphenol concentrations.

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MACHINE LEARNING MODELS IN ANTIVIRAL INHIBITOR RESEARCH: A PRELIMINARY INVESTIGATION

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The continuous fight against viral diseases highlights the necessity for novel approaches in developing antiviral drugs. Machine learning (ML) has appeared as a necessary tool in drug discovery processes, mainly through the application of classification models. This preliminary investigation explores the use of ML classification models in antiviral inhibitor research. We applied several ML algorithms, including Support Vector Classification (SVC), Multi-Layer Perceptron (MLP), Random Forest Classification (RFC), and Convolutional Neural Networks (CNN) to classify antiviral compounds based on their biological activity. Employing Chembl datasets with chemical and biological information, our preliminary analysis revealed that SVC provided high accuracy in distinguishing effective inhibitors (specified as actives) from less potent ones (indicated as inactive). The ML models offer a valuable understanding of compounds' structure-activity relationships and help researchers with the identification of promising new antiviral candidates. Our future work will focus on refining these models to enhance their predictive power, accuracy, and reliability in the exhaustive field of drug discovery.

MULTICOMPONENT ORGANIC CRYSTALS BASED ON THE BENZOIC ACIDS - ALKANOLAMINES SYSTEM

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Multicomponent crystalline materials such as salts, cocrystals, salt cocrystals, solvates, and coordination compounds, continue to drive important developments and a wide range of applications in numerous scientific domains. The precise control of intermolecular interactions through crystal engineering has allowed the development of new functional materials. The aim of this study is to present the synthesis of new multicomponent crystals based on the benzoic acids–alkanolamines system. A thorough examination of their ionicity, thermal stability, phase transitions, polymorphism, and intermolecular interactions is part of this. The results reveal that benzoic acids and alkanolamines play a crucial role in the formation of 1D, 2D, and 3D structural networks through strong and directional hydrogen bonds formed by cations and anions [1-4].

The current challenge in this area is to control the formation of multicomponent crystals with specific properties by identifying factors that influence changes in the ionization state in acid-base systems. For example, in systems comprising 4-nitrobenzoic acid and 2-chloro-5-nitrobenzoic acid with alkanolamines, our findings indicate that the solvent, rather than stoichiometry, primarily dictates the formation of various multicomponent crystals [1, 4].

The study of supramolecular synthons and the topologies formed through hydrogen bonds, π-π stacking, dipole-dipole interactions, and their combinations was also explored. The results demonstrated that these weak interactions are essential for studying the relationship between molecular structure, supramolecular structure, and solid-state luminescence properties.

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NOVEL LIQUID CRYSTALLINE DERIVATIVES CONTAINING FLUORENONE STRUCTURES

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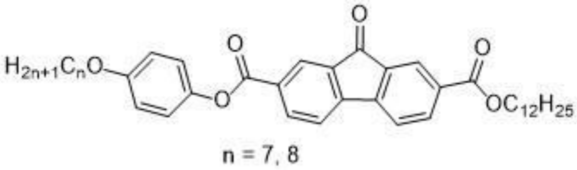
The design and development of novel fluorenone materials has gained an increased interest in the last decades due to their unique combination of chemical, structural, and optical properties [1]. Fluorenones are important building blocks for optoelectronic materials such as OLED devices [2], memory devices [3], nonlinear optical materials [4], as well as solar cells [5], sensors and imaging agents [6].

Considering the importance of fluorenone based LCs, herein we report the design, synthesis and characterization of novel potential fluorenone-based bicatenar mesogens. The compounds contain a central fluorenone mesogenic unit connected with 4-alkoxybenzoate unit at one end and dodecylcarboxylate chain at the other end (Scheme 1).



Scheme 1. Chemical structures of compounds

The purity and structural characterization of the intermediates and target compounds were carried out using 1D and 2D-NMR spectroscopy and elemental analysis. The effect of the chain length on the selfassembly behavior in LC was studied by differential scanning calorimetry (DSC), polarising optical microscopy (POM) and X-ray diffraction (XRD). The synthesized compounds displayed smectic and nematic phases.

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OPTICAL QUANTIFICATION OF MUREXIDE USING A METALLOPORPHYRIN WITH MANGANESE AS A SENSITIVE MATERIAL

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Murexide, with the IUPAC name ammonium 2,6-dioxo-5-[(2,4,6-trioxo-5-hexahydropyrimidinylidene)amino]-3H-pyrimidin-4-olate, is an synthetic compound frequently used in biochemical and histological applications [1]. Also, the vibrant and great coloring power of murexide make it particularly useful in various staining procedures.

In histochemistry, murexide is notably effective for identifying calcium deposits within biological tissues, such as skeletal structures [1-2]. This characteristic makes it an essential tool for researchers and clinicians, especially in the study and assessment of dental health, including the detailed examination of hemi-jaws for dental caries [3]. Its chemical versatility and staining capabilities underscore its importance in scientific investigations and diagnostic practice.

In this study, a porphyrin derivative functionalized with a carboxyphenyl group and metalated in the center of the porphyrin core with Mn(III) was used. The ability of porphyrin to detect murexide was demonstrated using the UV-Vis spectrophotometric titration method. The range of detection and quantification of murexide using this simple optical method is between 2.05×10^{-5} M and 4.35×10^{-5} M.

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SYNTHESIS OF TRIAZOLE HETEROCYCLIC INTERMEDIATES AND LIGANDS FOR ”CLICK” CHEMISTRY

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The copper(I)-catalyzed cycloaddition between a terminal azide and an alkyne (CuAAC), commonly called ”click” reaction, is an efficient method for introducing a covalent linkage between two molecular units, with the regiospecific formation of a 1,4-disubstituted 1,2,3-triazole [1]. The two functional groups, azide and alkyne, can be readily introduced into the scaffold of various biologically-relevant organic structures, and can be coupled efficently by virtue of their bioorthogonal nature [2]. Usually, the CuAAC reaction uses as catalyst Cu(I) complexed with a suitable chelating ligand [3] such as TBTA (tris(benzyltriazolylmethyl)amine) or THPTA (tris(hydroxypropyltriazolylmethyl)amine). It has been reported that the tris(triazolylethyl)amine ligands function by stabilizing Cu(I) ions against oxidation, thus accelerating the „click” reaction [4].

Our work focuses on the synthesis of a series of intermediates and novel heterocyclic triazole ligands, such as tris(hydroxymethytriazolylethyl)amine. We present a new method for synthesizing these compounds, together with the difficulties encountered during synthesis and purification, and strategies for overcoming them. All compounds were purified and characterized by physical and spectral analysis using ^{1}H–NMR, ^{13}C–NMR and Mass Spectroscopy.

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FACILE SPECTROSCOPIC DETECTION OF PANTOPRAZOLE USING A COBALT-METALATED PORPHYRIN

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Pantoprazole is a benzimidazole derivative with a structure consisting in a pyridine ring and a benzimidazole ring connected by a sulfinyl bridge. The active ingredient for the commercially available drug is named according to IUPAC: sodium 5-(difluoromethoxy)-2-([(3,4-dimethoxy-2-pyridinyl)methyl] sulfinyl)-1*H* -benzimidazole sesquihydrate [1].

Pantoprazole is a well-known proton pump inhibitor, commonly used to treat various gastrointestinal conditions, by reducing the amount of acid produced by the stomach [2]. Patients susceptible to heart failure must be carefully monitored as pantoprazole proved to have a negative effect on cardiac contractility [3].

A simple and efficient UV-Vis method for the detection of pantoprazole using Co(II)-2,7,12,17-tetra-tert-butyl-5,10,15,20-tetraaza-21H,23H-porphine as sensitive material is proposed. The detection of the drug using this spectrophotometric method can be accurate in the concentration domain 1.96×10^{-5} - 2.95×10^{-4} M.

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DESIGN, SYNTHESIS AND EVALUATION OF NOVEL MESO-PHENOTHIAZINYL PORPHYRIN AS PHOTOSENSITISER IN PHOTODYNAMIC THERAPY.

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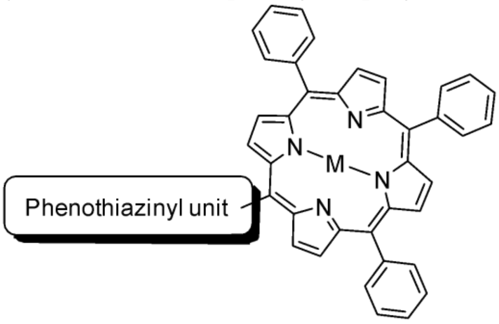
Organic dyes containing phenothiazine chromophore are well known for their medicinal applications derived from their metachromatic staining, antimicrobial and photosensitizer properties [1,2, 3].
The new meso-substituted AB_3-type phenothiazinyl-porphyrin were obtained by Suzuki-Miyaura or Mizoroki-Heck cross-coupling reactions from AB_3-type meso-substituted halogeno-porphyrin derivatives, the free base porphyrins were subsequently employed in the complexation reaction.



The potential of meso-substituted phenothiazinyl-porphyrins to act as photosensitizers in photodynamic therapy (PDT) was evaluated by measuring the generation of singlet oxygen under light irradiation and by studying the effects of PDT on mitochondrial function, reactive oxygen species (ROS) levels and modulation of nuclear factor erythroid 2-related factor 2 (Nrf2) in A2780 cells in the dark and under light irradiation.
It has been demonstrated that all the biological properties that can convey towards tumour growth inhibition are better expressed and enhanced in indium-functionalized porphyrins as the most active in dark conditions, exhibiting a good PDT activation.

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POLYPHENOLIC COMPOSITION OF GRAPE POMACE EXTRACTS OBTAINED BY SUPERCRITICAL FLUID AND MICROWAVE EXTRACTIONS: A COMPARATIVE STUDY

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Grape pomace is a winemaking byproduct which still contain important amounts of secondary metabolites with numerous therapeutic properties, such as antioxidant, antimicrobial, anti-inflammatory, antihyperglycemic, etc. [1]. Phenolic extracts obtained from grape pomace have a high potential to be used as food and cosmetic ingredients in order to develop functional products with enhanced therapeutic potential [2].

In this work, a comparison of the polyphenolic composition of extracts obtained from different red grape pomace by using both types of extraction, supercritical fluid extraction (SFE) and microwave extraction (MAE) is undertaken. The investigation of bioactive characteristics (total polyphenols, total flavonoids, catechins, tannins, and antioxidant activity) was carried out by UV-Vis spectrophotometric methods, while the individual polyphenolic composition was investigated by target UHPLC-HRMS/MS analysis.

Dehydrated grape pomace (Vitis vinifera L.) was subjected to: 1) SFE by running carbon dioxide coupled with ethanol as a modifier in 20:1 ratio, at 3000 psi and 2) MAE using a 70% ethanolic solution, at 1000 W applied power. Higher phenolic concentrations of extracts were attained by MAE, with a total polyphenolic content ranging between 2285 and 3298 mg GAE/L, total anthocyanin content ranging between 86 and 399 mg/L and an antioxidant activity between 112 and 530 mmoli TE. The chromatographic profiles confirmed the diverse nature of phenolic compounds occurring in extracts obtained from different grape pomaces. The obtained grape pomace extracts contain important amounts of catechin, epicatechin, gallic and syringic acids, quercetin, kaempferol, t-resveratrol, ellagic and azelaic acids, higher amounts corresponding to MAE extracts, comparing with SFE extracts.

Future studies aim at the use of polyphenolic extracts obtained from grape pomace as functional ingredients to obtain wines with high antioxidant potential.

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CRYSTALLOGRAPHY AND THERMAL BEHAVIOR OF TWO POLYMORPHS OF (E)–4-AMINO–N′–(1–(3–AMINOPHENYL)ETHYLIDENE)BENZOHYDRAZIDE

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The ability of a substance to crystallize in two or more crystalline phases, each having a different arrangements or conformations in the crystal lattice, is defined as polymorphism. Different polymorphs may have different chemical, physico-chemical and thermodynamic properties, including solubility, thermal stability, melting points, hygroscopicity, morphology, and density. Herein, we report the crystallography, solubility, melting points and thermal stability of two polymorphs (**α** and **β**) of (*E*)–4-amino–*N*′–(1–(3–aminophenyl)ethylidene)benzohydrazide prepared from 3′–aminoacetophenone and 4-aminobenzoic acid hydrazide by two different synthetic routes: direct condensation (**α**) and a template synthesis method using a Zn(II) salt (**β**).

Both polymorphs crystallize in the monoclinic crystal system, **α** in $P2_1/c$, and polymorph **β** in *Cc* space group. The **α** polymorph contains two identical molecules in the asymmetric unit, while **β** - three identical molecules. Despite this difference, both form the same supramolecular building block of H-bonded single chains. These chains then combine to form double chains in the **α** polymorph and triple chains in the **β** polymorph.

Despite minor crystallographic differences, both polymorphs have similar solubility: they are well soluble in *N,N*′-dimethylformamide at room temperature; in methanol, acetone and acetonitrile when heated, and insoluble in ethanol and water.

The thermal behavior of both crystalline forms was examined using TGA analysis, with a focus on the thermodynamic stability relationship of the polymorphic sets. Polymorph **α** is the thermodynamically stable polymorph with a higher melting point (172 °C) compared to **β** (166 °C). In addition, **α** is more thermally stable, beginning to degrade at 211 °C, while **β** starts decomposing at 199 °C. However, both polymorphs share the same maximum decomposition temperature, reaching 327 °C.

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ALTERNATIVE SYNTHESIS METHODS FOR MG-BASED METAL-ORGANIC FRAMEWORKS

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Alternative synthesis methods replaced the classic synthesis that uses heating and requires longer time. The alternative methods[1] as microwave synthesis, sonochemical synthesis and mecanochemical synthesis, have many advantages, for example: are greener, faster, economical, and in the case of mecanochemistry, there is no waste.

The aim of this study is to obtain Mg-based metal-organic frameworks using alternative synthesis methods, while taking into account the 12 principles of green chemistry, to characterize them, and, afterwards, to use the obtained materials for different applications. The Mg-based metal-organic frameworks were obtained from the reaction between etidronic acid (HEDP) and phosphonoacetic acid (PA) as the organic linker, and magnesium nitrate hexahydrate- as the inorganic component, under different conditions, such as: hydrothermal[2], mecanochemical, sonochemical and microwave assisted synthesis, while optimizing the parameters: temperature, metal: acid ratio, pH. The resulted solid materials (MgPA, MgHEDP) have been characterized by Fourier Transform Infrared Spectroscopy (FTIR), X-ray diffraction, elemental analysis and thermogravimetric analysis. As first evidence, from FTIR it was observed that the characteristic peak of the P-OH bond was absent, due to P-O-Mg bond formation, confirming that the MgPA, MgHEDP materials were obtained. The best performance was obtained for magnesium and phosphonoacetic based metal-organic frameworks under hydrothermal conditions, the time being reduced by one day and the yield was above 50%.

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A COMPREHENSIVE COMPUTATIONAL INVESTIGATION OF THE CHEMICAL DIVERSITY OF GLIPTINS

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In the present study, we performed an *in silico* characterization of 16 gliptins, a class of drugs used in the management of type 2 diabetes mellitus. These drugs, known for their ability to lower glycemic levels through inhibition of dipeptidyl peptidase 4 (DPP-4), were analyzed using a combination of physicochemical and pharmacokinetics properties, toxicity investigation, and Density Functional Theory (DFT) calculations. We aim to improve the understanding of drug efficacy and safety profiles to develop new strategies for combating type 2 diabetes.

This work was supported by Project No.1.1 from the "Coriolan Dragulescu" Institute of Chemistry Timisoara, Romania.

PREDICTION OF THE BIOLOGICAL ACTIVITY OF THE MAIN COMPONENTS OF THE ESSENTIAL OIL AND HYDRODISTILLATE OF *ARTEMISIA DRACUNCULUS*

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Artemisia dracunculus (common name tarragon) is a perennial plant that grows wild or is cultivated for its use in food, pharmacology and traditional medicine. This plant has been shown to have many beneficial properties: antibacterial, antifungal, anthelmintic, antiseptic, anti-inflammatory, antipyretic, carminative, digestive and stimulant activities. The main compounds in *Artemisia dracunculus* essential oil and respectively hydrodistillate were identified as sabinene, limonene, ocimene, estragole and eugenol methyl ester. The possible biological effects on humans of these compounds were evaluated using the ADMETLab2.0 computational tool. The toxicity of tarragon hydrodistillate against the aquatic organism *Lemna minor* was also evaluated using the growth inhibition test. The results obtained show that these compounds can inhibit cytochromes involved in endo- and xenobiotic metabolism and can produce skin sensitization, hepatotoxicity and some of them can also produce reproductive toxicity. Tarragon hydrodistillate is not toxic to *Lemna minor*. This information is particularly important for those who are occupationally exposed to higher amounts of these compounds and for completing eco-toxicological data.

TRADITIONAL MEDICINE A SOURCE OF PROMISING SMALL MOLECULE COMPOUNDS OF NATURAL ORIGIN AGAINST CANCER AND COVID-19

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Traditional Chinese medicine (TCM), Unani and Ayurveda are among the most ancient heritages, still being largely applied in Asia, China, Arabic countries, and India rescuing a considerable number of lives since the dawn of time [1]. For ages, plants are considered a major source of biologically active compounds, which are still being used medicinally. Nowadays, it was noticed an increased global interest in traditional medicine due to increased risk of side effects, unavailability of cure for some chronic diseases, huge cost of new drugs, antibiotic resistance, etc. which determined a revived interest in complementary and alternative medicines [2]. Therefore, in the context of COVID-19 pandemic there is a demanding need to discover new effective broad-spectrum drugs, with excellent safety profile, aiming at covering unmet needs of patients with comorbidities and a better understanding of the therapeutic potential of natural compounds for the treatment of cancer and COVID-19. Cancer and COVID-19 act on cells in similar way, e.g. when a cell is under stress a normal cell can be turned out into a cancerous one, similarly viral infections produce stress on cells which activate similar mechanisms [3]. Baicalein, is a flavone found in *Scutellaria Baicalensis* root, displaying a plethora of pharmacological effects including anti-inflammatory, antioxidant, antiviral, and antitumor which have been demonstrated by modulating targeted mechanisms and signaling pathways in cancer MAPK, Akt, caspase-9/-3 and MMP-2/-9, and has anti SARSCOV-2 effect at 0.1uM by modulating the interaction of spike protein with hACE2, the levels of IL-1β and TNF-α in serum [4]. Several pseudo-natural structure combinations were generated based on baicalein fragments in unique ways which are not identified in nature, aiming at the discovery of improved, unprecedented bioactivities [5].

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TREATMENT OF WATER WITH NITRATE CONTENT BY MICROFILTRATION

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In comparison with conventional water treatment methods such as adsorption, ion exchange, chemical precipitation, solvent extraction processes and so on, the use of microfiltration for advanced water treatment represents a green, compact and economical alternative system. This technique could separate organic and inorganic compounds from large streams with minimum energy consumption, high selectivity and technical feasibility, and produce low waste volumes.

A first important factor affecting the operational stability and selectivity of a membrane is the nature of the solid support. In this context, scientific research in recent years in the field of membrane technology has emphasized the importance of polysulfones (PSFs) - high performance polymers - due to their functional properties as some of the best materials used in many areas of everyday life.

The second factor influencing the operational properties of a membrane is the carriers. Therefore, ionic liquids (ILs) have been used as carriers to obtain efficient and selective membranes for water treatment processes.

In the present work, the efficiency of quaternized polysulfonic membranes in the treatment of nitrate-containing water by microfiltration was studied. The quaternized polysulphonic quaternized membrane (PSFQ) was used as such, or functionalized with different amounts of ionic liquids (3 and 15 %, respectively). Methyl trialkyl ammonium chloride (AmIL) and trihexyl tetradecyl phosphonium chloride (PhIL) were studied as ionic liquids. The PSFQ membrane was functionalized with the two ILs using two techniques, namely by: (1) incorporation/mixing of PSFQ solutions with ILs leading to polymeric inclusion membranes (PIMs), where ILs act not only as carriers but also as plasticizers; (2) deposition/immersion of the already obtained PSFQ membranes in ionic liquids. In this way, sustained ionic liquid membranes (SLMs) are obtained, where ILs are entrapped in the membrane structure.

The obtained membranes were used in the treatment of water containing 60 and 100 mg/L NO_3^- respectively. It was found that the presence of ionic liquids significantly improves the efficiency of the studied membranes. It increases with the increasing of ionic liquid amount in the membrane structure. PIM membranes show a higher efficiency than SLM membranes. These findings suggest that both the functional grouping of the ionic liquids and the membrane structure, through the porosity of the membranes, contribute to the removal of NO_3^- ions from water. For both PIM and SLM membranes, the ammonium-based ionic liquid had a greater influence on the microfiltration efficiency developed by the membranes than the phosphonium-based ionic liquid. In case of membranes obtained by inclusion and using methyl trialkyl ammonium, only one treatment cycle is sufficient, no permeate recirculation is necessary to achieve the desired efficiency.

This membrane has been successfully used in the treatment of underground water. It was found that metal ions present in real water samples do not negatively influence the microfiltration process, a slight decrease in their concentration is also observed. It results that the studied membrane has an affinity for anions. By using a two-membrane module in the microfiltration process, the efficiency of the process increases by about 20%.

QUATERNIZED POLYSULFONES/CELLULOSE ACETATE PHTHALATE/POLYVINYLIDENE FLUORIDE ELECTROSPUN MEMBRANES: AN APPROACH TOWARDS BIOACTIVE MATERIALS FOR BIOMEDICAL APPLICATIONS

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The fabrication of bioactive electrospun membranes is an active area of research because they have the potential to significantly enhance the hemodialysis process by increasing the removal efficiency of the harmful components of the biological liquid and overall treatment efficacy. In this context, membranes with tailored morphological and surface properties, constitute from quaternized polysulfone (PSFQ), cellulose acetate phthalate (CAP), and polyvinylidene fluoride (PVDF), and functionalized with antioxidants and anticoagulants were obtained. In this context, the membranes effectiveness was tested by monitoring the removal of key solutes, namely urea, creatinine, and uric acid from simulated biological fluid over a 4-hour dialysis period and was observed that there was 98.5% removal of creatinine, 93% of urea and 96% of uric acid. These findings reveal a significant relationship between the blend composition, surface properties, and the membranes' functional performance. Further, to assess the propensity of the membranes to be used in blood-contact devices, their biocompatibility and hemocompatibility were evaluated. Thus, the biocompatibility of these membranes was evaluated *in vitro* using human gingival fibroblast (HGF) cell lines by MTS test (ISO/IEC 17025:2005 (NABL accreditation and ISO 9001-2015 certification), which recommends the use of materials for biomedical devices when the cell viability is higher than 70%. In agreement with this standard, all the studied membranes achieved compliance with the requirements for application as medical purpose, demonstrating around 90% cell viability, indicative of good biocompatibility. Additionally, hemocompatibility was evaluated by measuring hemoglobin release from red blood cells upon contact with the electrospun membranes. Data obtained from the spectrophotometric analysis indicates a low hemolytic effect, which means used membranes tend to be more biocompatible and are less likely to cause side effects such as inflammation and activation of the immune system. This improves the patient's tolerance to treatment and reduces the risk of long-term complications.

Therefore, a biocompatible membrane, like electrospun bioactive polysulfone membranes, can be expected to prevent microaggregate formation during hemodialysis and avoid subsequent cell activation. Moreover, the structure-bioactivity relationship of the membranes, correlated with their microarchitecture, supports their promising application in blood-contact devices, such as extracorporeal devices.

EFFICIENT REMOVAL OF ANIONIC AND CATIONIC DYES FROM AQUEOUS SOLUTIONS USING MAGNETIC NANOCOMPOSITE

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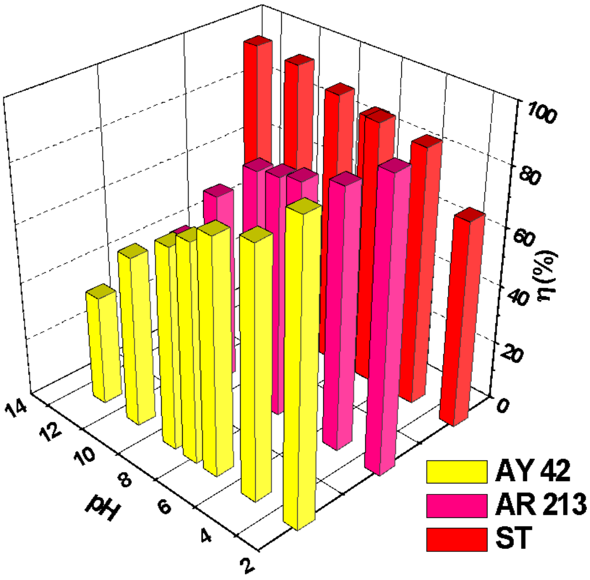
The magnetic nanoparticles embedded within a matrix of activated carbon [1] were tested as adsorbents for removal of two anionic dyes: Acid Yellow 42 (AY42), Acid Red 213 (AR213), and a cationic dye, Safranine T (ST), from aqueous solutions. The effects of process variables: solution pH, initial concentration of dye, adsorbent dose, contact time, temperature and their interactions on the adsorption capacity of the nanocomposite was investigated in order to optimize the process. The removal efficiency of pollutants depends on solution pH, and increases with the dose of *MC*, the initial concentration of the pollutants and temperature. Using an adsorbent mass of 1 g/L, an initial pollutant concentration of 50 mg/L, and working at 25°C, and natural pH of dyes solution, the removal efficiency was 80.95% for AR 213, 73.77% for AY 42 and 89.17% for ST, respectively.



Pseudo-second order kinetic model was fitted to the kinetic experimental data, and adsorption isotherm analysis and thermodynamics were used to elucidate the adsorption mechanism.
The combination of high adsorption capacity, excellent separation capability and the short equilibrium time, indicates that the investigated magnetite/carbon nanocomposites are very good adsorbent materials for colored pollutants.

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

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BFI IN KINASES: A PUBLIC RESOURCE FOR DOCKING REFINEMENT

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Protein-ligand docking, a cornerstone technique in cheminformatics, serves as a critical tool for virtual screening, pose prediction, and binding affinity calculations. However, the accuracy of docking simulations is dependent on the quality of crystal protein structures.

The B-factor index of the binding site (BFIbs) correlates atomic fluctuations within the binding pocket with the entire protein [1]. A large-scale docking study confirmed BFIbs' role in predicting ligand pose.

This work presents an updated and publicly accessible digital tool named BFI in Kinases (available at www.chembioinf.ro). This user-friendly resource provides researchers with computed BFIbs values alongside a comprehensive collection of crystallographic data, ligand descriptors, and valuable insights into protein-ligand binding interactions.

This resource empowers researchers to select optimal crystal structures for docking, ultimately improving docking accuracy and facilitating the discovery of novel kinase inhibitors.

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RAPID MICROWAVE SYNTHESIS OF UIO-66 METAL-ORGANIC FRAMEWORKS

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In the present paper, a fast and efficient microwave assisted synthesis method in the presence of acetic acid as modulator has been employed to prepare zirconium-based metal-organic framework UIO-66. XRD patterns for all the microwave synthetized samples exhibit similar patterns, in agreement with the literature for UIO-66 architecture and any impurity in its crystalline structure is not seen. The FT-IR spectra of the samples exhibit similar characteristic peaks and are in agreement with the data reported in the literature for UIO-66. From SEM images it can be observed that the samples are composed by small crystalline (confirmed by XRD measurements) agglomerated nanoparticles, with irregular shape. Additionally, 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 high thermal stability despite high linkers deficiencies per Zr_6 formula unit. The samples presented relatively good values of specific surface area, and had a combination of porosity, given by microporosity and mesoporosity. A preliminary evaluation of the materials performances regarding H_2 adsorption measurements at 77 K, up to 1 bar, were conducted and the differences values of hydrogen uptake are related to the surface area and porosity of the samples.

OPTIMIZATION OF THE ADSORPTION PROCESS OF RHODAMINE 6G FROM AQUEOUS SOLUTION USING MAGNETIC NANOCOMPOSITE

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Application of an efficient method for the removal of dyes from colored waters has become a necessity for researchers in order to improve the lifestyle and protect the environment [1, 2]. The present study combines two powerful tools: Factorial design and Response Surface Methodology (RSM) [3] in order to optimize the working conditions for the removal of Rhodamine 6G (R6G) from aqueous solutions by adsorption using magnetite/carbon nanocomposite (M/CN). The adsorbent was synthesized by combustion method and it was characterized in terms of structural, morphological and magnetic properties.

The experimental design and statistical analysis were carried out based on the most significant variables which influence the adsorption process such as: solution pH, initial dye concentration (C_{R6G}) and adsorbent dosage ($D_{M/CN}$). The interaction between the variables was studied and optimized using response surface methodology (RSM). A comprehensive regression analysis was performed using the experimental design matrix to find the most accurate empirical model for maximum R6G removal efficiency. Additionally, the analysis of variance (ANOVA) confirms the statistical significance of regressions at a 95% confidence level. The good agreement between the experimental and predicted results is reinforced by the low p-values and Fisher's test F-values exceeding the critical F critical values from statistical tables. Using contour maps and 3D representations for each pair of factors present in the model, the optimal working conditions were established to ensure a maximum efficiency (99%) of dye removal.

The pseudo-second order kinetic model describes the adsorption process for R6G dye. The equilibrium data were best fitted by the Sips isotherm model and a maximum obtained adsorption capacity was 266.87 mg/g. The thermodynamic parameters indicated the spontaneous and endothermic nature of the adsorption process.

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

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THE POLYMER SUPPORTS OF ACRYLONITRILE-DIVINYLBENZENE TYPE: THEIR CHEMICAL MODIFICATION WITH AMINOPHOSPHONATE GROUPS AND PRELIMINARY ANTIBACTERIAL TESTING

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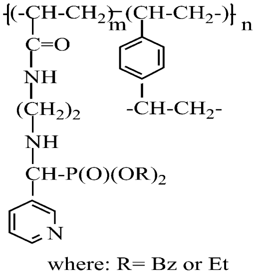
The chemistry of multicomponent reactions (MCRs) has been widely explored, since by MCR most atoms of three or more compounds are efficiently compressed into a single product [1].

A number of different MCRs have been discovered [2], among which the Kabachnik–Fields (KF) three-component reaction plays an important role [3]. Bioisosteres are chemical substituents or groups with physical or chemical properties that produce biological properties [4]. In the case of aminophosphonates, their bioisosterism is given by -OH and -NH groups. Phosphorus in the form of organic phosphates plays an essential role for biochemical processes. The functionalization of ion-exchangers containing primary amine groups (resulting from the aminolysis reactions with ethylenediamine) with dibenzylphosphite (code: Bz)/diethylphosphite (code: Et) and 3-pyridinecarboxyaldehyde was achieved by the "one-pot" Kabachnik-Fields method (see Scheme 1).



Scheme 1. The functionalized structure for Bz and Et samples.

The syntheses were carried out in tetrahydrofuran at a temperature of 55 °C. After the synthesis time of 20 hours, the product was filtered, washed with ethanol and dried at 50 °C for 24 hours. From the EDX analysis, the values of N = 18%, P = 1.2% were obtained for Bz, and N = 30%, P = 0.2% for Et. From the SEM image, a uniform structure of the functionalized copolymers was observed. The characteristic IR bands for the functionalized copolymers are: 3435.56 cm^{-1}, 2932.23 cm^{-1}, 1644.02 cm^{-1}, 1558.2 cm^{-1}. TG-DTG analysis was performed for Bz and Et samples and a 4-step loss was observed, the value of the residue left at 800 °C was 25.11% for Bz and 22.33% for Et, respectively. The reduction of more than 50% of the Gram-positive bacterial load was manifested after 9 hours of contact, a fact that was signaled for the Gram-negative ones only after 12 hours of contact. In

Staphylococcus aureus, the effect of sample Et is expressed at a bacteriostatic (94.8%) to bactericidal (99%) efficiency.

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STRUCTURAL AND PHOTOPHYSICAL STUDIES OF AN AMPHITROPIC METALLOMESOGEN BASED ON Zn(II) COORDINATION COMPLEX

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Due to their interesting photophysical and redox properties, luminescent coordination complexes can be used as functional materials for optoelectronic devices (e.g., optical storage and OLEDs) and biomedical tools.[1] Luminescent materials can theoretically be used in every physical state, but for practical applications they are used in condensed states as films or aggregates.[2] Compared to their behavior in dilute solutions, luminescent materials may exhibit in the condensed state reduced emission due to aggregation-caused quenching (ACQ) or enhanced emission through aggregation-induced emission (AIE).[3] Since the fluorescence behavior of AIE luminogens depends on their molecular packing and their interaction with the environment, the induction of liquid crystalline properties (LCs) appears highly attractive in the view of materials science.[4]

A metallomesogen (MM, **Zn_MM** – Figure 1) was reported by our group with record emission quantum yield in dichloromethane solution (θ = 95%) and in mesophase θ = 20.2%.[5] Water-soluble complexes may form aggregates depending on their molecular structure, amphiphilic and solvent nature, etc. Amphitropic MMs combine the thermotropic and lyotropic behavior of a LC, and their structure typically involves a balance between hydrophobic and hydrophilic segments, allowing them to respond to both thermal and solvent-based stimuli.[6]

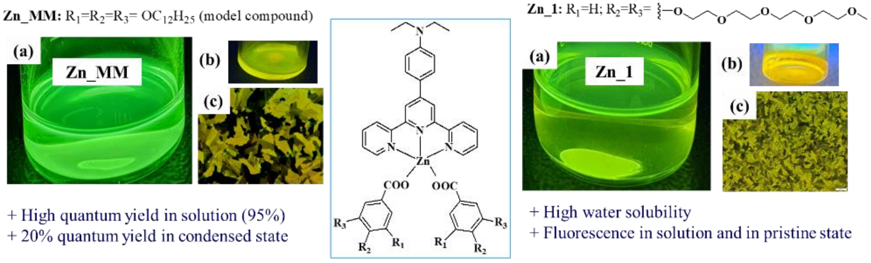

Figure 1. Chemical structure of **Zn_MM** and **Zn_1**; Photos: (a) in diclorometHane solutions and (b) in pristine condensed state under UV lamp (λ = 365 nm), (c) POM micrographs at r.t, magnification x20 - first cooling.

On this background, we present the synthesis and characterization of a water soluble penta-coordinated Zn(II) complex with benzoate as ancillary ligand decorated with two hydrophilic chains (**Zn_1** – Figure 1). The chemical structure and purity were determined by spectroscopic and analytic methods. The complex presented both thermotropic and lyotropic mesomorphism. The liquid crystalline properties were investigated in condensed state. The photophysical properties of the final complex were investigated in solvents of different polarity and at different concentrations.

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We acknowledge the **Romanian Academy, Program 4** and the project **ROOPENSCREEN, MySMIS code: 127952**, Contract no. 371/20.07.2020, co-financed by European Regional Development Fund through the Competitiveness Operational Program 2014-2020, for support.

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PESTICIDE RESIDUES IN GARLIC, LETTUCE AND ONION COMMERCIALIZED IN ROMANIA - A THREAT TO PUBLIC HEALTH?

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Several studies showed that pesticides contamination represents a public health problem. Food sustainability in Romania has not yet taken shape, because there has been a continuous increase in the possibility of theft, abuse, environmental damage, product piracy and health problems caused by an agriculture that does not conform to European standards. At the same time, there are still non-compliant practices and guidelines for the management of treatments applied to defend crops against pests, which can attack the plant at a certain stage of development, involuntarily transferring chemicals to the finished product. This is why the development and implementation of a traceability system, at the national level, on the path "*from the farm to the fork*" becomes a necessity. In this context, Romania is developing a surveillance program for pesticide residues in greengrocery. In this study 29 onion, 13 garlic and 10 lettuce samples were purchased from market and screened by GC-MS/MS for 74 pesticides. Residues of acetamiprid (0.0.018 and 0.009) and boscalid (0.021-0.022 mg/Kg) were detected in two onion samples (one white and the other red onion). However, these values did not overpass the MRL`s imposed by EU legislation (0.02 mg/Kg and 5.00 mg/Kg, respectively). Three pesticides were detected in two garlic samples; one of them contained clofentezine (0.023 mg/Kg against the EU MRL`s of 0.02 mg/Kg) and pirimicarb (0.032 mg/Kg against the EU MRL`s of 0.10 mg/Kg), the other one tebufenozide (0.016 mg/kg against the EU MRL`s of 0.01 mg/Kg). Only in one lettuce sample 3 pesticides were simultaneously identified: boscalid (0.234 mg/Kg against the EU MRL`s of 50.00 mg/Kg, cyprodinil (0.164 mg/Kg against the EU MRL`s of 0.15 mg/Kg) and pyraclostrobin (0.52 mg/Kg against the EU MRL`s of 2.00 mg/Kg). Although some of the pesticides detected within greengrocery overpassed the MRL2s imposed by the European legislation, considering the uncertainties of the detection method, the values can be considered as fitting the requested levels, but they must be under attention. Severely rules for prevention, control, and monitoring of food pesticides contamination will be developed and implemented to protect consumers pesticide poisonings and chronic effects.

Part of this complex research was conducted under Sectorial Plan-ADER 2026, Project ADER 6.3.7 – "*Applicability measures regarding the investigation of the organochlorine and organophosphorus contaminants distribution on the soil-plant-vegetable/fruit-finished product chain, following different types of* *soils in various areas*" financed by the Ministry of Agriculture and Rural Development – Romania; the other part was conducted under: Establishment and operationalization of a Competence Center for Soil Health and Food Safety – CeSoH, Contract no.: 760005/2022, Code 2 (PNRR-III-C9-2022 – I5), Project *"Improving soil conservation and resilience by boosting biodiversity and functional security of organic food products*", financed by European Union through Romanian Ministry of Research, Innovation and Digitization.

ANTIOXIDANT POTENTIAL OF ARISTOLOCHIA CLEMATITIS EXTRACTS WITH FOUR DIFFERENT SOLVENT SYSTEMS

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One of the most ancient medicinal plants, *Aristolochia clematitis*, contains aristolochic acids (AAs), which are responsible for its nephrotoxic and genotoxic effects. Despite this, it is also recognized for its diverse medicinal properties (eg., cancer, snakebite, wounds). The aim of this study was to investigate the antioxidant properties of *Aristolochia clematitis* herbal extracts reached via maceration using four different solvents, and to evaluate the antioxidant activity using 1,1-diphenyl-2-picrylhydrazyl (DPPH) radical scavenging assay, and total phenolic content measured by the Folin-Ciocâlteu method. The antioxidant activity values quantified through DPPH were compared to establish a difference between the four types of solvent extract, using Trolox as standard (2 mM). The obtained results showed that the lowest IC_{50} value was due to the solvent methanol with 0.1 formic acid with a value of 70.60 ± 0.02 μg/ml, indicating promising DPPH radical scavenging activity compared with Trolox. In contrast, the methanolic extract has an estimated IC_{50} value of 116.04 ± 0.08 μg/ml, suggesting that the highest value may reveal a lower antioxidant efficiency of the compound. The results of phenolic content were obtained from a calibration curve of propyl gallate and the *A. clematitis* plant extract using 0.1 formic acid and methanol as solvent systems, showed the highest content of 19.4 ± 0.020 mg GAE/g dry leaves. A low phenol content was obtained (12.5 ± 0.005 mg GAE/g) using 0.1 formic acid and ethanol as extraction solvent, suggesting that methanol is a better solvent extraction for phenols. Comparing results obtained from the two methods, both demonstrated that methanol in combination with formic acid is a better solvent system to increase the value of antioxidant capacity of an extract.

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NOVEL HALO-TAG PROBES FOR CELLULAR IMAGING APPLICATIONS

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Lipids are essential molecules that play crucial roles in numerous biological processes, including cell-cell signalling pathways [1-2]. While these pathways are deeply involved in normal embryonic development, they can be mis-regulated in various pathologies, including cancer and cardiovascular diseases [3]. In spite of their critical importance, however, the mechanisms of many signalling pathways remain unclear. To better dissect these mechanisms, there is still a need for novel and sensitive technologies to image various cellular components.

HaloTag is a powerful bio-orthogonal labelling technology that uses diverse synthetic ligands containing a chloroalkyl moiety, which specifically reacts with a catalytically-dead bacterial dehalogenase protein module (called HaloTag). If the chloroalkyl moiety is attached to a fluorophore, the resulting adduct with the HaloTag protein expressed in cells can be visualized by fluorescence microscopy [4]. Our goal is to use this technology to develop new, efficient and sensitive methods to image cellular lipids, including in live cell applications.

Herein, we present the synthetic approach for two promising probes containing a chloroalkyl moiety (for HaloTag attachment) and reactive moieties such as alkyne (for "click" azide-alkyne reactions [1-2]) or reactive esters (such as *N*-hydroxysuccinimide). The multi-step syntheses share a common key intermediate, a halogenated amine [5]. All synthesised compounds were characterized using physical and spectral techniques, such as NMR and HRMS spectroscopies.

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COLOUR DETERMINATION USING CIELab COLOUR SPACE OF ACID FAST VIOLET RR DYE

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The CIE 1976 L*a*b* color space is the most common used method for measuring and ordering object color. This color space can be visualized as a three dimensional space, where every color can be uniquely located. It is well-known that the above mentioned colorimetric space provides comparison samples of colors rated according to these properties: i. e. the CIE L* a* b* and the CIE L* C* h* systems. The colour is quantified by lightness (L*), redness (a*), yellowness (b*), chroma or saturation (C*) and hue angle (h°) calculated from the tristimulus values XYZ. The difference between two colors can be calculated easily using an equation developed by the CIE in 1976 called ∆ Eab and defined as the linear (Euclidian) distance between two points in the Cielab colour space. The CMC difference formula typically is known as a color tolerancing system and the metamerism is considered with respect to the human visual system [1] The colour of the single azo class dye: Acid Fast violet RR (C.I. 17.025) was evaluated in terms of above mentioned CIELAB parameters for the CIE D65 (natural day light), A (tungsten light), F2 (fluorescent light) and the standard 10° observer respectively. The colour differences: ΔE_{ab}^* and ∆ECMC were calculated against a standard namely Pigment White 6: titanium dioxide (C.I. 77.981) and reveal a good colouring power of the studied dye.

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SYNTHESIS AND PHYSICOCHEMICAL CHARACTERIZATION OF THE FIRST BINUCLEAR V(III,IV)-CITRATE COMPLEX

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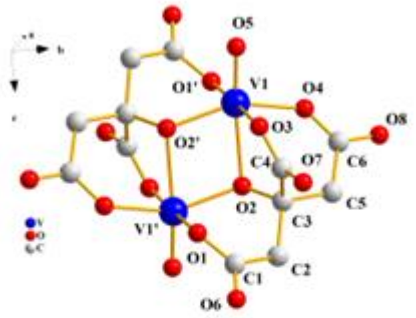
Vanadium has, over the past decades, drawn considerable interest in the realm of therapeutic medicine due to the plethora of various metal-based compounds exhibiting substantial efficacy against cancer. Extensive studies have been conducted on numerous vanadium-based binary and ternary compounds, recognized for their capacity to catalyze small molecule transformations and exhibit insulin-mimetic and antitumor properties.[1,2] Particularly noteworthy are V(IV) compounds, which, when paired with natural substrates, such as alpha-hydroxycarboxylic acids, have shown the potential to enhance insulin sensitivity and lower elevated plasma glucose levels - key factors in managing Diabetes Mellitus Type 2.[3] Furthermore, vanadium compounds have demonstrated significant anticancer activity through mechanisms, such as DNA cleavage, activation of xenobiotic enzymes, inhibition of cancer cell signaling pathways, and the production of free radicals.[4]



Despite these advancements, the clinical progression of vanadium compounds has been stalled in early trials due to the need for a more comprehensive understanding of their mechanisms of action, toxicity profiles, pharmacokinetics, and pharmacodynamics. Given the vast therapeutic potential in this field, our Lab has embarked on an in-depth investigation of vanadium systems combined with natural substrates to identify viable therapeutic profiles and enhance pharmacological functions. To this end, we successfully isolated a dinuclear V(III,IV) complex containing citric acid through three distinct synthetic approaches. The isolated crystalline material underwent thorough physicochemical characterization using techniques, such as Elemental analysis, X-ray crystallography, Fourier Transform Infrared Spectroscopy (FT-IR), Ultraviolet-Visible Spectroscopy (UV-Visible), and Cyclic voltammetry (CV).

The collective results project a realistic structural speciation of vanadium in three oxidation states in biological media. The abundance of vanadium species, dependent on the oxidation state of that element (V(III,IV,V)), denotes the a) structural diversity of vanadium complex assemblies, b) distinct physicochemical properties, which in turn presage the as yet unknown biological activity of those species (especially those of V(III)), and c) interwoven bioactivity of the three oxidation states of that element, which individually or concertedly contribute to the efficacy of the species when interacting with molecular targets, in particular, suggesting the potential roles of this metal ion in developing therapeutically competent metallodrugs.

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HYBRID PEROXIDO-VANADODRUGS AGAINST HEPATOCELLULAR CARCINOMA

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Hepatocellular carcinoma (HCC) is the predominant phenotype in liver cancer, ranking as the sixth most prevalent and the fourth most lethal malignancy. Due to the aggressiveness of the disease, HCC is often diagnosed at an advanced stage, limiting the available therapeutic options. At the same time, increasing evidence underlines the influence of tumor immune microenvironment on therapeutic effectiveness, enhancing the treatment response, or contributing to the resistance of the tumor to the administered therapies. [1]

Vanadium is an early first row transition metal of high physiological, environmental, and industrial importance. Various vanadium species have been found to exhibit significant effects as external cofactors either inhibiting or stimulating the function of a wide range of enzymes. In vivo, a key redox interplay emerges between the physiologically relevant V(V) and V(IV), while the V(III) form in found only in ascidians and fan worms. Various vanadium complexes are involved in immune regulation pathways, specifically in regulation of B and T cell signaling, promoting vanadium-based approaches in cancer-immunotherapies. [2]

Taking all that into consideration, research was launched in our Lab to delineate the *in vitro* potency of two well-characterized vanadium(V)-peroxido complex assemblies coordinated with betaines. The employed ternary species were synthesized in aqueous media through pH-specific synthetic methodologies, thereby providing physiochemically well-defined materials of high solubility and bioavailability. The cell lines that were chosen include HepG2 and Huh7, two commonly used cell lines for HCC research. To determine a comprehensive cytotoxic profile of the hybrid materials, not only was cell viability assessed, but also proliferation, chemotacticity, and morphology were studied, in a dose-/time-/cell line- dependent fashion. Moreover, to enhance the biological significance of the cytotoxicity profile and better mimic the tumor microenvironment, 3D spheroids (**Fig. 1**) were cultivated using the scaffold-free method, and the cytotoxicity of the hybrid materials was studied under similar conditions. The derived results show that the investigated hybrid species are potent against HCC, at small doses and timeframe, thereby supporting their potential merit as future vanadodrugs in anticancer chemotherapeutics

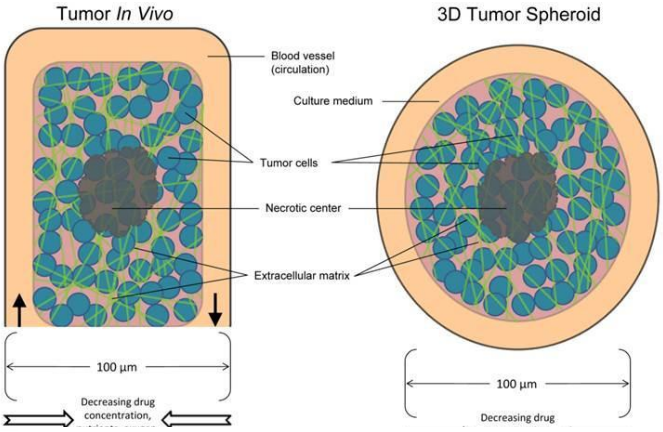

Fig. 1: In vitro 3D spheroids vs in vivo tumors [**3**]

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SYNTHESIS OF AMINO AZIDES AS BUILDING BLOCKS FOR "CLICK"-BASED CELLULAR IMAGING PROBES

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Azides are important in organic synthesis, as precursors for novel functionalities such as amines, heterocycles, phosphinamines, etc [1]. More recently, the discovery of the highly efficient and selective Cu(I)-Catalyzed Azide-Alkyne Cycloaddition reaction (**CuAAC**, Figure 1) [2, 3], has greatly expanded the scope and utility of organic azides. Furthermore, the bio-orthogonality of the CuAAC reaction [4] has made is indispensable in numerous applications beyond pure chemistry, including in biochemistry, cell biology and medicine.

Amino-azides are useful compounds for introducing azido groups into various molecules of interest, especially for biological applications such as fluorescent imaging, development of anti-hapten antibodies, or diagnostic tests [5,6].

In this context, we present herein synthetic strategies for obtaining several amino-azide precursors, carrying with various protecting groups (i.e. Fmoc, Alloc, Boc). These intermediates will be used in biological experiments that involve microscopic imaging of cellular processes. The various synthetic challenges encountered are discussed, as well as strategies to mitigate them. Finally, we present confirmation via spectral analysis (i.e NMR, HRMS) of the desired structures.

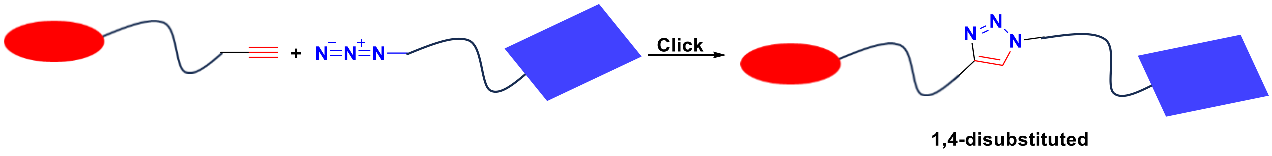

Figure 2 Copper - Catalyzed Azide - Alkyne Cycloaddition (**CuAAC)** reaction

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STRUCTURAL ANALYSIS OF GANGLIOSIDES ASSOCIATED TO KNOCKOUT TLR2D GENE

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Gangliosides, complex glycosphingolipids with critical roles in the central nervous system (CNS), are involved in various cellular processes such as cell adhesion, signal transduction, and cell-to-cell communication [1]. Alterations in ganglioside compositions are linked to numerous neurological disorders, making their study essential for a deeper understanding of their functions in the normal and diseased CNS [2]. The purpose of the current study is the comparative profiling and structural analysis of gangliosides in female and male brain tissues having the TLR2D (Toll Like Receptor 2) gene inhibited *vs*. age- and sex-matching control brains. Gangliosides from the following four distinct murine groups were extracted, purified and investigated under identical conditions: wild-type females (WF), knockout females (KF) with the TLR2D gene inhibited, wild-type males (WM), and knockout males (KM) with the TLR2D gene inhibited. The screening and structural analysis was performed by ion mobility separation (IMS) mass spectrometry (IMS) using nanoelectrospray ionization (nanoESI) on a Synapt G2S mass spectrometer operated in negative ion mode. Based on the separation of ions according to their mobility followed by MS detection at high resolution, the method allowed the discrimination and identification of numerous and complex ganglioside species across the different sample groups. The comparative analysis showed the occurrence of no less than 175 distinct ganglioside species in the KF samples, which represents an increase in the number of components as compared to the 130 species identified in the WF samples. Similarly, 140 ganglioside species were detected in the KM samples, whereas only 115 species were found in the WM samples. The gangliosidomes associated to the TLR2D knockout murine groups encompass a much higher variety of species and more complex structures, including components exhibiting several biologically significant modifications, such as *O*-fucosylation, *O*-acetylation, and CH_3COO^-. The analysis also revealed major dissimilarities in glycosphingolipid distribution among the four groups. KM samples exhibited a higher expression and diversity of GD1 species compared to KF samples, indicating specific metabolic or regulatory differences between these knockout variants. Detailed structural analysis by IMS CID MS/MS of the $[M-2H^+]^{2-}$ ion detected in KM at *m/z* 917.471, corresponding to GD1 (d18:1/18:0) as per mass calculation, confirmed also the presence of a GD1b isomer. In contrast to KM, KF extract showed an upregulation of GD2 type of gangliosides. Our study reveals that significant differences in the ganglioside profiles of WF, WM, KF, and KM mice exist, with a marked increase in ganglioside diversity observed in the knockout groups. These findings suggest metabolic or regulatory shifts due to TLR2D gene inhibition, with potential implications for understanding the role of gangliosides in neural function and pathology. The use of IMS MS has proven to be a powerful tool in elucidating such complex glycolipid profiles, paving the way for further investigations related to their biological roles.

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THE IMPACT OF TEMPERATURE ON CO_2 ADSORPTION ON AMINE FUNCTIONALIZED KIT-6 ADSORBENTS

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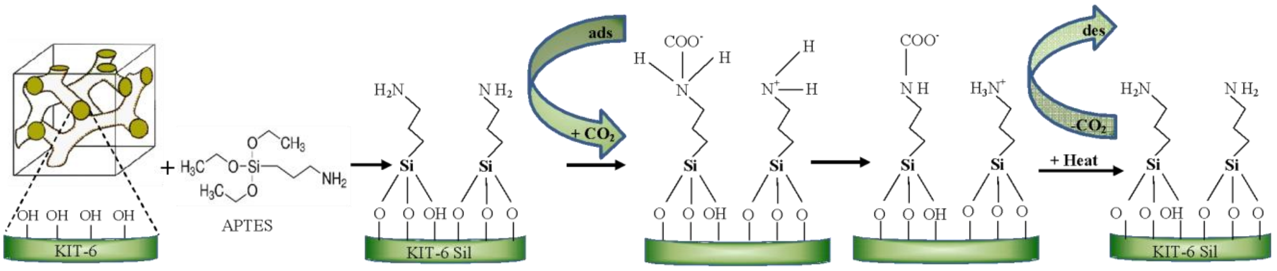
The mesoporous silica KIT-6 was synthesized and functionalized with 3-aminopropyltriethoxysilane by grafting at 110 ºC at three different concentrations of APTES: 20, 30 and 40 wt.%. Thermal gravimetric analysis in air and nitrogen atmosphere, Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction, and nitrogen adsorption-desorption were used to characterize the samples.



In this work, CO2 adsorption-desorption was investigated using a temperature-programmed desorption-mass spectrometer (TPD-MS) at different temperatures of 40-70°C.

The results indicate that adsorption capacities remain stable even after nine adsorption/desorption cycles.

AN ELECTROCHEMICAL IMPEDANCE SPECTROSCOPY STUDY OF METAL PHOSPHONATES BASED ON COBALT AND ZINC AND ETIDRONIC ACID IN SALINE SOLUTION

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Phosphonic acids, organic phosphorus compounds, are known for their ability to adhere on the metal surface, which gives them the property of corrosion inhibitors. Their ability to bind monodentately, bidentately or tridentately to the surface of the metal determines the ease of absorption of these compounds. The formation of a thin layer on the metal surface is possible by using this bonding technique [1, 2].

The aim of this study was to investigate the efficiency of metal-organic inhibitors in preventing the corrosion of metallic materials. Electrochemical tests electrochemical impedance spectroscopy spectra (EIS) and polarization curves (CP) were performed to evaluate the corrosive effect of chloride ion on iron in the absence and presence of organic phosphorus compounds. Before each determination, metal phosphonates were dissolved in 3% NaCl solution acidified to pH~2.5 adjusted with HNO_3. The examined metal phosphonates, Co-HEDP, and Zn-HEDP were hydrothermally synthesized at 80°C from bivalent metals such as Co and Zn, as well as from etidronic acid (HEDP) [3].

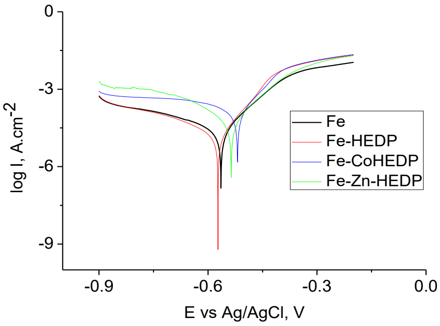

Figure 1. Polarization curves of the Fe electrode immersed for 60 minutes in 3% NaCl solution (pH~2.5) and with 200 ppm organic phosphorus compound

In the presence of HEDP the protective film formed on metallic surface improve the corrosion resistance. Earlier experimental results suggest the possibility that metal phosphonates are promising candidates for the role of corrosion inhibitors [4]. The release of HEDP occurs with a delay and this allows the corrosive species present in the system to attack the iron surface before the HEDP binds to the metal surface. The Co-HEDP and Zn-HEDP concentration must be lower than 0.01mM. At 200 ppm of metal phosphonate its inhibition efficiency decreases due to the dissolution of the oxide layer as corrosive species attack the metallic surfaces.

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MULTIDISCIPLINARY APPROACH IN ELECTROCHEMICAL STUDIES. II. COMPUTATIONAL AND EXPERIMENTAL CHARACTERIZATION OF NICKEL OXYHYDROXIDE

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Electrosynthesis, the synthesis of chemical compounds using an electrochemical setup, continues to be of great importance to the scientific community, especially in light of the current attempts to transition towards a sustainable society [1]. Nickel-based oxyhydroxides have been extensively studied for their potential use as oxidizing agents in organic synthesis and in the construction of electrochromic devices, sensors and nickel-based batteries [2-5]. This paper presents a multidisciplinary approach to the investigation of the properties of the nickel oxyhydroxide molecule, using theoretical and experimental methodologies. This combined approach is designed to enhance the current understanding of the reaction mechanism of oxygen evolution on oxyhydroxide, with the ultimate goal of improving the electrochemical performance of the compound. The theoretical study, which included optimization of the NiOOH molecular geometry and frequency calculations, was carried out using the DFT/B3LYP method with the 6-31G basis set. The calculated results for HOMO-LUMO energies show that the NiOOH molecule has a lower tendency to donate electrons to the acceptor molecule, with the negative value for ΔE indicating easier charge transfer between orbitals. The low value of the dipole moment implies high structural stability and low polarizability for the molecule. The results of the ESP analysis (Fig. 1a) indicate that the electrophilic sites are primarily located on oxygen atoms [6]. Experimentally, the employed electrochemical method was cyclic voltammetry. A Ni plate working electrode, a Pt plate counter electrode and the Ag/AgCl (sat. KCl) reference electrode were connected to a potentiostat and immersed into 1 M KOH electrolyte solution. When in contact with this strongly alkaline environment, the surface of the Ni electrode is covered with a layer of $Ni(OH)_2$. The voltammograms were recorded in the potential range between -0.2 and 0.8 V, at the scan rate of 0.1 V/s. In the anodic direction, $Ni(OH)_2$ is oxidized to NiOOH ($E_{pa} = 0.403$ V), which is reduced back to $Ni(OH)_2$ during the cathodic scan ($E_{pc} = 0.295$ V). As more cycles are traced, the oxidation peak shifts towards more positive values, while the reduction peak shifts in the opposite direction, towards more negative ones (Fig.1b). The two peaks are single peaks, which indicates that the electrode reaction unfolds only between $Ni(OH)_2$ and NiOOH. The electrode also displays good stability during the cyclic voltammetry experiment [7].

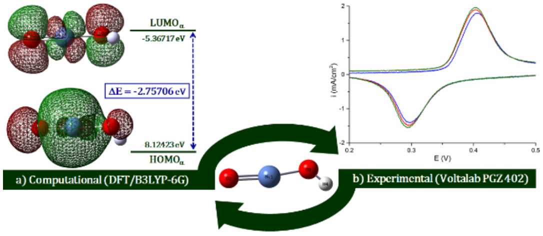

Figure 1. NiOOH: a) Representation of HOMO$_\alpha$ and LUMO$_\alpha$ orbitals; b) Cyclic voltammograms recorded on the Ni electrode.

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Ni-DOPED HETEROPOLY COMPOUNDS FOR THE ETHANOL DEHYDRATION TO ETHYLENE

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Heteropoly compounds (HPCs) with the general formula $Cs_xNiH_{3-x}PW_{12}O_{40}$ (x=2, 2.25 and 2.5) were prepared and used as catalysts for the ethanol dehydration to ethylene and other organic compounds used as starting materials for the organic industry. The effects of Ni on the structure and catalytic activity of the catalysts were investigated. The thermal decomposition was evaluated using thermogravimetric differential thermal analysis (TG-DTA) and consists of water release: physically adsorbed water, hydrogen-bonded water and constitutive water. The release of constitutive water leads to the destruction of Keggin units and the formation of WO_3 and P_2O_5 oxides. FTIR spectra showed that the Ni-doped catalysts maintained the Keggin structure of the undoped catalysts. X-ray diffraction results indicated that all synthesized compounds exhibit the reflections corresponding to cubic phase. Catalytic activity of catalysts in ethanol conversion was studied by continuous flow reaction technique (CFRT) and the products were analyzed on gas-chromatography (GC) with FID and TCD detectors. The introduction of large counter-cations, like Cs, into acid increases surface area and enhances catalytic activity. Nickel doping prevents the formation of coke and improves the burning of coke. The Keggin structure is not affected by coke formation during ethanol dehydration, which led us to conclude that these catalysts can be regenerated.

MISCIBILITY STUDIES OF FUNCTIONALIZED CARBON DOTS WITH CU(II) BASED METALLOMESOGEN

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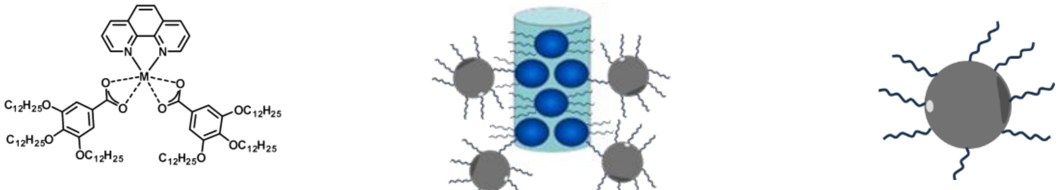
Hybrid systems composed of liquid crystals and carbon-based materials are promising supramolecular "soft" functional materials for advancements in sensing [1,2,3] and electro-optics [4]. Structural studies on the hybrid systems may bring important information related to their activity, mechanism of action or inducement of new synergistic properties. In this regard, the control of supramolecular arrangement of the hybrid material is very important. When physically mixing two different nature compounds is very difficult to obtain homogeneous materials at molecular level. Thus, the reproducibility in terms of obtaining the same homogeneous mixture is quite impossible. Therefore, to improve the compatibility to yield a more homogenous, the functionalization of carbon dots with long alkyl chains was carried out.

In this work, N-doped carbon dots obtained by microwave synthesis from citric acid and diethylenetriamine (DETA) were functionalized with long alkyl chains to introduce lipophobic units for a better compatibility with the hydrophobic parts of the metallomesogen. The functionalized carbon dots (f-CDts) were characterized by spectroscopic methods (FT-IR and RAMAN).

Hybrid systems were obtained by physically mixing f-CDts with a Cu_MM, whose chemical structure is presented in Figure 1, in 1 to 5 ratio (% w/w). The final hybrid system was investigated by spectroscopic (FT-IR and RAMAN) methods and their liquid crystalline properties were determined by polarized optical microscopy (POM) and differential scanning calorimetry (DSC).



Cu(II) metallomesogen

Carbon dots

Figure 1. Physically mixing of f-CDts with Cu_MM in 1 to 5 ratio (% w/w)

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