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MAIN GROUP ORGANOMETALLICS AS METALLOLIGANDS FOR TRANSITION METALS - DISCRETE HETEROMETALLIC SPECIES, COORDINATION POLYMERS AND SUPRAMOLECULAR ARCHITECTURES

Alexandru SAVA, Ahmad BEN KIRAN, Raffaele FONTANA, Sabina VIERIU, Levente KISS, Cristian SILVESTRU

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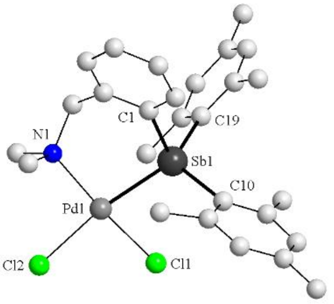
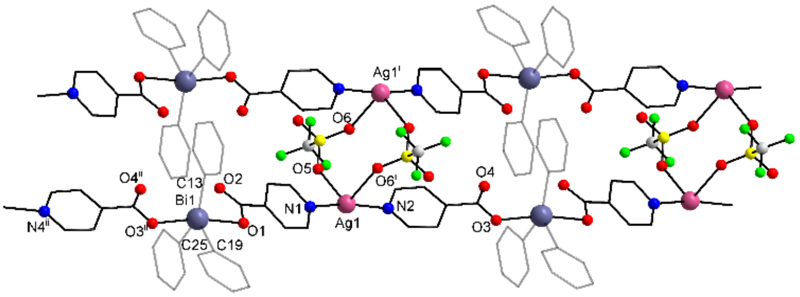
Main group organometallics with appropriate design can be used as robust, air stable, neutral or anionic ligands for transition metals, thus providing discrete heterometallic species or coordination compounds of different dimensionality. Nonmetal atoms from functionalized organic groups attached to the metal atom or even the central main group metal atom, in low oxidation state, can behave as connecting centers to other metal atoms. Ditopic or multitopic tectons can be designed taking advantage of the nature of the main group metal and its coordination properties, the nature of organic groups bearing recognition sites, or the nature of the anionic groups attached to the central metal atom of the potential metalloligand. Recent examples of such organometallic tectons based on a main group metal, *e.g.* Sn, Sb, Bi, or Hg, will be presented as well as transition metal molecular complexes or coordination polymers. Supramolecular solid-state networks of different dimensionalities (1D, 2D or 3D) and architectures based on various types of interactions will be discussed. [1-10]



[{(*N*,*Sb*)-[2-(Me_2NCH_2)C_6H_4]Mes_2Sb}$PdCl_2$]



[Ag{$Ph_3Bi[O(O)CC_6H_4N\text{-}4]_2$}($O_3SCF_3$)]$_n$

Acknowledgements. Financial support from National University Research Council (CNCSIS, Romania; Research Projects No. PN-II-ID-PCCE-2011-2-0050, PN-III-P4-ID-PCE-2016-0857 and PN-III-P4-ID-PCE-2020-2651) is highly acknowledged.

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BIO-BASED PLATFORM CHEMICALS UPGRADING VIA DIALKYL CARBONATE CHEMISTRY

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Over the last two decades, there has been a growing demand for renewable feedstock as an alternative to finite resources such as petroleum. As a result, carbohydrates and their derivatives has emerged as promising building blocks for the development of cost-effective and high-performance renewable materials and added-value chemicals. In this prospect, the US Department of Energy (DOE) has published a list of 15 target molecules, starting from 300 original candidates that were considered of special interest for biorefinery development. [1] These compounds have been selected by taking into consideration numerous factors such as available processes, economics, industrial viability, size of markets and their possible employment as a platform for the production of derivatives. Over the years, due to the considerable progress in biorefinery development, this list, as well as the criteria used to identify bio-based products have been revised. However, among the original selected chemicals, some bio-based platform chemicals such as D-sorbitol, 5-hydroxymethylfurfural (HMF), together with ethanol and glycerol, still occupy top positions as they encompass all of the desired criteria for bio-based platform compounds.

D-Sorbitol is a sugar alcohol, found in nature as the sweet constituent of many berries and fruits from which it was isolated for the first time in 1872. Its large-scale manufacture began in the 1950s, due to the growing applications as humectant in cosmetology and sugar substitute in confectionery. Nowadays the global market of D-sorbitol is estimated around 800 kt, half of which is produced in China with a demand currently growing at 2–3% rate annually. The reason of such interest relies on the fact that D-sorbitol has all the characteristics of a typical bio-based platform chemical in terms of sustainability, applications and market value. In fact, dehydration of D-sorbitol produces anhydro sugar alcohols, including sorbitan and isosorbide. Both these products have achieved commercial importance and can be used to synthesize numerous intermediates of industrial interest. [2]

Similarly, HMF stands out as a versatile bio-based platform chemical capable of undergoing diverse chemical transformations, including oxidation, hydrogenation, hydrolysis, and esterification, offering a wide range of industrially relevant compounds. [3] As a result HMF has found numerous applications in the synthesis of chemicals, materials, bio-based polymers and fuels.

However despite D-sorbitol and HMF are renewable starting materials, their derivatizations often do not always follow the green chemistry principles. In this prospect, this presentation will focus on the reactivity of D-sorbitol, isosorbide and HMF with green reagent and solvent dimethyl carbonate (DMC). [4]

The reactions between these bio-based chemicals with DMC, [5] are very appealing as they encompass the preparation, as well as the transformation of a renewable resource into industrially relevant products via a chlorine-free and green approach.

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MAX PHASE AND MXENE A NEW TREND IN CATALYSIS

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In the last two decades, a new class of materials known as MAX phases ($M_{n+1}AX_n$) and MXenes ($M_{n+1}X_nT_x$) have been discovered (with n = 1-4, M = early transition metal, A = A-group element, X = carbon or nitrogen, and T_x = various surface terminations, like -O, -OH, and -F). [1–3] Their many remarkable chemical and physical features have made a significant impact. For instance, MAX phases merge previously separate categories of materials (ceramics and metals) by combining desirable attributes of both (high thermal and electrical conductivity, mechanical strength, resilience to high temperatures or oxidation, and low density, among others).

Over thirty MXenes of varying compositions and more than one hundred fifty MAX phases [4] have already been synthesised. [5] Because of their lamellar structure, metallic/covalent bonds, and relatively weak bonding between the M and A layers, MAX phases exhibit unusual features.

In order to produce MXene, 2D materials, the A elements (mainly Al) in MAX phases are etched out, leaving behind 2–4 layers of M–C sheets. Many of them are good conductors like metals and are also hydrophilic. High conductivity is maintained even in polar fluids due to the presence of oxygenated terminations. [2]

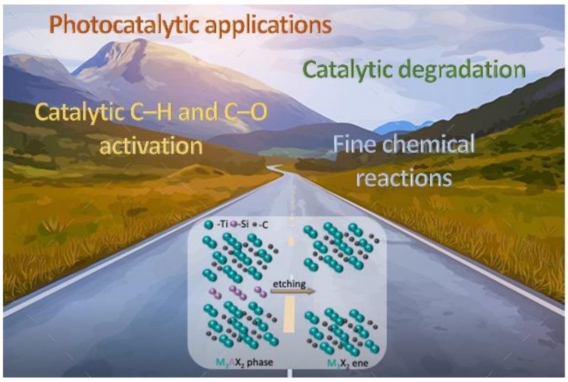

Figure 1. The MAX phases and MXene derivatives: a roadmap to potential applications.

Consequently, MAX phase and MXene are extremely envisioned and appealing materials for catalysis due to their unique features; yet, despite evidences that promote them as catalysts, their catalytic capabilities were just recently explored. [6,7] (Figure 1).

Herein we will emphasize the great potential of these materials to act as catalysts, as well as supports, creating a synergy with various active species by presenting few examples of successful application of MAX phase and MXene. To enhance the activity of MXenes and to introduce functional groups helpful in certain chemical processes, it may be able to manipulate their surface chemistry. For example, new acid solvent development that can depolymerize PET back into raw materials is of paramount importance right now. Sulfonated groups were introduced into MXenes using aryl diazonium sulfanilic acid's sulfonated aryl diazonium salt to graft $-SO_3H$ groups onto the surface. Several methods (XRD, DRIFT, RAMAN, SEM, TEM) were used to examine the modified MXenes and found that their lamellar structure had not collapsed throughout the sulfonation procedure. High acidity and efficiency as catalysts for PET depolymerization characterize the materials developed. MAX phase and MXene are efficient also in selective hydrogenation of C=O bond and also are able to produce oxidative products as a result of oxdidation reaction of key platform molecules in fine chemistry.

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METAL PHOSPHONATE INCLUSION COMPOUNDS: EXPLORING THE VIABILITY OF THE 'BOTTLE AROUND THE SHIP' APPROACH TO INCLUSION OF NANOPARTICLES IN METAL PHOSPHONATES

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The synthesis of porous materials is often goal of the 'Inorganic Phosphonate chemist'. The superior chemical and physical properties with respect to many carboxylate-based MOFs leads to metal phosphonates being the material of choice for a number of applications, particularly the inclusion and stabilisation of particles and guest molecules.

The synthesis of materials with pores and channels in the nanometre regime remains challenging with few such materials being reported in the literature, the majority tending to be in the range angstroms. Their synthesis relies on the use of long chain organophosphonates, which can be difficult to synthesize/purify or obtain commercially as well as an ability to control synthesis conditions to yield a materials with a porosity that remains once the solvents are removed prior to inclusion of guest species, otherwise called the Ship-in-the-Bottle approach 1.

An alternative approach to the synthesis of inclusion materials is to construct the host material around the (preformed) guest species; the so-called 'Bottle-around-the-Ship' method 2. In this paper we will explore the possibility of using this including a variety of guest species, including both molecular species and nanoparticles, in a number of well known materials whose synthesis is well understood and highly reproducible but whose crystal structures would exclude the possibility of a Ship-in-the-Bottle approach.

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THE CHEMISTRY AND BIOLOGY OF AN EARLY TRANSITION METAL ION INDUCING CELL DIFFERENTIATION AND MATURATION IN DIABETES MELLITUS II

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Metal-based materials have been increasingly gaining ground toward a multitude of industrial and biological applications. Among them outstanding are organometallic and metal-organic compounds with biological properties justifying their use in (patho)physiological aberrations in humans. Of the multitude of examples presently used in the therapeutics of human diseases, platinum, ruthenium, and gold emerge predominantly in the form of drugs addressing diseases, such as cancer, diabetes, neurodegeneration, etc.. Diabetes has undoubtedly been a disease of global proportions with a single molecule (i.e. insulin), a hormone, playing a crucial role in the major types of the disease encountered in humans of variable medical background, age, lifestyle and genetic disposition. Efforts to overcome problems associated with the administration of insulin and its daily injections have prompted the scientific community to seek alternative drugs to lower hyperglycemia and/or a plethora of aberrant medical complications. To that end, vanadium and zinc have been used to investigate the aqueous chemistry with organic substrates capable of providing soluble species that atoxically facilitate glucose uptake and catabolism by mature adipocytes.

Cognizant of the complexity of the aqueous chemistry of vanadium with organic substrates and the equally intricate web of interactions with cellular targets in adipocytes, the early transition metal ion Ti(IV) (isoelectronic to V(V)) was employed to pursue analogous aqueous chemistry with physiological substrates at the binary and ternary level. To that end, the structural speciation of Ti(IV) with α-hydroxycarboxylic acids (citric, quinic, 2-hydroxyisobutyric, etc.) was investigated synthetically, leading to a well-defined web of species as function of pH and molecular stoichiometry. [1, 2] The analytical, spectroscopic, and structural characterization of the resulting binary species in the solid state and in solution (elemental analysis, FT-IR, TGA-DTG, cyclic voltammetry, ESI-MS, NMR) led to the formulation of a well-defined physicochemical profile. The latter was crucial in selecting the species for further biological perusal of their properties.

The in vitro biological investigation of select Ti(IV)-(α-hydroxycarboxylato) complex species included a) biotoxicity exploration in a time- and concentration-dependent fashion, followed by morphology, migration and proliferation work, and b) cell differentiation (3T3-L1 cells) experimentation on immature adipocytes supported by genetic markers revealing the state of maturation of differentiated adipocytes capable of taking up glucose and catabolizing it. [3] Exposure of immature fibroblasts to select Ti(IV)-(α-hydroxycarboxylato) species showed which ones were atoxic and as such their biological potential in inducing cell differentiation and adipocyte maturation. The collective experimental data on the investigated systems reveals well-defined binary Ti(IV)-(α-hydroxycarboxylato) complex species, the atoxic biological profile of which supports cell differentiation potency in producing mature adipocytes capable of fighting hyperglycemia and exhibiting structure-specific synergistic activity with insulin. Undoubtedly, the global profile of the Ti(IV)-hydroxycarboxylic acid chemistry reflects merit in the specific metal ion delivering biological activity as a metallodrug in Diabetes mellitus II in the future.

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RESPONSIVE SOFT MATERIALS FOR ADVANCED APPLICATIONS

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Soft materials are ubiquitous in our daily life and are key players in many industries, such as electronics, automobiles, environment, and robot engineering. Hard and heavy materials used 50 years ago have been replaced by soft and light materials such as polymers, liquid crystals, gels or colloids. [1] Moreover, a high percentage of our body is made of soft materials having complex structural and dynamic properties. [2] Thus, much scientific effort has been devoted to developing highly functional soft materials. Among soft materials, hydrogels are a promising material platform, especially in view of their biomedical applications such as drug delivery, tissue engineering, ocular devices, and tissue and organ replacement. [3] Hydrogels can be obtained from synthetic and/or naturally occurring polymers through chemical or physical cross-linking processes. While a multitude of synthetic hydrogel materials strategies have been reported, they all come hand in hand with shortcomings that can limit their applicability. [4]

In this respect, poly(2-isopropenyl-2-oxazoline) (PiPOx), has attracted increased scientific attention as a reactive polymer for the synthesis of advanced functional materials. [5] PiPOx is a versatile polymer soluble in water and various organic solvents, can be prepared with well-defined characteristics, and exhibits high thermal and good hydrolytic stability [6, 7]. Furthermore, PiPOx was shown to be biocompatible, rendering it suitable for medical and pharmaceutical applications. [8] The pendent 2-oxazoline group can be transformed in an efficient, mild, and selective manner, providing an extremely valuable toolbox for the synthesis of advanced materials. The post-polymerization modification reaction with (di)carboxylic acids enabled access to a wide variety of structures with defined and controlled properties.1 The versatility of this modification method allows the synthesis of a wide variety of functional polymers with tunable properties from soft to hard materials. [9-11]

Recent developments from our research group that illustrate the potential of PiPOx as smart (bio)materials will be discussed in this lecture, ranging from fundamental studies on ring opening addition of PiPOx with carboxylic acids to emerging applications of these polymers as biomaterials, nanosensors, and drug delivery vehicles.

Acknowledgements. The authors acknowledge the Romanian Ministry of Research, Innovation and Digitalization, CNCS/CCCDI – UEFISCDI, project number PN-III-P2-2.1-PED-2021-2544 within PNCDI III, for the financial support.

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SMALL MOLECULE ACTIVATION AT BIOLOGICAL METAL-MACROCYCLE COMPLEXES: CONTRASTS BETWEEN HEME AND VITAMIN B_{12}

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In heme-containing proteins, redox-active agents such as peroxides or oxyanions of halogens/sulfur/nitrogen offer a rich chemistry involving high-valent iron, free radical reactions and small molecule activation. [1,2] By contrast, until recently our knowledge of the reactivity of cobalamin with oxidizing agents has been confined to processes where, especially with strong oxidizing agents, the corrin ring is covalently modified by oxygenation or halogenation, or where Co(I) or Co(II) are oxidized to Co(III) in an outer-sphere manner – but no complexes of Co(III) with oxidizing agents, and no ensuing high-valent Co centers. [3] We have, however, recently reported that H_2O_2 does in fact form a stable and reversible complex with cobalamin, assigned as Co(III)-hydroperoxo based on UV-vis and NMR spectra complemented by DFT calculations. [4] We describe here a combination of spectroscopic and computational results showing that m-chloroperoxobenzoic acid also yields a relatively stable complex with Co(III) cobalamin. Using the same experimental toolkit – centered on ^{1}H-NMR spectroscopy and DFT calculations – we then describe a stable adduct of Co(III) cobalamin with chlorite – which in contrast to the known instability of the putative heme-chlorite complex in the catalytic cycle of the enzyme chlorite dismutase. Also described are the adducts of cobalamin with hypochlorite – again more stable than their heme counterparts. Differences in reaction mechanisms between Fe(III) heme and and Co(III) cobalamin complexes in such processes are rationalized.

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LACCASES: BLUE ENZYMES FOR GREEN CHEMISTRY

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Laccases are oxidoreductases belonging to the multinuclear copper-containing oxidases. The overall outcome of their catalytic cycle is the reduction of one molecule of oxygen to two molecules of water and the concomitant oxidation of four substrate molecules to give four radicals. [1]

Typical substrates of laccases are phenols and aliphatic or aromatic amines, the reaction products being mixtures of dimers or oligomers derived by the coupling of the reactive radical intermediates. For instance, these biotransformations have been exploited to isolate new dimeric derivatives of natural phenolic derivatives (resveratrol and its analogues, chalcones, β-estradiol, totarol). [2] In these studies, a significant influence of the solvent on the reaction outcomes has also been observed. [3]

In other studies, we have described the use of laccase-catalyzed reactions for the selective hydroxylation of ergot alkaloids and for the synthesis of the bisindole alkaloid anhydrovinblastine, [4] and more recently the outcomes of the oxidation of aromatic amines. [5]

Additionally, laccases oxidation of non-phenolic groups, particularly benzyl and primary alcohols, is also possible thanks to the ancillary action of the so-called “mediators” (i.e., TEMPO, HBT, ABTS), accordingly, a series of sugar derivatives and of natural glycosides have been oxidized. [6]

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s- AND p-BLOCK WONDERS: A TALE OF OFFBEAT MAIN GROUP METAL COMPLEXES

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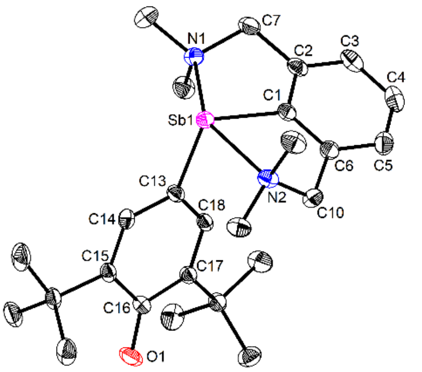
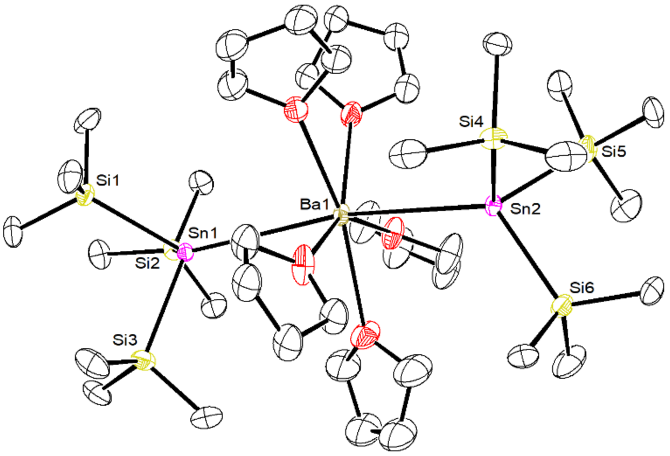
In recent years, main group metals have emerged as viable alternatives to more traditional, and sometimes more toxic, transition metals for a range of applications in organic chemistry, for instance as homogeneous catalysts for a variety of metal-mediated transformations or for site-selective functionalisations.

Our group has been involved for nearly 15 years in the design of highly reactive, electron-deficient complexes based on main group metals that have often been overlooked, e.g. the large alkaline earths (Ca, Sr and Ba), tetrels (Sn, Pb) and pnictogens (Sb, Bi). In this lecture, the synthesis of a suite of unusual, highly electrophilic complexes based on these elements will be detailed. Their applications as molecular catalysts for dehydrocoupling reactions and for C-H activation processes will be discussed.





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DEVELOPMENT OF ION MOBILITY MASS SPECTROMETRY FOR THE ANALYSIS OF CHONDROITIN/DERMATAN SULFATE GLYCOSAMINOGLYCANS

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Proteoglycans (PGs) represent a group of proteins covalently linked to sulfated linear *O*-glycan chains called glycosaminoglycans (GAGs), primarily expressed in the extracellular matrix where they are responsible for crucial biological events and implicated in various interactions as well as the onset and/or progression of severe pathologies. [1] Although the majority of PGs contain *N*-glycans as well, GAGs represent more than a half of the PG molecular weight, hence, the properties and biological activities of proteoglycans are given by their glycosaminoglycans.

Among GAGs, chondroitin sulfate (CS) and dermatan sulfate (DS) are found in a variety of PGs with an extensive expression in mammalian tissue. CS is composed of glucuronic acid-(β-1,4)-*N*-acetylgalactosamine-(α-1,4) disaccharide repeats, usually sulfated at GalNAc; however, during the biosynthesis, the sugar moieties may undergo modifications, thus, the glucuronic acid (GlcA) can be epimerized to L-iduronic acid (L-IdoA), to yield dermatan sulfate (DS). Hence, hybrid chains, in which DS sequences are randomly interspersed among CS motifs of regular and irregular sulfation patterns occur. This structural diversity gave rise to efforts for development of efficient analytical methods, among which, in the last decade, mass spectrometry (MS) contributed the most to the progress of the field. [2,3]

In this context, we report here on the development of ion mobility (IMS) MS and MS/MS for profiling and detailed structural analysis of CS/DS and the introduction of this approach in glycomics of CS/DS from human decorin (DCN) and biglycan (BGN). The CS/DS chains were released by β-elimination, depolymerized using specific lyases, fractionated by size-exclusion chromatography and subsequently subjected to detailed compositional and structural analysis by IMS MS and MS/MS. The present protocol, connecting IMS separation, MS screening and tandem MS, allowed: i) the discrimination of isobaric species by their separation according to the mobilities of their corresponding ions; ii) the detection in the CS/DS domains of DCN and BGN of novel over- and undersulfated sequences which, in view of their sulfation status are, more likely, biologically active, and iii) a detailed structural analysis including the identification of CS/DS sulfation code. The optimized IMS CID MS/MS provided a series of diagnostic fragment ions crucial for the characterization of the misregulations, which occurred in the sulfation pattern of CS/DS motifs in DCN and BGN.

Our approach, based on an integrated technique, offered the structural analysis of CS/DS species, at ultrahigh sensitivity, in a single run, in high-throughput mode. By performing an online separation, mass analysis and fragmentation on a single instrument, IMS MS was able to cut across the traditional methodologies existing in MS-based glycosaminoglycomics, which assume physical coupling of separation instruments to MS, with the entire arsenal of shortcomings that accompany such procedures. Considering these results, we believe that the present concept addresses to a better extent the needs of glycosaminoglycomics for faster, more reliable and more sensitive methodologies on one side and a few of the many questions still open, related to the structure and sulfation status of biologically active CS/DS domains.

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Ca(II) CONTAINING HYBRID BOROSILICATE AEROGELS FOR BONE REGENERATION

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On the last decades, bioactive glasses have attracted great attention due to their ability to stimulate the body's own repair process called "osteostimulation". [1,2] One important class of these porous non-crystalline solids are the borosilicates which possess a fast decomposition and adsorption rate in the human body. [3-5] In order to extend the knowledge on the correlation between biological activity and the borosilicate materials structural properties, a bunch of Ca(II) containing hybrid borosilicate aerogels have been designed, prepared and investigated systematically. Moreover, an in-depth structural characterization has been done, taking in account the effect of the used Ca(II) sources ($CaCl_2$, β-$Ca_3(PO_4)_2$ and $Ca_{10}(PO_4)_6(OH)_2$) and PVA (mw: 13000, 49000, 83000). Complementary characterization method was employed to obtain information about the chemical structure (FT-IR spectroscopy and solid state NMR), textural properties (N_2 sorption and SANS), morphology (TEM and SEM), elemental analysis (EDS), X-ray diffraction and zeta potential. The applicability of the hybrid aerogels in the field of bone regeneration was tested by viability and proliferation of mesenchymal stem cells.

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SUPRAMOLECULAR PHOTOSWITCHING SYSTEMS

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Host-guest pairs (H:G) offer attractive noncovalent binding motifs for constructing diversified supramolecular systems (e.g., rotaxanes), molecular machines, and self-assembled materials. In recent years, our research group has been interested in the design and development of water-soluble photoresponsive host-guest binding pairs, envisioning potential applications in biology and materials science. [1–5] We have developed and characterized photoswitchable dithienylethene (DTE) – cucurbit[*n*]uril (CBn) supramolecular systems with sub-picomolar affinities that can be exploited for drug delivery (Figure 1). [1–3] In a different approach, using as guests our group's well know flavylium/chalcone photoswitching pair, [4, 5] we have developed pseudorotaxanes, [6, 7] and supramolecular polymers based on homoternary HG_2 complexes, these latter exploited as photorheological fluids.

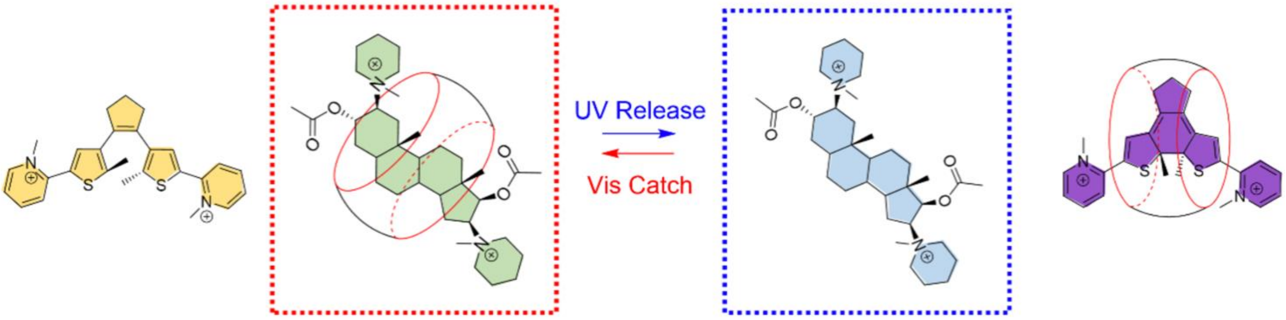

Figure 1. Light-controlled binding and release of a steroidal drug from a cucurbituril receptor using a DTE as a competitor with photocontrolled affinity.

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G-PROTEIN COUPLED RECEPTORS AS THERAPEUTIC TARGETS: A BRIDGE NOT TOO FAR BETWEEN CHEMISTRY AND BIOLOGY

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G protein-coupled receptors (GPCRs) represent a prominent class of cell surface receptors, with over 800 members in humans, each responding to diverse ligands, including neurotransmitters, hormones, ions, and photons. They function as molecular switches, initiating intricate intracellular signaling cascades upon ligand binding. Given their ubiquitous presence in various physiological processes, GPCRs have emerged as crucial therapeutic targets in drug discovery, with more than 30% of the FDA-approved drugs targeting them as agonists or antagonists [1, 2].

The dynamic conformational changes within GPCRs serve as a central hub for transmitting extracellular signals into intracellular responses. Consequently, targeting GPCRs with small molecules or biologics has proven to be an effective strategy for modulating numerous physiological processes and treating various diseases, ranging from cardiovascular disorders to neuropsychiatric conditions. Moreover, the development of cutting-edge screening technologies, such as high-throughput screening (HTS) and virtual library screening (VLS), has accelerated the identification of novel GPCR ligands. These approaches, combined with computational methods, have significantly expanded the repertoire of GPCR-targeting molecules and expedited drug discovery efforts. The chemistry aspect of GPCR targeting involves the rational design and synthesis of ligands that can selectively activate or inhibit these receptors. By implementing HTS and synthesis of ligands we identified and characterized GPCRs that are involved in the regulation of energy metabolism and demonstrated their in vivo relevance by employing genetically modified mouse models. Further studies entailing cellular biochemistry, molecular biology, and medicinal chemistry identified novel metabolites of arachidonic acids with opposing effects on vasculature and insulin metabolism [3-6].

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CHALLENGES IN THE DEVELOPMENT OF ANTIVIRAL AGENTS

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In recent years, this issue has become increasingly relevant and is set by the media and the public. In May 2023, the WHO declared the end of COVID-19 global health emergency pandemic, but warned that the next pandemics are "knocking on the door" and we must be prepared for them. This is especially true for us – the scientists, on whom the entire society relies to find quick and adequate solutions to medical crises.

The purpose of our presentation is to summarize the main challenges to the development of antiviral agents.

They are related to the nature of viruses, the peculiarities of their structure and life cycle; as well as testing their activity in preclinical studies in cell cultures and animal models. These include the simple structure of viruses, their dependence on cell infrastructure and physiology, which makes targeting virus-specific molecules and processes difficult, and the genetic variability of these infectious agents. These obstacles can only be overcome by the joint efforts of chemists, biologists, doctors and pharmaceutists. What are the viruses that attract the attention of the scientific and medical community today? Do we need to have antiviral agents if vaccines are available and vice versa? Can artificial intelligence help us? Examples of antivirals against influenza, HIV, SARS-CoV-2 and hepatitis viruses will be discussed.

The presented interdisciplinary topic will provide an opportunity to discuss one of the leading scientific, medical and social challenges of our time - the fight against viral infections; will contribute to the next steps in the combined efforts of the biomedical and chemical scientific community to overcome it.

Keywords: viruses, antiviral agents, drug resistance, vaccines

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ANTIMICROBIAL PEPTIDES AND THEIR POTENTIAL IN BIOMEDICAL APPLICATION

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Antimicrobial peptides (AMPs) possess unique properties that make them valuable tools for studying membrane structure and function and promising candidates for therapeutic applications. [1, 2, 3, 4] AMPs exhibit diverse structural features, including amphipathic structures and specific amino acid residues, enabling selective interaction with multiple membranes. Their mechanisms of action involve disrupting lipid bilayers through different pathways, depending on peptide properties and membrane composition. [1] We present the development of six newly designed AMPs based on buforin II sequence with low toxicity to normal human cells and high antimicrobial activity against bacterial strains tested. Exploring AMPs holds promise for developing novel therapeutic strategies against infections, cancer, and drug delivery challenges. [1, 2, 3, 4, 5]

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HOW CAN ZEOLITES CLOSE THE LOOP OF ENVIRONMENTAL REMEDIATION TECHNIQUES?

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In the quest for a sustainable future, environmental remediation techniques play a pivotal role in mitigating pollution and safeguarding our ecosystems. Among the diverse array of materials available, zeolites have emerged as promising candidates for addressing environmental challenges. [1] With their unique properties, zeolites offer the potential to close the loop of remediation by effectively removing pollutants from aqueous solutions taking into account toxicity effects behind remediation procedure. [2] This contribution focuses on exploring the application of zeolites in the removal of pesticides and other contaminants, highlighting their pivotal role in environmental remediation.

Zeolites and porous materials possess well-defined pore structures, large specific surface areas, and negatively charged frameworks. These features offer opportunities for incorporating various functionalizing phases to enhance their performance and enable tailored removal of specific contaminants. The combination of zeolites with functional materials, such as heteropoly acids/salts [3, 4], functional carbons [5], and conducting polymers [6, 7], has resulted in synergistic effects, enhancing the adsorption capacity, catalytic performance, and overall environmental applicability of these composites. Moreover, the incorporation of antibacterial agents into zeolite composites has shown promise in tackling microbial contamination in water systems. [8]

Furthermore, spent zeolite adsorbents require regeneration and/or reuse. After reaching their adsorption capacity, zeolites can be subjected to regeneration processes, such as thermal treatment [9], desorption, or solvent extraction or they can be further treated to produce novel materials for electrochemical applications. [10] The reuse in subsequent remediation cycles and the onset of new applications minimize waste generation and promote resource efficiency.

By harnessing the unique properties of zeolites, we can pave the way for efficient and sustainable solutions to addressing environmental pollution challenges. Understanding the adsorption mechanisms, catalytic and regeneration processes, and the subsequent reuse of zeolites is crucial for developing effective remediation strategies and achieving a cleaner and healthier environment.

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CHEMICAL BIOLOGY TOOLS FOR HEPATITIS C VIRUS RESEARCH

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Hepatitis C Virus (HCV) infects 55 million people worldwide. Although major breakthrough has been done in the standard of care by clinical use of direct acting antivirals, there are still infections which may not be reversed from their evolution to liver cirrhosis and hepatocellular carcinoma. Thus, understanding further host-pathogen interaction is needed beyond fundamental research reasons. Moreover, the incidence of HCV infection is increasing justifying the quest for a HCV vaccine. Herein, we will present several chemical biology tools developed to help address the above-mentioned problems.

To image the HCV assembly process, we have used genetic labeling at tetracysteine tags. Real-time imaging techniques have been complemented by interactomic proteomics in HCV cell culture system. New chemical probes which target active cysteine proteases were designed and tested. For a more efficient glycoprotein purification a new polyaminopolycarboxilic probe was designed. To identify new antiviral compounds, a targeted compound library was selected by chemoinformatic techniques. Using these tools, new endogenous proteins involved in HCV assembly process were identified and dynamics of HCV core and NS5A proteins were monitored in living cells. A more efficient HCV E2 protein purification was accomplished using the new chelator probe. New chemical scaffolds were identified against NS2 protease which are able to inhibit HVC replication.

Chemical biology will be instrumental in molecular virology research for target identification and validation, antiviral drug screening and vaccine development.

GREEN HYDROGEN FROM SOLAR WATER SPLITTING USING TRANSITION METAL OXYNITRIDES

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Although hydrogen is a zero-emission energy carrier, its current global production still heavily relies on fossil fuels. Current momentum on renewable energy and environmental remediation is unprecedented because of fast climate change. We all know that the world is hurrying up to achieve the United Nations Sustainable Development Goals (SDGs) by 2030 without pausing even during the COVID-19 pandemic. One of the important SDGs is Goal 7: Affordable and Clean Energy. As a replica of natural photosynthesis, a semiconductor-based artificial photosynthetic system is regarded as one of the most economically viable, highly efficient, and environmentally benign chemical processes to generate green hydrogen energy from solar water splitting. [1-2] However, to harness solar energy efficiently, it is necessary to enhance the visible-light-driven photocatalytic performance of the existing materials and to discover novel visible-light-active materials. Mixed-anion compounds offer new opportunities in this regard. As a 600 nm-class photocatalyst, $BaTaO_2N$ has received particular attention due to its small bandgap (E_g = 1.9 eV), suitable band edge positions for visible-light-induced water splitting, chemical stability, and nontoxicity. [3] $BaTaO_2N$ is routinely synthesized by a two-step method: (i) the synthesis of a corresponding oxide precursor and (ii) its high-temperature nitridation under an NH_3 atmosphere for a prolonged period. This two-step method leads to the formation of various defects that negatively affect the water splitting performance.

Therefore, we have (i) applied an NH_3-assisted direct flux growth approach to reduce the defect density of $BaTaO_2N$, (ii) engineered the bandgap by cation substitution, and (iii) explored the effects of the altered morphology, size, and porosity on the visible-light-induced water oxidation activity and photoelectrochemical performance of $BaTaO_2N$. The findings revealed that the photocatalytic activity and photoelectrochemical performance of $BaTaO_2N$ were significantly influenced by its morphology, size, porosity, substituent type, and substitution concentration. Particularly, the $BaTaO_2N$ crystal structures obtained by nitridation of oxide precursor without KCl flux exhibited a higher surface area and high anodic photocurrents compared to the $BaTaO_2N$ crystal structures obtained by nitridation of oxide precursor with KCl flux due to the high number of dangling bonds acted as nucleation centers for the highly dispersed CoO_x cocatalyst nanoparticles. Also, an NH_3-assisted direct flux growth approach reduced the density of intrinsic defects in $BaTaO_2N$ crystals, leading to a substantial enhancement in water oxidation activity. The Mg-substituted $BaTaO_2N$ and Al-substituted $BaTaO_2N$ independently exhibited the highest amounts (in 5 h) of evolved O_2 (503.6 μmol) and H_2 (117.4 μmol), respectively, whereas the Zr-substituted $BaTaO_2N$ showed the high photocatalytic activities in both O_2 (446.8 μmol) and H_2 (80.4 μmol) half-reactions due to the altered potentials of the valence and conduction bands and an increased density of charge carriers.

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EXPLORING (HETERO)ARYLAZO CHEMICAL SPACE FROM SYNTHESIS TO APPLICATIONS

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Heteroaylazo compounds [1] have been recently reported as a promising class of photoswitches. [2] Initially developed as alternatives to the widely known azobenzenes in order to overcome their major drawbacks, such as such as incomplete conversion between the isomers or rather short half-life of the least stable isomer, the field of heteroayl azoswitches has steadily grown, each heterocycle reported in the structure displaying novel features. However, there are still unanswered questions regarding their structures, properties and mechanisms of actions relationships.

The presentation refers to work regarding novel (hetero)arylazo compounds involving various azole moieties [3] moieties (i.e. 1,3,4-oxadiazole, 1,3,4-thiadiazole, pyrazole) from synthesis to study of the main parameters that characterise a photoswitch. In the design of the compounds, we considered grafting the heterocyclic cores with functional groups known for providing enhanced features (*i.e.* fluorine). Besides thorough structural characterisation of the new compounds (e.g. NMR, XRD), we used UV-Vis and NMR spectroscopies to determine the absorption properties, photostationary states, fatigue resistance and thermal stability of the metastable isomer at irradiation. Our results indicated interesting behaviour of the compounds with respect to previously reported structures, with improvements in band separation or thermal stability.

Aknowledgments. This work was supported by a grant of 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, contract 609/PED, within PNCDI III. The University of Bucharest - UniRem project is also gratefully acknowledged.

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1D-NANOFILAMENTS TIO_2-BASED LEPIDOCROCITE FOR PHOTOCATALYTIC HYDROGEN PRODUCTION THROUGH WATER SPLITTING

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Water and sunlight are often regarded as the most pristine, highly sustainable, and plentiful resources available on our planet. Photocatalysts have the capability to harness solar energy and facilitate the decomposition of water into its elemental components, namely oxygen and hydrogen. The latter refers to a type of environmentally friendly fuel that is now being developed as a potential substitute for fossil fuels. Its purpose is to mitigate carbon dioxide emissions.

The pursuit of cost-effective and scalable photocatalysts with exceptional stability for hydrogen generation has been a longstanding aspiration of the scientific community. However, despite extensive efforts, there are presently no commercially accessible materials that satisfy all the necessary criteria for widespread implementation. These criteria include high light quantum efficiency, stability, safety, and affordability. From a cost analysis standpoint, the production of H_2 using photocatalysis is now projected to have a cost of ~ \$10 per kilogram, with the primary cost driver being the photocatalyst itself. Simultaneously, the production of H_2 using fossil fuel reformation, which is considered environmentally unsustainable, incurs a cost of around \$1 per kilogram. In order for photocatalysis to achieve competitiveness, a significant reduction in its price is necessary, on the order of magnitude or greater. This reduction is crucial for the realization of a solar-H_2 world economy.

Based on these premises, in this study [1], we provide findings on the synthesis of one-dimensional lepidocrocite-based sub-nanofilaments (NFs) with a cross-section of around 5×7 Å^2. These NFs have the ability to produce H_2 when exposed to simulated sunlight in a combination of water and methanol (80:20 v/v). The NFs exhibited stability when kept in such mixtures for durations exceeding 4,300 hours, with 300 hours of the period involving irradiation. Quantum yields reaching a notable magnitude of 11.7% were successfully achieved.

Based on the findings obtained from the analysis of deuterated water, it can be inferred that water serves as the source of H_2. Moreover, the analysis did not reveal any presence of CO_2 resulting from the process of photocatalytic destruction of methanol. Hence, these novel materials demonstrate the necessary characteristics of an efficient photocatalyst, including proficient charge separation, rapid charge transfer, and notably, enduring stability in aqueous surroundings. The findings of this study provide novel opportunities for investigating energy generation systems utilizing one-dimensional NFs derived from inexpensive, environmentally safe, and widely available source materials through a straightforward, cost-effective, and easily scalable synthesis approach.

Aknowledgments. This work was partially supported by grants of the Ministry of Research, Innovation and Digitization, CNCS-UEFISCDI, project numbers PN-III-P4-PCE-2021-1461 and PN-III-P4-ID-ERC-2021-0007, all within PNCDI III.

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WHEN A NITRONYL NITROXIDE LIGAND MEETS AMINES TO FORM SCHIFF BASES. LIGANDS DESIGN AND THEIR COMPLEXES WITH 3d AND 4f METAL IONS

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Novel nitronyl nitroxid ligands, HL^1 and HL^2, have been synthesized starting from 2-hydroxy-3-(hydroxymethyl)-5-methylbenzaldehyde (HL^a) and 2,6-diformyl-*p*-cresol (HL^b), respectively, [1] following the synthetic protocol reported in the literature. [2] Using the ligand HL^1, three 2p-4f binuclear complexes, $[Ln_2(L^1)_2(hfac)_4]$, have been obtained and characterized, where Ln = Gd, Tb, Dy and hfac = hexafloroacetylacetonate anion (Figure 1a). [3] Moreover, 2,6-diformyl-*p*-cresol (HL^b) can be used to obtained the corresponding diradical. Its synthesis and crystal structure are known in the literature, [4] and, more recently, a copper trinuclear complex has been reported. [5] In this work we show that the monoradical HL^2 can be also synthesized and further employed as a ligand.

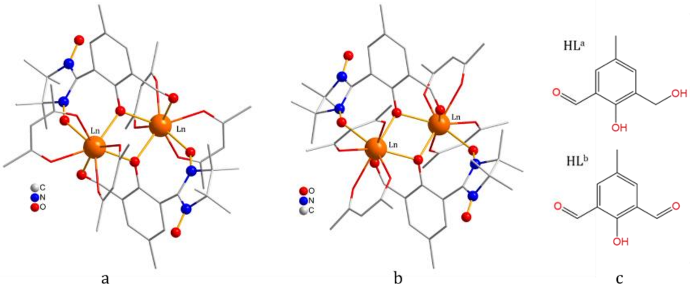

Figure 1 Perspective view of the molecular structures of (a) $[Ln_2(L^1)_2(hfac)_4]$ and (b) $[Ln_2(L^2)_2(hfac)_4]$ (monoclinic crystal system). Florine and hydrogen atoms have been omitted for clarity. (c) Structures of HL^a and HL^b aldehydes.

Hence, a new family of of 2p-4f binuclear complexes, $[Ln_2(L^2)_2(hfac)_4]$, has been obtained and characterized bearing similar features (Figure 1b). X-ray diffraction studies on single crystal and on powder reveal that these compounds present polymorphism as they are crystalizing both in a monoclinic and a triclinic crystal system. Due to the fact that HL^2 has a free formyl group, Schiff bases with primary amine could be formed, enhancing the number of heteroatoms from the molecule available for coordination. Thus, several diradicals have been synthesized using 1,3-diaminopropane, 2,2′-(ethylenedioxy)bis(ethylamine), 4-amino-TEMPO. A tripodal triradical has been synthesized using tris(2-aminoethyl)amine, and it was characterized via X-ray diffraction on single crystal. The polydentate paramagnetic ligands have been reacted with different 3d and 4f hexafluoroacethylacetonato complexes giving rise to mono- and oligonuclear complexes with exciting properties.

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TUNING THE SIGN AND MAGNITUDE OF COMPLEXATION-INDUCED pK_a SHIFT IN CUCURBIT[7]URIL HOST-GUEST COMPLEXES BY MOLECULAR ENGINEERING

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Cucurbit[n]urils (CBn) became popular macrocyclic receptors in supramolecular chemistry because they can recognize complementary guest molecules with high affinity in aqueous environments. CBn selectively bind positively charged guest molecules, including ionizable ammonium cations which frequently display much higher affinity than their neutral counterparts. This selectivity for the protonated species is translated into an increase in the basicity of encapsulated guest: in other words, CBn stabilize the protonated form of guest molecules and then increase the pK_a value of the conjugate acids of amines. [1–3] Despite being very rare, negative pK_a shifts can be observed for specific guests. Following a previous work from our group [4] reporting slightly negative pK_a shifts for flavylium and chalcone dyes featuring N-diethylamino substituents ($\Delta pK_a = -0.2$), in this communication we report a systematic study on the complexation of N-dialkylaminochalcones with CB7. The results show that the pK_a shifts of these host-guest complexes can be rationally tuned by the nature of the N-dialkylamino groups and also by target substitutions on the skeleton of the dye, allowing design of a CB7 1:1 host-guest complex with a $\Delta pK_a = -0.6$ (Figure 1).

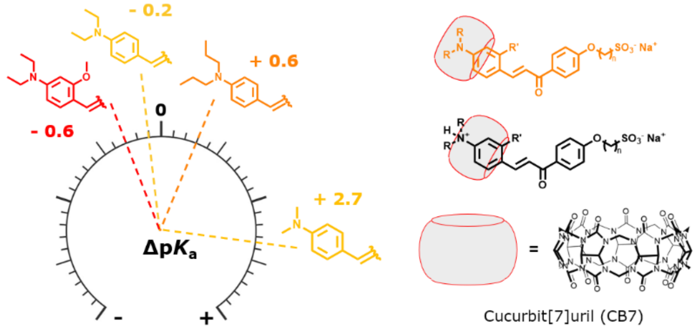

Figure 1. Schematic representation of the complexations of N-dialkylaminochalcones with CB7 and their corresponding pKa shifts observed by our group.

Acknowledgements. This project has received funding from the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement N° 814299 - CHARISMA. This work was supported by the Associate Laboratory for Green Chemistry LAQV, which is financed by national funds from FCT/MCTES. FCT/MCTES is also acknowledged for the CEECIND/00466/2017 research contract (N.B.).

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SUSTANAIBILE BIOCONTROL OF BIOLOGICAL AGENTS ON APPLE AND POTATO AT HIGH TEMPERATURES

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Products of microbial origin in combination with para-aminobenzoic acid (PABA) derivatives can be the basis for organic farming and plant resistance to unfavorable environmental factors inducing, as well as for the crop yield increasing. The article presents the results of the study of efficiency of fruit-cultures and potato plantations treatment with aqueous suspensions of entomopathogenic bacteria *Bacillus thuringiensis* subsp. *kurstaki* and *Bacillus thuringiensis* var. *thuringiensis* with addition of para-aminobenzoic acid derivatives solutions in concentrations 10^{-2}, 10^{-4}, 10^{-6} mol/l. An increase in the average weight of fruits and tubers and a reduction in disease and insect damage were observed in all variants of the experiment compared to the control. The studied derivatives exhibited higher biological activity at the lower concentration than PABA. The best trial was treatment with a mixture of *Bacillus thuringiensis* subsp. *kurstaki* with the addition of an aqueous solution of PABA at concentrations of 10^{-4} and 10^{-6} mol/l. It was shown that the use of *Bacillus spp.* with the addition of the para-aminobenzoic acid derivatives solutions, leads to an improvement in the functional state of plants, contributing to the activation of the active resistance mechanisms to the action of the stress factors. The results obtained demonstrate the possibility of using entomopathogenic bacteria in a tank mixture with PABA for the creation of biological preparations as alternatives to pesticides and the development of biological methods of plant protection.

PEACH PIT DERIVED ACTIVATED CARBONS: EFFECT OF RAW MATERIAL FORM AND SYNTHESIS PARAMETERS ON POROSITY FEATURES AND H_2 ADSORPTION CAPACITY

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The production of activated carbons (ACs) starting from economic precursors using eco-sustainable synthesis processes appears to be a particularly interesting research field nowadays [1], allowing the reintroduction of waste materials into the economic system, transforming them into a new resource. Peach pits represent an interesting possibility for the production of ACs through synthesis processes with low environmental impact. The resulting activated carbons, in fact, show interesting nanostructure in terms of specific surface area (S_{BET}), total pore volume (V_T) and an excellent microporosity that make them functional for a wide range of applications, such as supercapacitors, gas storage (e.g. H_2, CH_4, CO_2 etc.), filters, sensors, etc. In the present experimental work, ACs were produced by pyrolysis, through two main phases, i.e. carbonization and physical activation of the raw material [2]. The main goal was to study how the key process parameters (gas type and temperature) and the starting form of biomass influence the structural properties and, consequently, the hydrogen adsorption capacity. Chemical and morphological properties were investigated through different energy dispersive x-ray (EDX) analysis, Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM) while textural features and H_2 adsorption capacities were determined using volumetric techniques. All porous carbons derived from peach pits through the optimization of synthesis process own high specific surface area up to 1317 m^2/g, total pore volume up to 0.6 cm^3/g with microporosity percentage (< 2nm) between 85-100% and excellent H_2 adsorption capacity at low pressure (wt% =1.85 at 77 K and 1 bar).

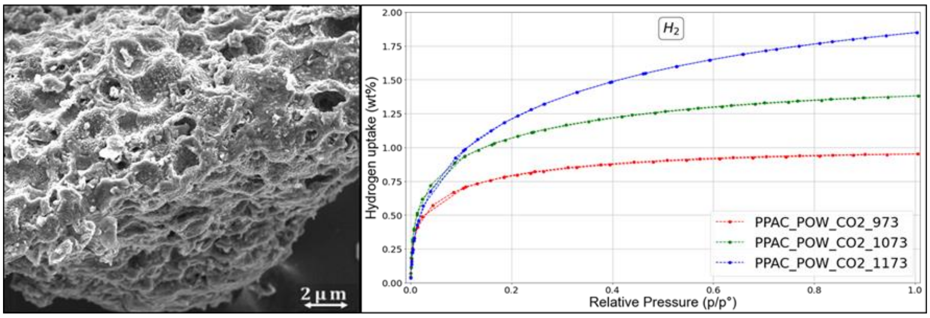

Figure: Left – Scanning electron microscope image of PPAC_POW_CO2_973 sample on a 2 μm scale; Right - H_2 adsorption isotherms at 77K up to 1 bar.

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METABOLIC PROFILE DURING TOMATO JUICE DEGRADATION

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While tomato (*Solanum lycopersicum)* is one of the most produced vegetables in the world, with 189 million tons in 2021 [1], it's processing also produces large amounts of waste that can be further recycled. Waste composition and its evolution in time can be characterized by NMR metabolomics.
Metabolomics is a rapidly emerging field that studies the small molecules (metabolites) biosynthesized in a living organism. For metabolomic studies there are two main techniques broadly used, i.e., Mass Spectrometry (MS) and Nuclear Magnetic Resonance Spectroscopy (NMR) [2]. NMR can provide quantitative information on the targeted metabolites while also providing an untargeted profile of the sample with a minimum sample preparation prior to analysis.
Although there are studies done on the characterization of tomatoes varieties [3] and during various growth stages [4], to our knowledge there are no metabolomic studies regarding tomato juice degradation.
This study follows the concentration profiles of 26 metabolites during a period of 224 days in various simulated conditions. The presentation will focus on γ-aminobutyric acid (GABA) (Figure 1) in degrading tomato juice monitored by NMR spectroscopy.

Figure 1. analysis of γ-aminobutyric acid during tomato juice degradation in various conditions shown different concentration profiles that varied with oxygen.

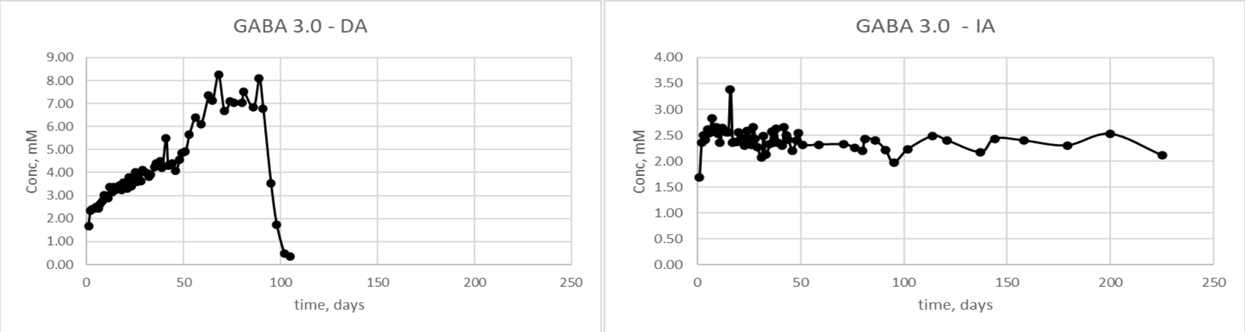

Figure 1. γ-aminobutyric acid concentration (mmol/L) evolution during tomato degradation in aerobic (DA) and anaerobic (IA) condition.

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REVERSIBLE THERMOCHROMIC SMART LABELS BASED ON ENCAPSULATED FLAVYLIUM LEUCO DYES

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In this work, a series of five flavylium spirolactone dyes were successfully synthesized and spectroscopically characterized. [1] Their acid-base behavior and abilities to evolve into leuco forms in certain media were studied by UV-Vis's absorption spectra. The thermochromic properties were evaluated in the presence of weak bases/acids and water-insoluble solvents. The thermochromic dyes were encapsulated through an in-situ polymerization process using an appropriate surfactant as an emulsifier agent and a resin as a shell coating of the emulsion droplets. This leads to the synthesis of thermochromic pigments. The spirolactone flavylium dyes were used as colour formers. Weak bases and acids were used as colour developers, and different co-solvents as phase change materials. The encapsulated materials were printed on a self-adhesive matt inkjet paper, Figure 1. These printed films are visual thermal sensors (which fall in the definition of smart labels) for the industry of temperature indicators where cold chain market is targeted. [2, 3]

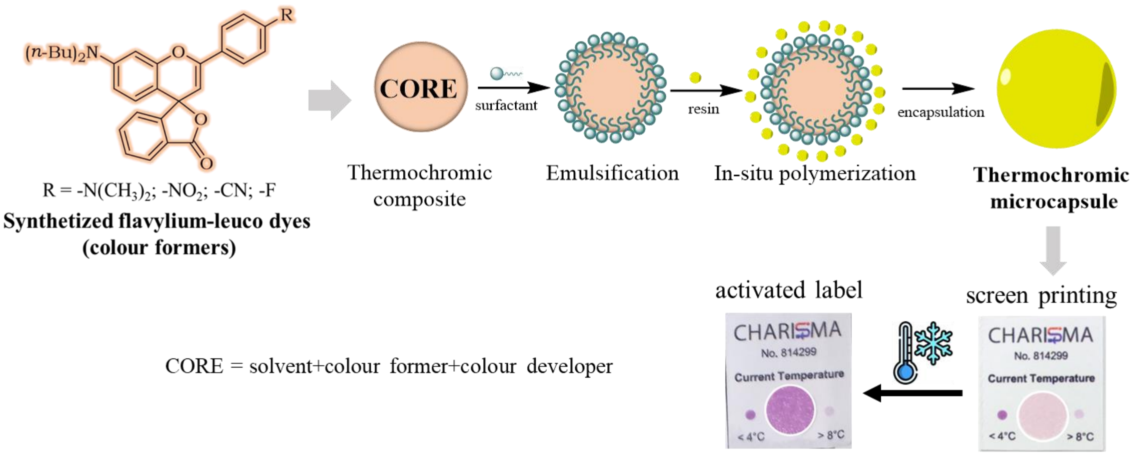

Figure 2. The experimental pathway that led to the development of reversible thermochromic smart labels.

Acknowledgements. This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sokolowskis-Curie grant agreement No 814299.

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HYDROGEL SYSTEMS FOR BIOMEDICAL APPLICATIONS: DIFFERENT APPROACHES IN SCHIFF BASE DYNAMIC BONDS

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Polymeric materials play a critical role in many current technologies. Particularly, the dynamic bonds introduce unique properties, such as self-healing and injectability, to materials and thus provide exciting opportunities for various future technologies. "*Significant efforts have been made to synthesize a variety of dynamic linkers, creating a diverse library of materials. In addition to the development of new dynamic chemistries, fine-tuning of dynamic bonds has emerged as a technique to modulate dynamic properties*." [1] This gives grounds for further research, both fundamental in materials science and applicative in various domains. [2]

The imine bonds are often chosen for hydrogel manufacturing, being the *key ingredient*. The interest in these bonds in biomedical technologies relies on the two critical advantages of these systems: they are (1) injectable and (2) self-healing hydrogels. The former is a highly suitable solution for 3D printing and clinical challenges, since it is based on an *in situ* crosslinking reaction, which occurs fast, easyly and safe. The latter is most promising for cell encapsulation and tissue engineering applications. Our focus, however, has been on the controlled drug delivery and wound dressing.

The active interest in hydrogels as a prime choice for modern applications is owing to their structural versatility, as well as their advanced performance, as numerous studies have revealed. Moreover, the hydrogels features are determined to a large extent by their polymeric components. The innate properties of natural polymers, *i.e.*, proteins and polysaccharides, highly recommend them for medical applications. [3]

Our report is an assessment of some of the most relevant aspects of imine-based hydrogels. First, we used our experience in polysaccharide and protein chemistry to tune the structure (and available moieties) of these polymers, with focus on the selective oxidation of polysaccharides (*i.e.*, cellulose, pullulan, starch etc.). Second, we varied the hydrogels properties by optimizing the two fundamental components of the imine bond: the amine and the aldehyde. We tuned the amine/aldehyde ratio, the polymer components, and the crosslinking conditions. Therefore, various systems were obtained using selectively oxidized polysaccharides as aldehyde bearing component; for the amine bearing counterpart, we have explored compounds with low and high molecular weight, namely dopamine, chitosan and gelatin. Third, different characterization techniques were employed for structural (FTIR and NMR spectroscopy), morphologic (SEM) and functional evaluation (swelling, injectability etc.). From our point of view, based on literature reports and on our own achievements, the research on imine-based hydrogels is reaching a pinnacle and ongoing development of innovative chemical functionalization techniques can lead to materials with advanced properties suitable for biomedical applications.

Acknowledgments. This work was supported by a grant of the Romanian Ministry of Research, Innovation and Digitization, CNCS/CCCDI – UEFISCDI, project number PN-III-P1-1.1-TE-2021-0597, within PNCDI III

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HYDROGELS WITH TUNABLE DEGRADABILITY BASED ON POLY(2-ISOPROPENYL-2- OXAZOLINE) FOR DRUG DELIVERY APPLICATIONS

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Hydrogels are three-dimensional networks of crosslinked hydrophilic polymers capable of absorbing large amounts of water and have emerged as promising candidates for drug delivery applications due to their biocompatibility and their ability to preserve and deliver the activity of pharmacologically active compounds.[1] However, the existing hydrogels face challenges regarding biodegradability and potential toxicity of crosslinking agents, which often hinder their applicability in the biomedical field. Poly(2-isopropenyl-2-oxazoline) (PiPOx) recently emerged as a novel and versatile platform to develop advanced functional materials, showing high potential to be used in the development of hydrogels. [2-7]

In this study, we explore the use of poly(2-isopropenyl-2-oxazoline) (PiPOx), a biocompatible polymer with favorable characteristics such as increased hydrophilicity, thermal stability, and immuno-modulative properties, to develop synthetic degradable hydrogel materials for drug delivery applications. PiPOx was crosslinked with natural, nontoxic dicarboxylic acids to obtain a library of hydrogels. Stability studies and drug release experiments were conducted in several simulated body fluids, to prove the versatility of the hydrogel material as a drug delivery system. The degradability of the hydrogels was assessed using various methods, demonstrating their potential for drug release under physiological conditions. Experimental results indicate successful modification reactions (crosslinking) and reveal the influence of the crosslinker's nature on hydrogel degradation. Moreover, the drug release rate was found to be influenced by the choice of the crosslinker. This study presents PiPOx-based hydrogels with tunable water uptake, drug release profile, and degradability, offering a promising approach for drug delivery applications.

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EVALUATION OF THE EFFECTS OF SOME PESTICIDES ON HUMANS AND ENVIRONMENT

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Pesticides are heterogeneous chemicals widely used on farmland and private gardens, but also in some industries. Pesticide use is expected to increase based on world population growth and the need for more food supplies. Furthermore, many pesticides are chiral compounds and commercial products are mixtures of enantiomers, even though the enantiomers are known to usually have distinct biological activities. Consequently, it is necessary to evaluate the effects of pesticides taking into account their enantiomers and even their metabolites on both human health and the environment. In this study, some herbicides and fungicides are considered, and their effects on human health and the environment are evaluated taking into account their enantiomeric forms and combining a computational and an experimental approach. The experimental approach revealed that the pesticides studied usually decreased the activity of soil enzymes, changed the population structure of soil microorganisms and affected organisms living in the aqueous environment. The computational approach highlighted that the investigated pesticides were capable of producing multiple types of toxicity in humans and that enantiomers typically have distinct toxicological potential in humans and distinct interactions with soil enzymes.

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BODY CLEARANCE OF A MAGNESIUM SUPPLEMENT FOLLOWED BY NMR METABOLOMICS

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Magnesium is a mineral important for the good health of the organism as it contributes to keeping the heart rhythm and blood pressure in normal ranges as well as maintaining the bones strong. In addition to this, magnesium deficiency was correlated with higher inflammatory markers. There are also some medical drugs, particularly those used in treating acid reflux, known for lowering the magnesium level in organism.

Recommended dietary magnesium doses for adults range between 300-450 mg/day. These doses may be easily filled up from natural foods including vegetables with leaves (e.g. spinach), nuts, beans, and whole-grain cereals [1]. However, there are currently several magnesium products available as food supplements or over-the-counter pharmaceuticals. These products include either magnesium alone as metallic ion, or in combination with other ions like calcium and zinc. Human use magnesium is conditioned either as inorganic salt (e.g. oxide, chloride, hydroxide, carbonate) or organic salts (e.g. citrate, orotate, lactate, aspartate) the organic ligands presumably enhancing the body absorption.

High doses of magnesium and its organic ligands from supplements can interact with some medicines, including some types of antibiotics, and in some cases even with diagnosis of some disease.

NMR metabolomics is an emerging field allowing simultaneous identification and quantitation of several metabolites in biological fluids. We have previously applied this technique for both pharmacokinetic studies [2] and medical diagnosis [3, 4].

The present study describes preliminary pharmacokinetic results on follow-up of an organic magnesium medicine by NMR metabolomics. Our findings show a total clearance of the organic ligand in 26 hours after a single dose of 1/3 of daily recommended quantity of the medicine.

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DIVERSITY ORIENTED SYNTHESIS OF FUNCTIONAL MONOMERS STARTING FROM 2-ISOPROPENYL-2-OXAZOLINE

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Nowadays, the field of smart polymeric materials is witnessing a continuous expansion and undergoing studies focused on fulfilling three main requirements: functionality, adaptability, and autonomy. [1] Thus, new synthesis methods are being developed, while current ones are being adapted to synthesize materials that encompass all three characteristics. Generally, smart polymeric materials can be obtained by either polymerization of functional monomers or by post-polymerization reactions with functional moieties, while both methods come hand in hand with advantages and disadvantages. [2] The synthesis of functional monomers, although a straightforward approach to preparing functional polymers, can often be laborious, requiring advanced purification techniques, while post-polymerization reactions are dependent on reactive groups availability and organic functional precursors.

2-Isopropenyl-2-oxazoline (iPOx) is a monomer with dual polymerizable groups, that can undergo cationic polymerization via the oxazoline ring, [3] and radical or anionic controlled polymerization via the isopropenyl group. [4] The first approach enables the preparation of a poly(N-acyl ethylene imine) with the retention of the vinyl functional group, while the second approach enables the preparation of well-defined poly(2-isopropenyl-2-oxazoline)s (PiPOx) with the retention of the oxazoline functional ring. PiPOx has recently emerged as a versatile platform to develop new functional polymeric materials based on the post functionalization chemistry between the oxazoline sidechain rings and (di)carboxylic acids. [4-7] The simple post-polymerization conditions, the high reactivity of iPOx units towards carboxylic acids, and the lack of catalysts and by-products generated during the reaction has inspired the herein monomer synthetic approach from iPOx. Therefore, an oversimplified bottom-up synthetic procedure to design functional monomers with both reactive polymerizable groups and stimuli responsive groups was developed from 2-isopropenyl-2-oxazoline. The reaction takes place in mild conditions with a high chemical rate and allows the design of diverse functional monomers based on the large number of commercially available carboxylic acids. Thus, monomers containing specific responsive units such as azobenzene, terpyridine, pyrene, indomethacin, and others, were obtained and characterized, while their responsive properties regarding different stimuli have been investigated.

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FUNCTIONALIZATION OF 5-BROMOSALICYLALDEHYDE AS MANNICH, SCHIFF-BASE, AND NITRONYL-NITROXIDE LIGANDS AND THEIR COMPLEXES

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5-bromosalicylaldehyde has a great potential of forming various ligands, due to the possibility of Mannich and Schiff functionalizations [1], as well as conversion of formyl groups into nitronyl-nitroxide free stable radical moieties [2] (Figure 1).

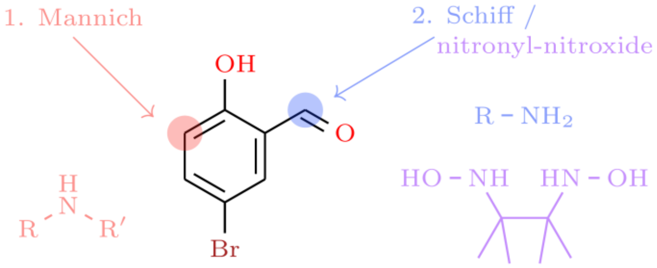

Figure 1. Functionalization of 5-bromosalicylaldehyde

In this work, three Mannich reactions were conducted, starting from 5-bromosalicylaldehyde, resulting in simple, double, and triple condensation products. The amines employed were N-methylpiperazine, piperazine, and tris[2-(methylamino)ethyl]amine. Further, Schiff bases were synthesized, using amines bearing one, two, or three NH_2 groups, leading to compartmental ligands. Alternatively, the Mannich bases were also functionalized as nitronyl-nitroxide radicals, such ligands having paramagnetic properties. The new ligands have been characterized by NMR spectroscopy and mass spectrometry. Complexes of Mannich, Schiff-bases, and nitronyl-nitroxide radicals with Cu(II), Ni(II), and Mn(II) metal ions were obtained. Their structures were determined by single-crystal X-ray diffraction measurements (Figure 2).

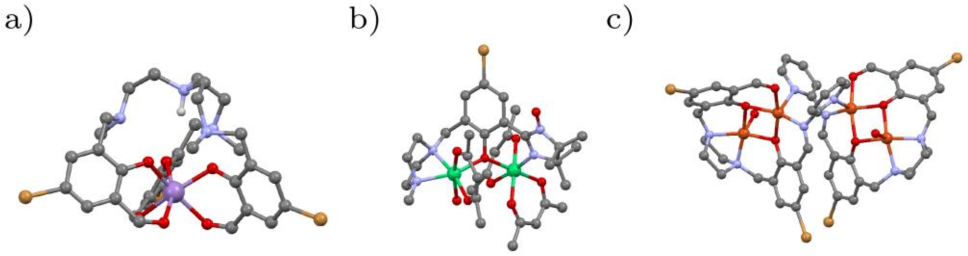

Figure 2. Coordination compounds of: a) a tripodal Mannich base with Mn(II); b) a imino-nitroxide radical with Ni(II); c) a Schiff base with Cu(II).

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COMPUTATIONAL STRUCTURAL BIOCHEMISTRY STUDY OF BENZODIAZEPINES

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Objective

Benzodiazepines are a type of psychotropic drug. They are generally known as tranquilizers and were introduced initially as anxiolytics. However, benzodiazepines are highly addictive, and a person who abuses them faces a host of symptoms. Moreover, the market for new psychoactive substances is growing. The aim of this study is to predict *in silico* chemical structures on benzodiazepine skeleton with affinity for the GABA A receptor.

Methods

A set of 50 benzodiazepine-based compounds was analysed to develop a QSAR training set with respect to published binding values to GABA receptors. In order to develop mathematical model, physicochemical properties (partition coefficient, molar refractivity, molar volume) were used for correlation with biological activity ($logIC_{50}$). To test our model, we estimated the $logIC_{50}$ and compared them with the observed values. So as to create the ADMET profile, we used the ADMETlab2.0 program. The molecular target for diazepam and nitrazepam molecules was predicted using SwissTargetPrediction. The visualization of the target structure was achieved with the Chimera program. The SeamDock molecular docking program was used to study molecular target interactions with diazepam and nitrazepam drugs.

Results

The best results of univariate correlation are shown by molar volume. The best statistics were obtained for univariate correlation. Diazepam and nitrazepam are small molecules with good oral availability that cross the blood-brain barrier, affecting the nervous system The target predicted most likely to interact with drugs is the alpha-1 subunit of the GABA A receptor. The molecular docking study showed a favorable interaction between the molecular target and the drugs diazepam and nitrazepam. This shows that the drugs have the effect of potentiating the activity of the predicted molecular target.

Conclusion

This QSAR model will allow rapid prediction of the binding activity of emerging benzodiazepines in a rapid and economic way, compared with expensive *in vitro*/*in vivo* analysis. Diazepam and nitrazepam interact with GABA A receptors, potentiating their activity.

POTENTIAL ANTITUMOR ACTIVITY OF ZN(II)/AU(I) COMPLEXES WITH SCHIFF BASES IN GLIOBLASTOMA MULTIFORME CELLS

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Introduction

Glioblastoma multiforme is one of the most common primary brain tumors in humans, accounting for 48.6% of all CNS malignancies. There are many challenges to the therapy of this type of tumor due to (multiple) drug resistance of glioblastoma cells, their escape from the immune response, tumor heterogeneity, limited access of drugs to the tumor due to the blood-brain barrier and high invasiveness of the tumor. Despite advances in treatment of glioblastoma multiforme the median survival of patients after diagnosis is 15 months (only 5% of patients survive more than 5 years) [1]. Currently, the main treatment of glioblastomas is aimed at increasing the overall survival of the patients [1, 2].

Aim

The aim of the study was to evaluate the influence of newly synthesized complexes of Zn(II), Zn(II)/Au(I) with Schiff bases (derivatives of 2,6-diformyl cresol (diald) - Aepy, Ampy, Dmen, as well as Salen, Salampy, Saldmen) in one of the most common and aggressive tumors characterized with high mortality in human - glioblastoma multiforme.

Materials and methods

As an experimental model was used permanent cell line 8MG BA (human glioblastoma multiforme). Cytotoxic/antitumor activity of the compounds was evaluated by: i) short-term (24-72h) experiments –using MTT test, neutral red cytotoxicity assay, crystal violet staining technique, double staining with acridine orange and propidium iodide and ii) long-term experiments (37 days) –by 3D colony-forming method.

Results and conclusions

The results obtained show the promising antitumor activity of the compounds investigated. They decrease in time-and concentration-dependant manner viability and proliferation of treated glioblastoma cells. Metal complexes are more effective compared to their ligands alone. The higher cytotoxic/antitumor activity exhibit ZndmenAu and ZnsaldmenAu. They induce cytopathological changes and inhibit the 3D growth of tumor cells in a semi-solid medium. More experiments are needed to clarify the mechanism of action of these compounds.

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EFFECTS OF TRIAZOLE FUNGICIDES ON COMMON DUCKWWED GLUTATHIONE PEROXIDASE, GLUTATHIONE TRANSFERASE AND ATP-SYNTHASE. A MOLECULAR DOCKING APPROACH

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Triazole fungicides can reach the aquatic environment and have ecotoxic effects on the present aquatic organisms, such as the common duckweed (*Lemna minor)*, a free-floating aquatic macrophyte. By uptake, the fungicides can interact and exert an effect at a biochemical level on some plant enzymes. To study this potential biochemical effect, four model protein sequences were selected in this study, with 3D structures available in the UniProt database: glutathione peroxidase, glutathione transferase and ATP-synthase, subunits alpha and beta. The studied fungicides were flutriafol, metconazole, myclobutanil, tebuconazole, tetraconazole and triticonazole, and the effects of these fungicides on the four protein sequences were studied by molecular docking, using the SwissDock program. Results showed that not all six fungicides bound in the active site of all four protein sequences. All analyzed fungicides bound in the active site of only glutathione transferase and the beta subunit of ATP-synthase. Regarding glutathione reductase, only the fungicides flutriafol, myclobutanil and tetraconazole were bound in the active site, while in the case of the alpha subunit of ATP-synthase, only tetraconazole and triticonazole were bound. The highest binding energy was obtained in the case of tetraconazole against the alpha subunit of ATP-synthase, followed by the binding of the same fungicide to glutathione peroxidase. The lowest binding energies were observed for metconazole and myclobutanil against the beta subunit of ATP-synthase. The enzyme with the highest average binding energy to the studied fungicides was the alpha subunit of ATP-synthase, the beta subunit having the lowest average binding energy. The highest average binding energy was observed for tetraconazole, while metconazole had the lowest average binding energy. These results highlight the binding of the six analyzed fungicides to the selected protein sequences, in their active site. The studied fungicides can thus potentially prevent the interaction of the respective enzymes with their specific substrates, potentially leading to the inhibition of their enzymatic activity. Experimental studies are to be carried out to confirm/deny the predictions of the modeling made in this study.

LIFE CYCLE ASSESMENT FOR BIOETHANOL PRODUCTION FROM MICROALGAE

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Biofuels that are renewable, non-hazardous, and biologic-based are alternative energy sources to petroleum. Bioethanol which is widely used in transportation is one type of biofuel. Because bioethanol has crucial features. It has high octane number and oxygen content. Selecting algal biomass to produce bioethanol can be preferred regarding the properties of algae. Since algae can be grown at a high rate. They are non-edible and cheap feedstock. The Cultivation of algae can be done in wastewater. In addition, it can be possible to obtain carbon-neutral fuels by using them as feed [1]. Life Cycle Assessment (LCA) provides researchers to achieve the effects of any products on the environment. LCA provides an opportunity to reach carbon dioxide emissions from raw materials, energy, and waste throughout the process [2].

The study aimed to display the effect of raw materials, manufacturing, delivering, and waste management strategies of bioethanol production from one-tone Spirulina sp. microalgae on the environment by utilizing a LCA software tool, CCalC2. Data that belongs to the algae cultivation, bioethanol production, and occurring waste during the process were provided in the previous research and were put and modified for the software [3,4]. Results were displayed in Greenhouse Gases amounts on the CO_2 based.

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A PRELIMINARY STUDY ON FATTY ACID METHYL ESTERS COMPOSITION IN MITOCHONDRIA HOMOGENATES OF RAT ORGANS

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It has been shown that mitochondria is the energy source of cells, generating up to 90% of the energy in a cell and how metabolism of mitochondrial fatty acids can influence the energy production in cells. The link between fatty acid metabolism and mitochondria are a considerable number of cellular processes, an important field in science for understanding the fundamental processes of cellular energy production and the mechanisms to develop new therapeutic strategies for disorders and information about the regulation of lipid metabolism and how it is affected by various factors, such as diet, exercise, and disease. The aim of our study was to elaborate a comparative analysis of the fatty acid profile in mitochondrial homogenates from three types of organs. Kidneys, brain and testis were collected from a healthy Sprague Dawley rat. Mitochondrial homogenates were obtained from each organ and processed for a modified protocol for fatty acids (FAs) derivatization to obtain fatty acids methyl esters (FAMEs). The gas-chromatography coupled to mass spectrometry (GC-MS) method was used to obtain the FAMEs profile in mitochondria homogenates.FAMEs percentages were calculated and a comparison between saturated, monosaturated and polyunsaturated is presented. Our analysis highlighted differences in FAMEs composition when compared the types of organs, suggesting that fatty acids are involved in mitochondrial function and in lipid metabolism.

ANTIMICROBIAL ACTIVITY AND *IN VITRO* ANTIPROLIFERATIVE POTENTIAL OF GREEN SYNTHESIZED SILVER NANOPARTICLES USING *POPULI GEMMAE* EXTRACT

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Introduction: "Green-synthesis" techniques of silver nanoparticles (AgNPs) have attracted extensive attention in recent years due to their promising activity with many biomedical and pharmaceutical applications [1, 2]. Moreover, the green synthesized AgNPs prepared from a wide range of medicinal plant extracts are recognized for their antimicrobial and anticancer activities [3]. *Populus nigra* L. buds extract (Pg) has been endowed with a wide range of active components, therefore, in recent years this vegetal product has been in the spotlight in various research studies.

Aim: The current study is designed to evaluate the antimicrobial and antiproliferative potential (MCF7 breast adenocarcinoma and A549 lung adenocarcinoma cell lines) of AgNPs obtained from an ethanolic extract of *Populi gemmae* (Pg) collected from the western part of Romania- further noted as Pg-AgNPs_S1 and Pg-AgNPs_S2.

Materials and methods: The antimicrobial activity of Pg-AgNPs was evaluated using disk diffusion and dilution methods, and the antiproliferative activity by MTT assay.

Results: Both Pg-AgNPs presented an antibacterial activity on Gram-positive bacteria as well as on fungi. Lack of activity can be seen for Pg-AgNPs_S1 on Gram-negative bacteria. The difference between the Pg-AgNPs can be attributed due to their particle size (Pg-AgNPs-S1 was synthesized using 1 M $AgNO_3$, resulting in nanoparticles with smaller dimensions than Pg-AgNPs-S2, which were designed using 5 M $AgNO_3$) and due to different wall structures of the respective microorganisms. Related to their antiproliferative activity, it was proved that different concentrations (10, 25, 50, 75, 100, 150 mg) of Pg-AgNPs_S1 provoked a dose-dependent decrease in cell viability in both cancer cell lines, however, the most affected was the A549 cell line. On the other side, the MCF7 cell line was more sensitive to Pg-AgNPs_S2 when compared to the A549 cell line. In terms of antiproliferative IC_{50} values, Pg-AgNPs_S2 was more active on both cell lines (3.24 µg/mL in case of MCF7 cells and 5.03 µg/mL in case of A549 cells), Pg-AgNPs_S1 showed a much weaker activity with higher IC_{50} values (4.39 µg/mL in case of A549 cells and 40.23 µg/mL in case of MCF7 cells).

Conclusions: The results have shown that the Pg-AgNPs presented a good antibacterial potential, with a superior activity of Pg-AgNPs_S2. Additionally, in set of experimental conditions, Pg-AgNPs showed an antiproliferative activity in a dose-dependent manner, however, Pg-AgNPs_S2 presented a stronger activity on both cancer cell lines.

Keywords: *Populus nigra* L.; silver nanoparticles; antimicrobial potential; antiproliferative activity.

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GREEN SYNTHESIS OF NANOSELENIUM PARTICLES AS A FUNCTIONAL PRODUCTS AGAINST *IN VITRO* AND *IN VIVO* CADMIUM TOXICITY

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Cadmium (Cd) is a heavy metal with high toxicity at low concentrations, causing serious damage to the kidney, liver, brain functions, and central nervous system as a result of produced reactive oxygen species, which cause DNA damage. Cadmium, along with other heavy metals (arsenic, chromium, lead, and mercury), has been listed as a human carcinogen by the United States Environmental Protection Agency and the International Agency for Research on Cancer. Our study is divided into three parts. The initial step is the biogenic synthesis of selenium nanoparticules (SeNPs) by *L. casei*, which is followed by structural and morphological examination of the nanoparticles. The second part was to demonstrate *in vitro* the potential protective role of SeNPs against toxicity and Cd binding ability in probiotic bacteria (*L. casei*). The third part highlighted the protective effect of SeNPs-enriched probiotic administered orally to mice for 30 days in varied concentrations (0.1, 0.2, and 0.4 mg/kg b.w.) against the toxic effects of cadmium at the hepatic and kidney levels. Multiple acquisition of micro-Raman spectra, recorded in the low wavelength region, clearly demonstrated that formation of endogenous SeNPs is a time-dependent reaction, the maximum intensity being reached after 48 h of fermentation. Homogenous, spherical shape SeNPs and sharp size distribution with maximum 200 nm were obtained via reduction route, using *L. casei* and Na_2SeO_3. The XRD pattern, demonstrates quasi-amorphous form of selenium [1]. The protection effect of SeNPs was demonstrated by the features of dynamic growth curves of L. casei treated with Cd. The efficiency of Cd remediation is increased by SeNPs intake, the ratio of 1:2 LAB/SeNPs being more efficient for both bacteria [1]. On the other hand, *in vivo* the protective effect of SeNPs against Cd liver toxicity was demonstrated by the restoration of blood hepatic markers (AST, ALT, GGT and total bilirubin) and antioxidant enzymes, such as catalase (CAT) and glutathione peroxidase (GPx). Moreover, the antioxidant capacity of mice plasma by the FRAP assay, revealed the highest antioxidant capacity for the 0.2 mg/kg LSeNPs group [2]. Histopathological analysis demonstrated the morphological alteration in the group that received only cadmium and was restored after the administration of SeNPs [2]. The blood marker of renal injury (creatinine) significantly decreased in groups where the mice were treated with SeNPs. The antioxidant capacity of plasma revealed that SeNPs in co-treatment with Cd, promotes maintaining antioxidant activity at the control level [3]. Histopathological analysis of kidneys demonstrated morphological alteration in the group that received only Cd and restored after administration of SeNPs. A functional product that includes elemental SeNPs could be successfully used to annihilate Cd-induced liver and kidney toxicity, and to improve both nutritional values and health benefits.

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BIOHYBRID POLY(2-ISOPROPRENYL-2-OXAZOLINE)-GELATINE NANOFIBERS FOR WOUND HEALING APPLICATIONS

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Nanofiber dressings have recently emerged as an interesting alternative to known wound dressing materials,[1] having distinct advantages, such as: (i) better coverage and protection of the wound against infection, (ii) nanoporosity that allows efficient permeability for water and oxygen, increased interchange of nutrients as well as exclusion of metabolic wastes, (iii) large surface area of interaction with the cells, available in the wound bed, through an extracellular matrix, and (iv) enhance hemostasis due to their high surface area and interstices.[2] These advantages make nanofiber dressings suited for ultrasensitive, fast-responding, and user-friendly sensors. Although complex smart systems, that show real-time monitoring of the wound situation, high sensitivity, and high stability, were reported, none of these systems reached commercialization.[3, 4] The production of water-stable, hydrophilic and biocompatible nanofibers remains subject of further optimization, e.g., by exploring more facile and eco-friendly production methods.

Poly(2-isoproprenyl-2-oxazoline) PiPOx represents an excellent candidate as a base material for the synthesis of reactive hydrophilic nanofiber networks, which has just been reported in the literature.[5] To address the current limitations concerning synthesis, sensing, fabrication, biocompatibility and antimicrobial properties, herein we used in the construction of the target biohybrid nanofibers the electrospinning technique of two distinct polymers: (a) a synthetic PiPOx that allows facile, modular, and reproducible synthesis protocols of functionalization and crosslinking, and sensing properties and (b) a natural polymer (gelatin) that endows the nanofibers with biomimetic properties to alleviate the problems associated with tissue regeneration. The influence of the processing parameters such as flow rate, voltage, and polymer concentration on the morphology of the resulting nanofibers was systematically investigated as well as the post-fabrication crosslinking. The formed PiPOx-GelMa nanofibers with a porous and uniform morphology were characterized using scanning electron microscopy (SEM), and Fourier transform infrared (FTIR) spectroscopy, before and after crosslinking.

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MULTIDISCIPLINARY APPROACH IN ELECTROCHEMCAL STUDIES. I. REGRESSION ANALYSYS IN DETERMINING THE STANDARD ELECTRODE POTENTIAL

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Given the current socio-economic context, there is growing interest in the scientific community for the development of advanced research methods in electrochemistry, aimed at reducing experimental costs (e.g., material waste and time-saving). For this purpose, it may be necessary to introduce a theoretical stage (of analysis and testing) prior to the experimental one, so that the reaction conditions can be selected from the theoretical stage, with the best-obtained model being tested experimentally. Starting from these considerations, the present work aims to outline the advantage of the multidisciplinary approach and the need for conducting a statistical analysis to explain electrochemical reactions at the theoretical level.

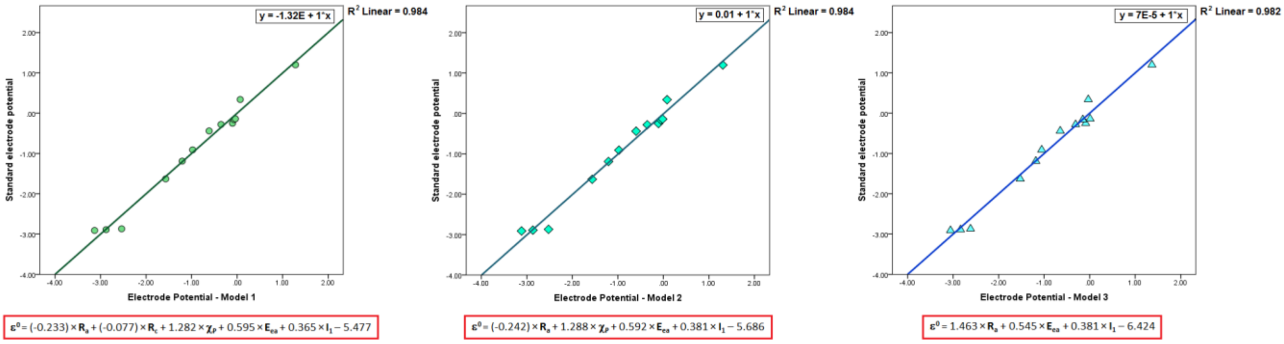

Figure 1. Literature data vs. computed values for standard electrode potential

For this purpose, the values of the standard electrode potential for a series of metals were selected from the literature together with their associated physical-chemical parameters (i.e., atomic radius, covalent radius, Pauling electronegativity, electron affinity and first ionization energy), and the collected data were analyzed using the SPSS 21 and SPSS AMOS 21 software. The Pearson correlation analysis was used to determine the univariate association between the parameters considered in the study, while hierarchical multiple regression was employed to identify their most significant statistical combination usable to predict the standard electrode potential. Subsequently, the linear association between the parameters was comparatively estimated, and the total, direct and indirect effects of each parameter in the model were assigned with path analysis. According to the Pearson correlation index, the standard potential correlates strongly in the positive direction with electronegativity, electron affinity and first ionization energy, and strongly in the negative direction with covalent radius and atomic radius. After applying the regression analysis, three different prediction equations were obtained, all of them fitting the literature data (R^2 = 0.984 for the first two models and R^2 = 0.982 for the third one). The results from the path analysis showed that the total effect of all parameters used in the study is significant in the prediction equation only when the mediating effect of covalent radius, electronegativity, ionization energy and electron affinity are also taken into account.

IN SILICO MODELING OF AHAS (WILD TYPE/MUTANT) HERBICIDE-ENZYME INTERACTIONS IN WEEDS

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According to the International Survey of Herbicide Resistant Weeds Database [1] herbicide resistant weeds have been reported in 72 countries, 269 species being involved. Weed resistance was observed for 21 of the 31 known herbicide sites of action and to 166 different herbicides, the most targeted site being the enzyme acetohydroxyacid synthase (AHAS). Usually, resistance occurs by alteration of amino acids in the target binding site, decreasing the sensitivity to target-specific herbicides [2]. Thus, mutations that confer herbicide resistance are the main concern for the management of invasive plants and are often under-characterized structurally and functionally [3]. Computational modeling of herbicides action on susceptible and resistant biotypes for invasive species was engaged in order to elucidate the differences in the pattern of interactions inside the AHAS binding site. For the generation of reliable 3D structural models for AHAS enzyme (susceptible and resistant), homology modeling, the most accurate theoretical method, was utilized. It was investigated mainly the Trp574Leu mutation which is responsible for the acquisition of herbicide resistance in many weeds. The molecular docking of a series of known herbicide that induce resistance led to the identification of the key features responsible for the loss of herbicidal activity. It was observed that the indole ring of Trp574 plays a defining role in the vast majority of cases by realizing pi-pi interactions with aromatic rings of many herbicides. This could be one of the explanations according to which replacing Trp574 with a leucine leads to the loss or significant decrease in biological activity.

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THE COMPOSITION OF HUMAN CEREBELLUM ASSOCIATED GANGLIOSIDES IS HIGHLY COMPLEX AS REVEALED BY ION MOBILITY TANDEM MASS SPECTROMETRY

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Cerebellum represents a highly specialized region of the brain encompassing approximately 80% of the total brain neurons and regular arrays of neuronal units involved in motor control, learning, cognitive and emotional functions [1, 2]. In recent years, human cerebellum started to be investigated at the molecular level, in order to correlate its functions with the expression of various biomolecules, especially gangliosides, sialylated glycosphingolipids highly expressed in the central nervous system. Among the bioanalytical methods employed so far in the analysis of cerebellar biomolecules, mass spectrometry (MS) provided the most comprehensive information [3].

We report here on the first introduction in cerebellum research of ion mobility separation (IMS) mass spectrometry for a systematic mapping of cerebellar gangliosides and determination of the species associated to development and aging. For this purpose, gangliosides extracted from post-mortem tissue biopsies of fetal -in the 15 and 40 gestational weeks (samples 15GW and 40GW)- and 65 years of age (sample 65Y) cerebellum were analyzed by nanoESI IMS MS in the negative ion mode under identical conditions. Altogether, no less than 734 molecular ions corresponding to 551 gangliosides, fucogangliosides and species modified by *O*-acetylation, *O*-GalNAc and CH_3COO^- were identified by IMS MS separation and screening, which represents almost five times more cerebellar structures than ever reported before.

In the next stage of the research, using CID MS/MS at low and variable collision energy after mobility separation in the transfer cell, were confirmed and characterized the structural conformation of the glycan core and ceramide moiety of three precursor ions that are common in all samples. The optimized isolation and fragmentation conditions induced efficient ion dissociation with high sequence coverage and a significant number of fragment ions diagnostic for the proposed structures of GD1 (d18:1/18:0), GQ1(t18:18:0) and GQ1(d18:1/18:0).

The comparative analysis revealed for the first time that: i) 40GW contains the highest number of species (373), followed by 15GW (327) and 65Y (192); ii) fetal cerebellum gangliosidome is characterized by a much higher sialylation degree and species altered by carbohydrate and non-carbohydrate type of modifications than the gangliosidome of aged cerebellum; iii) significant developmentally- and age-regulated changes in the expression and structure of cerebellum gangliosides exist. These variations are to be correlated in the future with the neurological diseases, leading to the discovery of pathways to more effective therapeutic schemes.

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EVALUATION OF THE QUALITY OF GOAT'S MILK BY CHEMICAL ANALYSIS

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Milk is an important component of the human diet, being considered a complete food due to its content of vital nutrients, such as proteins, essential fatty acids, lactose, vitamins and minerals. However, milk and milk products may contain chemicals and contaminants, which represent a risk for the health of the consumer. Analyzing and monitoring the quality of milk from the point of view of its chemical composition, but especially of the content of heavy metals, is a very important activity. In this study, the analysis of raw milk samples from 2 micro-farms located in the western part of Romania was carried out. The analysis of the physicochemical parameters involves the determination of the pH value and the content of lactose, fat, protein, dry defatted substance. Heavy metals and trace elements levels in milk were determined for: Fe, Mn, Zn, Cr, Cu, Pb, Cd by flame atomic absorption spectrophotometer. Regarding the content of heavy metals and trace elements in analyzed milk, the values do not exceed the limits stipulated in the quality standards, in none of the 2 farms. There is no risk of contamination with heavy metals due to milk consumption. We recommend paying more attention to determine the concentration of heavy metals in milk samples intended for human consumption to prevent heavy metal contamination and the adverse reactions resulting from it.

EVALUATION OF THE IMPACT OF NICOSULFURON ON THE SOIL BY ENZYMATIC METHODS

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Nicosulfuron is a systemic selective herbicide, from the group of sulfonylurea herbicides, herbicide frequently used in agricultural crops to combat a wide range of annual or perennial broadleaf weeds in maize crops. The application of herbicides leads to an increase in agricultural productivity and crop yield, but their inadequate and excessive use can have adverse effects on the environment, especially on the community of microorganisms in the soil. Microorganisms in the soil and implicit their enzymatic activity are considered basic indicators of soil fertility, as they quickly respond to changes caused by pollution and contamination. The evaluation of the impact of nicosulfuron on the community of microorganisms in the soil was carried out based on the determination of the enzymatic activities when different doses of the herbicide were applied. The analyzes consisted in the determination of 4 enzymatic activities determined by soil microorganisms: dehydrogenase, urease, phosphatase and catalase activity, in laboratory conditions at soil level, over a period of 28 days. Also, throughout the duration of the experiment, the physico-chemical parameters of the soil were determined: the temperature, the pH, the electrical conductivity, the organic matter content, the contents of water, ammonium, nitrate-nitrogen, and phosphate. Nicosulfuron showed an inhibitory effect on the enzymatic activities: dehydrogenase, urease and catalase regardless of the concentration applied the effects was evident starting from day 7 of the analysis. For phosphatase activity, the inhibitory effect of nicosulfuron occurs only when high doses were applied. Catalase and phosphatase activity were positively correlated with pH, organic matter content, nitrogen as nitrate, nitrogen as ammonium and phosphorus content. Dehydrogenase activity showed a statistically significant positive correlation with organic matter content. Overall, the effect of nicosulfuron on the metabolism of soil microorganisms is different, its action is dependent on the dose applied and the exposure time.

COMPUTATIONAL EVALUATION OF THE INTERACTIONS OF SOME DI-ISONONYL PHTHALATE METABOLITES WITH FAMILY 1 SULFOTRANSFERASES

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Sulfotransferases (SULTs) are phase II enzymes that metabolize xenobiotics by catalyzing the sulfonation of a wide variety of endogenous and exogenous chemical compounds. In humans, SULTs are classified into five families SULT1, SULT2, SULT3, SULT4 and SULT6 which can be found in different tissues [1]. The main members of the SULT1 family are SULT1A1, SULT1A2, SULT1A3, SULT1B1, SULT1C1, SULT1E1. This computational study aims to predict the toxicological effects and evaluate the interaction with SULT1 enzymes of the metabolites resulting from the bioprocessing of di iso-nonyl phthalate (DiNP), a phthalate that is used as a plasticizer and is found in many objects with which humans come into contact [2].

The prediction of toxicological effects was possible by using the AdmetLab2.0 program, the docking was done with the help of the SwissDock and SeamDock programs, and the visualization and analysis of the docking results was done with the UCSF Chimera program. Following the study, it was observed that DiNP metabolites reveal relatively low elimination rates from the human body, which underlines their potential to produce toxicological effects. These metabolites can cause liver damage and have the potential to inhibit peroxisome proliferator-activated receptors. DiNP metabolites show the ability to interact with sulfotransferase family 1 enzymes and thus can inhibit the activity of these enzymes. Since the sulfonation activity of SULT1 is biologically important, any xenobiotic that inhibits this process or initiates the desulfonation process may lead to adverse effects on human health [3].

Keywords: di-isononyl phthalate monoesters, sulfotransferases, molecular docking, toxicological effects.

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EFFICIENCY OF COPPER ACCUMULATION IN VARIOUS STRAINS OF RECOMBINANT MICROORGANISMS FOR BIOREMEDIATION OF HEAVY METAL-POLLUTED WATERS

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The purpose of this study was to use different genetically modified bacteria and yeasts to treat synthetic water with high concentrations of copper through the bioremediation process. Several genetically altered strains of *Saccharomyces cerevisiae* (EBY100, INVSc1, BJ5465, and GRF18), *Pichia pastoris* (X-33, KM71H), *Escherichia coli* (XL10 Gold, DH5α, and six types of BL21 (DE3)), as well as *Escherichia coli* BL21 (DE3) OverExpress expressing two different peroxidases were used to determine the efficiency of copper ions accumulation. Bacteria are viable at copper concentrations up to 2.5 mM, and yeasts are viable at concentrations up to 10 mM, according to experiments performed on several yeast and bacterial strains. The tolerance of bacterial strains on media containing 1 mM copper was found to be lower than the tolerance of yeast strains at the same copper concentration, according to optical emission spectrometry with inductively coupled plasma analysis (ICP-OES). The *E. coli* BL21 RIL strain had a copper accumulation efficiency that was 1250 times more efficient than the control strain (4.79 mg/L of culture adjusted at an optical density of 1.00). Out of the six yeast strains studied, *S. cerevisiae* BJ5465 was the most effective at accumulating copper, doing more than 400 times more than the negative control strain. Additionally, compared to cells that produced periplasmic recombinant peroxidases, *E. coli* cells that internally expressed recombinant peroxidase from *Thermobifida fusca* were able to accumulate copper 400 times faster.

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PEGYLATED SQUALENE-BASED NANOTHERAPEUTICS: ENHANCED *IN VITRO* ANTITUMOR ACTIVITY OF COMMERCIAL DRUGS

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Nanomedicine, an extensive scientific research field, encompasses diverse studies exploring various types of nanotherapeutics. Over the past decades, nanomedicine has gained significant attention due to its potential to offer improved treatment for severe diseases such as cancer, neurological disorders, and cardiovascular pathologies, as well as benefits in diagnostics, contrast reagents, and medical devices.[1-3]

Newly discovered drugs, such as peptides, siRNA, therapeutic nucleic acids, or proteins, often require delivery systems to overcome poor bioavailability in conventional formulations and instability in biological environments. Nanotechnology has emerged as a promising approach to address these challenges.[4,5]

Nanotherapeutics exhibit superior characteristics, including minimal toxicity, enhanced bioavailability, and improved therapeutic impact, making them viable candidates for clinical trials or applications.[6,7]

Considering our previous research, we explored the biocompatible amphiphilic conjugate, PEGylated squalene (SQ-PEG), which self-assembles into micellar structures in an aqueous environment.[8] These micelles' hydrophobic regions can safely encapsulate hydrophobic drugs for targeted delivery to various tissues. To showcase our contribution in this field, we utilized SQ-PEG as a carrier to encapsulate antitumor drugs, aiming to enhance their biological characteristics. We investigated the stability and release kinetics of the obtained SQ-PEG-based nanotherapeutics in PBS solutions at pH values of 6.5 and 7.4 using UV-Vis and DLS analysis, which revealed improved stability and drug release profiles. STEM images demonstrated a spherical morphology with nanometric dimensions.

In vitro tests evaluated the cell viability of the micellar entities on NHDF-healthy cells and their antitumor activity on HeLa and MCF-7 tumoral cells. The encapsulation of commonly used antitumor drugs in SQ-PEG micelles improved their biological properties, rendering these nanotherapeutics potential candidates for further *in vivo* testing.

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A TOOL TO ENHANCE THE PROCESS OF SELECTING CRYSTAL STRUCTURE COMPLEXES FOR DOCKING PURPOSES

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Protein-ligand docking is a widely utilized technique in the field of cheminformatics, serving as a valuable tool for virtual screening, posture prediction, and the calculation of binding affinity. The outcomes of docking are dependant of the quality of the crystal protein structures.

The B-factor index of the binding site (BFIbs) is a measure that establishes a correlation between the atomic fluctuations occurring inside the binding site and those observed throughout the entire protein [1]. In a comprehensive docking exercise involving a substantial number of 26,019 protein-ligand complexes, it was observed that BFIbs had a significant correlation with the ability to accurately anticipate the pose of the ligand during docking.

In this paper, we present an updated digital tool called BFI in kinases, which is accessible to the public at www.chembioinf.ro. This tool offers researchers computed BFIbs values, together with a comprehensive collection of crystallographic data, ligand descriptors, and valuable insights into protein-ligand binding. The dataset comprises 2433 crystal structures that specifically capture kinases.

This resource has the potential to enhance the process of selecting crystal structure complexes, leading to enhanced docking outcomes and ultimately streamlining the search for novel kinase inhibitors.

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CHARACTERISTICS AND PROPERTIES OF SOY HULL PECTIC FIBER EXTRACTED BY DIFFERENT PROTOCOLS

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Effect of different protocols for pectin extraction on characteristics and properties of isolated fiber was studied. Soy hull, a by-product of soybean processing, was used as a source of pectic fiber. Pectic fibers were extracted with 0.05 M HCl for 1 h at 80 ˚C (APF), ultrasound treatment in 0.05 M HCl for 30 min (USPF) and with 0.05 M HCl for 1 h at room temperature (RTPF). Obtained results showed that ultrasound treatment accompanied with acidic extraction enabled the highest achieved yield of pectin fiber, 32 mg_{PF}/g_{DW}. FTIR spectras of extracted pectic fibers (Figure 1) showed some differences, indicating possible differences in their characteristics and properties. APF showed the highest solubility in water (61.85%) compared to other two pectic fibers. Moreover, results showed that highest water holding capacity was obtained at APF sample (16.17 g_{H2O}/g_{sample}) while pectic fiber produced using ultrasound treatment had highest oil holding capacity (2.24 g_{Oil}/g_{sample}) (Figure 2). RTPF had the highest content of galacturonic acid 54.7%, 23% higher compared to APF, and 28% higher then USPF. Pectic fiber extracted from soy hull showed desirable characteristics that may be suitable for usage in various food products and therefore in the food industry.

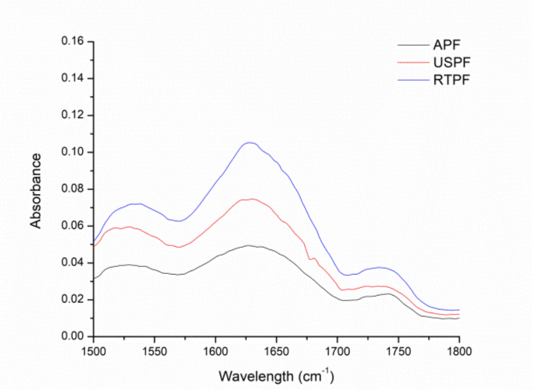

Figure 1. FTIR spectras of APF, USPF and RTPF extracted soy hull pectic fibers

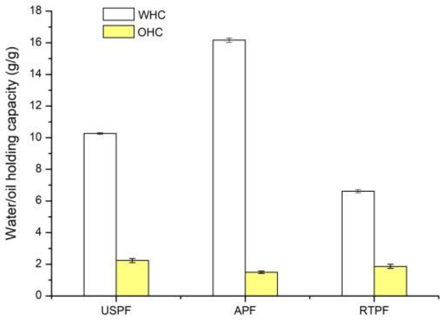

Figure 2. Water and oil holding capacities of extracted soy hull pectic fibers

Acknowledgement. This research was funded by Ministry of Education, Science and Technological Development, Republic of Serbia, project number E!13082.

ASSESSMENT OF THE MYCLOBUTANIL EFFECTS ON THE ACTIVITIES OF SOME ENZYMES FOUND IN SOIL

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Within this study, the effect of different doses of myclobutanil, a triazole fungicide, on soil enzyme activities (dehydrogenases, phosphatases, catalase, urease and protease) has been assessed. Myclobutanil used in high doses negatively affected the activities of dehydrogenases, protease and urease. Because myclobutanil as a commercial product is a racemic mixture of the (R)- and (S)-steroisomers, a molecular docking study has been considered to assess the possible stereoselectivity of the fungicide. Both enantiomers of myclobutanil were able to bind to the active sites of dehydrogenase, phosphatase and protease, the interacting energies being to some extent higher for the (S)-myclobutanil, the enantiomer that is known to be less active against target organisms and to manifest higher toxicity against non-target organisms. It underlines the enantioselective effects of the triazole fungicide myclobutanil on the activities of enzymes found in soil. It also accentuates that the racemic mixtures that are used in crop and food management practices should be replaced by the enantiomer revealing the higher activity against target organisms and the lower toxicity against non-target organisms.

NEW APPROACHES TO BIOLOGICAL IMAGING. COORDINATION OF BORON COMPOUNDS TO DIFFERENT PORPHYRINS FOR LASER DYES AND FLUORESCENT LABELING

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The coordination of boron compounds to tetrapyrrolic ligands, such as porphyrins, are applied for laser dyes and fluorescent labeling in biological imaging [1, 2]. In this study we aimed to create a new complex between 5,10,15,20-(tetraphenylporphinato)dichloro-phosphorus(V) chloride (P(V)-porphyrin) and MgB_2, to create a new type of linkage [3].

UV-Vis spectrum of P(V)-porphyrin in ethanol ($c=6.1316\times10^{-6}$ M) is presented in Figure 1 and the formation of the complex with MgB_2 (isosbestic points at 556 nm and 578 nm) was UV-Vis monitored (Figure 2).

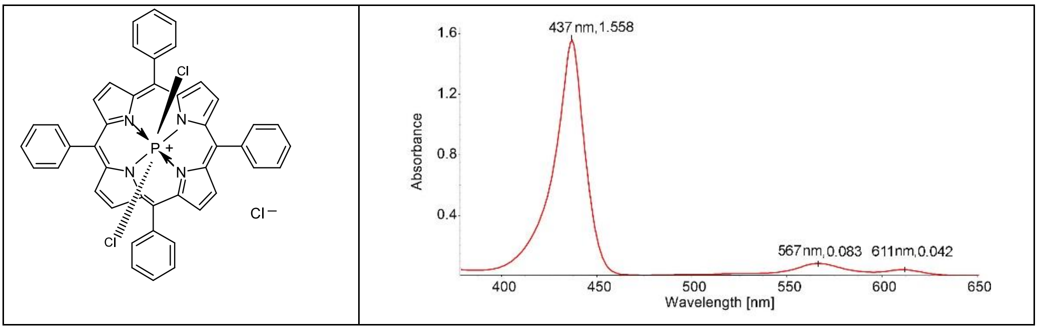

Figure 1. The structure and UV-Vis spectrum of P(V)-porphyrin

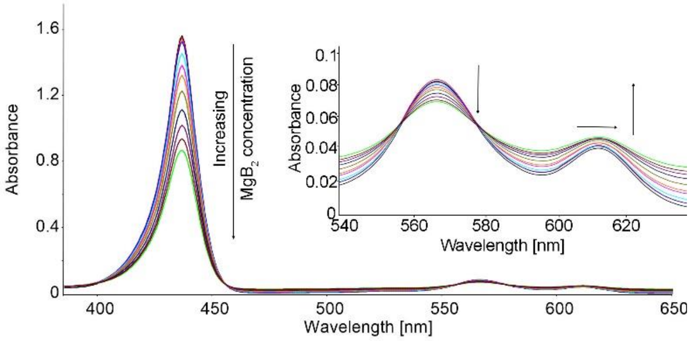

Figure 2. Overlapped UV-Vis spectra presenting the complex formation between MgB_2 and P(V)-porphyrin in ethanol.

The Q bands of porphyrin in the visible region are weak, probably because of the changes regarding extended conjugation, but they also undergo changes regarding the position –red shift. The lower Q band gains in intensity and is shifted to the red at the expense of the upper Q band [4]. Magnesium and phosphorous have anomalous electron affinity. In magnesium the electron should be added to 2p orbital, a less stable structure compared to that of the atom $[Ne]3s^2$. In phosphorous the electron should be added to 3p orbital which is half filled and thermodynamically stable. There is a long way to establish the mechanism of interaction in this complexation process (we cannot disregard the strong affinity between Mg and P-containing molecules).

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OPTIMIZATION OF ENZYME-ASSISTED EXTRACTIONS OF PROTEIN FROM PUMPKIN LEAVES

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The growing global population lead towards increase in demand for protein sources. Proteins from alternative sources including plants, microbes, and insects have drawn a lot of attention due to potential ability to feed a growing global population. Besides, production of new food items with less environmental impact is perceived as the advantage. Plant-based proteins represent promising ones due to their long history of use and cultivation, lower cost of production, and easy access in many parts of the world. Plant proteins are also more environmentally sustainable [1]. In this study enzyme-assisted extraction of protein from pumpkin leaves as sustainable and eco-friendly technique was optimized. Pumpkin leaves are waste material after harvest of pumpkin and they can be potential source of protein. The intention was to find optimal conditions for efficient protein isolation with the assistance of commercial cocktails of carbohydrases. Independent variables were enzyme dosages and time while concentrations of protein [2] and reducing sugars [3] were determined as responses. Optimal conditions for enzyme-assisted extraction with Viscozyme were 12.1 FBG/g and 1 hour resulting in release of 1.37±0.04 mg protein/mL and 11.16±0.06 mg reducing sugars/mL. When pumpkin leaves were treated with Enzyme complex at dosage 7.5 FPU/g for 30 min maximal concentrations of protein, 1.46±0.07 mg/mL, and reducing sugars, 21.16±0.16 mg/mL, were attained. Optimization of enzyme-assisted extraction of pressed pumpkin leaves regarding cocktails dosages and extraction time indicated that at optimal conditions Enzyme complex was more efficient judging by concentration of released protein and reducing sugars than Viscozyme. Extraction of protein aided with carbohydrases cocktails as green technique could be promising method for more efficient and eco-friendly exploitation of waste leaf materials.

Acknowledgements. The financial support by the Science Fund, Republic of Serbia, Project MultiPromis, Grant No.7751519 is greatly acknowledged.

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PORPHYRIN-BASED NANOMATERIALS ABLE TO QUANTIFY WATER IN FOOD PACKAGING

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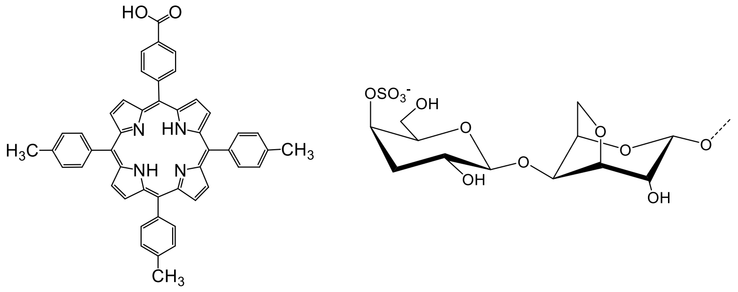
The importance of preserving food in dry conditions and extending the shelf life of products is an ongoing task in industry [1]. Intelligent food packaging, based on natural extracts, in association with biopolymers, are currently created, in order to improve the quality and sustainability [2].

k-Carrageenan (Figure 1 a) is a polysaccharide able to perform water swelling. It is well known that porphyrins exhibit optical properties that recommend them for diverse sensing applications. For this experiment we selected 5-(4-carboxyphenyl)-10,15,20-tris (4-methyl-phenyl)-porphyrin (5-COOH-3MPP) (Figure 1 b), on the premise of its possible interactions with k-carrageenan, based on hydrogen bond formation.



a b

Figure 1. Structure of 5-(4-carboxyphenyl)-10,15,20-tris (4-methyl-phenyl)-porphyrin (a) and k-carrageenan (b)

The synergic effect between these two types of compounds led to a material able to detect, quantify and retain traces of water. Under the presence of increased quantities of water, the intensity of absorption of the Soret band, located at 418 nm, decreases in a linear fashion in the concentration domain 3.14×10^{-3} M – 1.79×10^{-2} M (Figure 2).

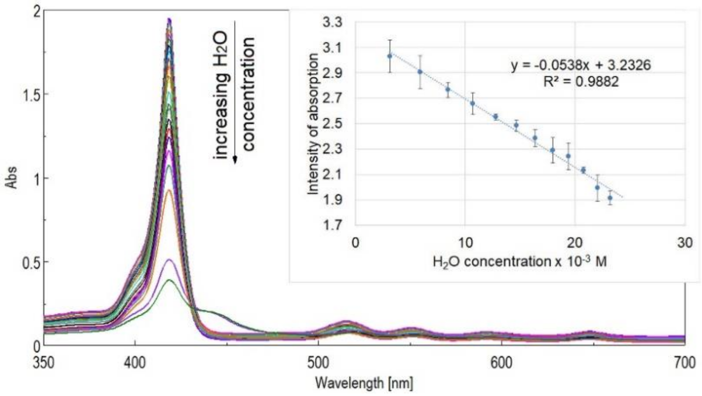


Figure 2. UV-Vis spectra during adding of water. Linear dependence of the absorption intensity read at 418 nm and the water concentration.

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COMPLEX BETWEEN AN A_3B PORPHYRIN, AuNPs AND K-CARRAGEENAN USED FOR DETECTION OF 1-METHYLIMIDAZOLE

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Taking into account the applications of 1-methylimidazole both in medicine for the design of antibacterial compounds and in technology for the development of more efiicient solid-state dye-sensitized solar cells [1], the need to accurately detect this compound becomes a priority.

The synergistic behavior between porphyrin-k-carrageenan composite and AuNPs (porphyrin-k-carrageenan-AuNPs) that gave a wide-band absorption material [2] encouraged us to extend its functionality toward 1-methylimidazole detection. The UV-Vis monitoring of 1-methylimidazole is presented in Figure 1.

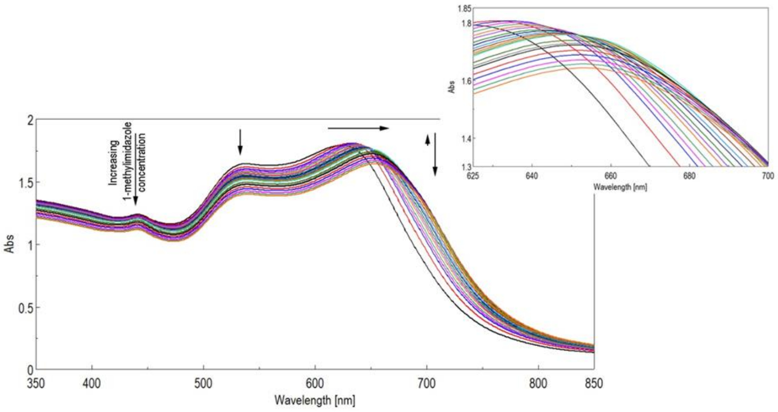

Figure 1. Overlapped UV-Vis spectra when adding to each step 0.02 mL 1-methylimidazole (c= 1 × 10^{-2} M) to (porphyrin-k-carrageenan-AuNPs) plasmonic complex, in acid medium pH= 2.

As can be seen from Figure 1, the maximum of absorption is bathochromically shifted from 632 nm to 653 nm, associated with a decrease of the intensity of the spectra.

The dependence between the absorption intensity of the (porphyrin-k-carrageenan-AuNPs) plasmonic complex, read at 528 nm and the concentration of is linear (Figure 2) in the concentration range 7.9×10^{-5} - 42×10^{-5} M.

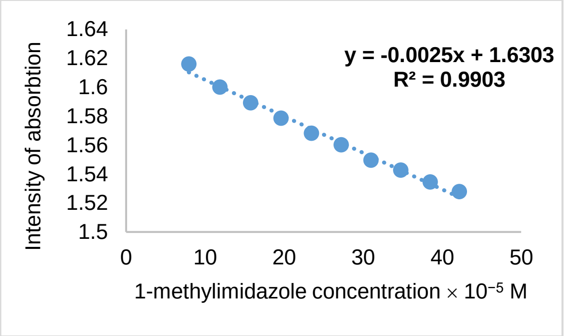

Figure 2. Linear dependence between the absorption intensity of the (porphyrin-k-carrageenan-AuNPs) plasmonic complex, read at 528 nm and the concentration of 1-methylimidazole.

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ADVANCED ANTIBACTERIAL COMPOUNDS. COMPLEXES BETWEEN 1-METHYLIMIDAZOLE AND A CARBOXY –A_3B PORPHYRIN

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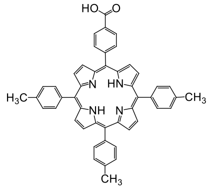
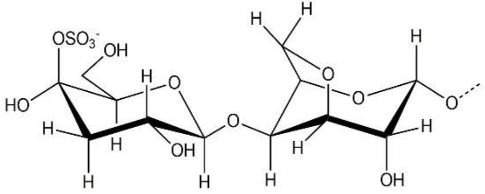
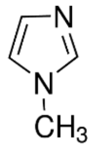
1-Methylimidazole, is a compound used in proteomic research and also as electrolyte for the solid-state dye-sensitized solar cells. New antibacterials for gram-positive *S. aureus*, evidenced that *N*-methyl benzimidazole substituted with biomimetic compounds have excellent potential [1].

 5-COOH-3MPP	 k-carragenaan	 1-methylimidazole

New complexes between 1-methylimidazole and 5-(4-carboxyphenyl)-10,15,20-tris-tolylporphyrin (5-COOH-3MPP), in k-carrageenan polymeric matrices have been obtained from 5-COOH-3MPP and k-carragenaan in THF brought to reflux for 160 min [2]. To a small quantity of this composite, 1-methylimidazole ($c = 1 \times 10^{-3}$ M) was continuously added (UV-Vis monitored in Figure 1).

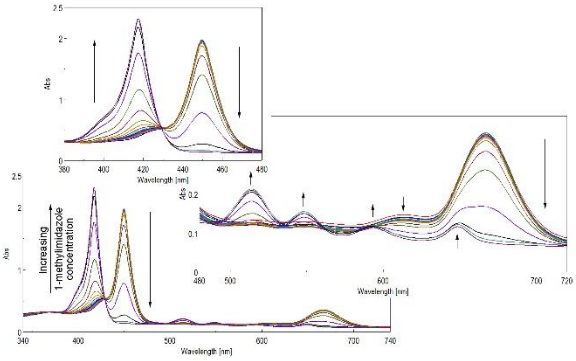


Figure 1. UV-Vis monitoring of equilibrium processes when adding 1-methylimidazole to 5-(4-carboxyphenyl)-10,15,20-tris-tolylporphyrin

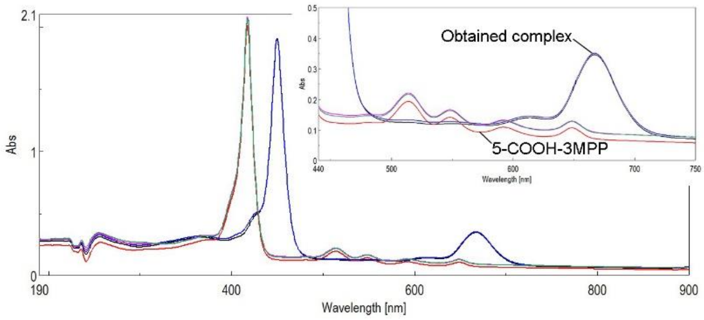


Figure 2. Final UV-Vis spectrum representing the complex formation between 1-methylimidazole and a carboxy-substituted A_3B porphyrin in k-carrageenan polymeric matrices

The new obtained complex has improved optical properties that recommend it for antibacterial photosensitization, namely a significant bathochromic shift of all bands with at least 30 nm accompanied by a strong hyperchromic effect regarding QI band.

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UP-SCALING THE RECYCLING PARADIGM: NOVEL THERMOPLASTIC COMPOSITES FOR STRUCTURAL APPLICATIONS MADE ENTIRELY FROM WASTE

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In recent years, a great deal of interest has been invested in innovating materials based on waste, through re- and up-cycling, intended for structural applications. Thus, academic and industrial R&D offerred, and still does, new solutions to actual environmental issues, intended to limit the negative impact of pollution. [1-4]

The present study is subscribed to this trend and presents new thermoplastic composites based on high density polyethylene waste (HDPEw) reinforced with natural fibers from agriculture (sorghum baggasse, SB) and inorganic powders (concrete waste from demolition sites, CWP). These new composites made entirely from recycled materials have been characterized (mechanical tests, thermal properties, water sorption) in order to assess their level of performance in relation with the amount of filler and reinforcement, and to envisage their range of applications.

The experimental results indicated that SB fibers increased the elasticity of samples, expressed as improved impact strength, while CWP enhanced the hydrophobicity and the ultimate tensile strength. An optimized formulation will provide the best combination of properties for the intended applications.

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NEW BIOMATERIALS BASED ON POLYSACCHARIDE DERIVATIVES FOR MINIMALLY INVASIVE ADMINISTRATION OF LOCAL DRUG DELIVERY SYSTEMS

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Minimally invasive procedures are continuously of interest for the medical community due to their undisputable advantages: low negative impact on the patient's well-being, fast recovery, and maximal clinical benefits. However, these procedures exhibit a series of drawbacks when applied to drug delivery systems. The most prevalent obstacle is the needle clogging during the administration. Another problematic aspect is the fact that after administration the polymeric mixture does not crosslink fast enough and the components are readily dispersed in the neighboring tissues, so that the effectiveness decreases. The key point to maintain both structural and functional integrity is a very good optimization of the self-healing behavior. This will ensure efficient, controlled drug delivery and improved therapeutic effect. Gelation can occur *in situ* due to changes in pH, temperature or type of ions, therefore not requiring an initiator or crosslinker [1].

In our study, we exploited the functional groups naturally occurring in the structure of polysaccharides. Particularly, selective oxidation protocols are attractive for obtaining derivatives with added value, improved properties, and increased reactivity [2]. Aiming to explore the impact of different types of interactions, we focused on derivatives either with carboxylic or aldehyde groups. When coupling these macromolecules with chitosan, which is a highly versatile amine-bearing polysaccharide, the resulting biomaterials achieved advanced properties [3,4]. Most importantly, the networks exhibited injectability, as well as readily tunable gelation and mechanical properties. In addition, the structures had good hydrophilicity and the pore size varied with the density and strength of the interactions between the polymers.

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PRELIMINARY ANALYSIS REGARDING THE DETERMINATION OF THE ACTIVITY OF ACIDOPHILIC BACTERIAL STRAINS IN SYNTHETIC MEDIA CONTAINING DIFFERENT CONCENTRATIONS OF HEAVY METALS

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One of the most critical problems facing both humans and animals, with direct effects on their health, is water pollution. The main sources of water pollution come from industrial, agricultural, and domestic activities. Industrial agricultural activities are necessary for a country's economic development, but they generate industrial spills, agricultural run-off, and wastewater discharges, which contribute to water pollution. Mining activities are also responsible for heavy metal pollution of water.

Environmental solutions are now being sought to bioremediate contaminated water. One such solution involves bioremediation of heavy metal-contaminated water using microbial strains. Two strains of acidophilic bacteria have been used for this purpose: *Acidithiobacillus ferrooxidans* and *Leptospirillum ferrooxidans* and were tested in synthetic water with known concentrations of copper or iron.

The results suggest that these strains are resistant to relatively high concentrations of heavy metals due to their metabolism adapted to extreme environmental conditions. These adaptations allow certain microorganisms to be successfully used in the bioremediation of heavy metal-contaminated water bodies.

Keywords: pollution sources, mining activities, acidophilic bacteria, bioremediation.

Acknowledgement. This research was funded by the Project RoRS 337- ROmania Serbia NETwork for assessing and disseminating the impact of copper mining activities on water quality in the cross-border area (RoS-NET2), implemented under the Interreg-IPA Cross-border Cooperation Romania-Serbia Programme that is financed by the European Union under the Instrument for Pre-accession Assistance (IPA II) and co-financed by the partner states in the program.

POLYOXAZOLINES – STABILITY, BIO- AND HAEMOCOMPATIBILITY STUDY

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INTRODUCTION

Osteomyelitis (OM) is an infection and inflammation of the bone and bone marrow that affects about 2 out of every 10,000 people. If left untreated, the infection can become chronic, causing blood loss to the affected bone, and possibly leading to bone death. We hypothesize that PiPOx, an emerging polymer in biomedical applications, combined with well-known antimicrobial agents such as nafcillin, metronidazole and antimicrobial peptides will result in synergetic antiseptic properties able to alleviate the problems associated with bacterial infection in osteomyelitis. Little data is known about PiPOx coupled with antibiotics, therefore, an initial study on stability, cytotoxicity and hemocompatibility of these polymers, as such or modified, has been performed.

EXPERIMENTAL METHODS

Life-dead and MTT assays on L929 murine fibroblasts were used to assess the cytotoxicity of PiPOx samples. The cytokine profiles of TNF-α and IL-6, known pro-inflammatory markers, were investigated on RAW264.7 macrophages. Haemocompatibility was evaluated by determination of the activated partial thromboplastin time (APTT) using whole blood and a ST4 StagoMax coagulometer. Endotoxin level in PiPOx extracts was determined by using Limulus Amebosyte Lysate (LAL) chromogenic endpoint assay.

RESULTS AND DISCUSSION

Extracts after 4h up to 2 weeks in which PiPOx hydrogels were incubated, were used to indirectly determine the cytotoxicity and endotoxin levels. Basal levels for pro-inflammatory cytokine production post macrophages interaction with extracts and normal endotoxin levels were obtained. APTT coagulation times were within normal levels.

CONCLUSION

The bio- and haemocompatibility of PiPOx hydrogels was proven by in vitro testing on L929 murin cells and RAW264.7 macropages. Further application of these polymers in the biomedical field is encouraging, offering a versatile platform to develop novel candidates for drug delivery purposes.

Acknowledgement. The authors acknowledge the Romanian Ministry of Research, Innovation and Digitalization, CNCS/CCCDI – UEFISCDI, project number PN-III-P2-2.1-PED-2021-2544 within PNCDI III, for the financial support.

HYDROGEN EVOLUTION REACTION - USAGE OF BISMUTH OXIDES AS CATALYSTS

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The major priority in H_2 energy science is to create a special catalytic system with increased activity in order to lower costs in industrial and residential applications that involve big scale production. In order to greatly increase the efficiency of H_2 production using green pathways like photochemical, electrochemical, it is necessarily to develop an efficient catalytic system. Bi-based nanocatalysts are environmentally friendly, very inexpensive materials with exceptional capabilities. In this context, in present study three composite materials based on bismuth oxide sulphate ($Bi_2O(SO_4)_2$), Bi_xO_y-C-6% PVA were prepared by using sol-gel method. In order to highlight the specific crystalline morphology, the composite materials were characterized by scanning electron microscopy (SEM), small-angle neutron scattering (SANS) and atomic force microscopy (AFM). Existence of electrocatalytic properties with the ultimate goal of obtaining hydrogen, was proved by using electrochemical techniques. AFM data indicates a pronounced roughness only on the surface of material, also confirmed by the small specific surfaces obtained from nitrogen adsorption-desorption isotherms (Brunauer–Emmett–Teller (BET) theory). After synthesizing, the three materials were tested in order to verify the existence of the catalytic properties necessary for hydrogen evolution reaction (HER), the linear voltammetry data showed overpotential values between 0 and -0.2 V. The experimental data confirmed the catalytic properties necessary for the HER reaction. The Bi_xO_y-C-6%PVA material presents the highest electrical conductivity value of $5.33\text{x}10^{-04}$ S·cm^{-1}, and the highest specific capacity according to cyclic voltammetry is given by the Bi_xO_y material. Based on the results obtained, it can be concluded that materials based on bismuth oxides have catalytic properties and that they can be used in the hydrogen production process.

Acknowledgment. This paper was financially supported by the Project "Network of excellence in applied research and innovation for doctoral and postdoctoral programs"/InoHubDoc, project co-funded by the European Social Fund financing agreement no. POCU/993/6/13/153437.

THE EFFECT OF CELLULASE-AIDED EXTRACTION ON RECOVERY AND FUNCTIONAL PROPERTIES OF WHITE PROTEIN FRACTION FROM PUMPKIN LEAVES

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The intention of this study was to examine potential of cellulolytic complex to affect isolation of white protein fraction from pumpkin leaves and its functional properties. Pumpkin leaves represent waste material that can be used as the source of this protein. The findings demonstrated that green protocols with usage of enzymes enabled improved recovery of RuBisCO protein from pumpkin leaves. By using different dosages of enzyme and changing duration of extraction process, the highest concentration of released protein (Figure 1) and reducing sugars (Figure 2) were achieved with 30 FPU/g during 1 hour. Improvement of recovery of white protein fraction with Cellulase complex was approximately by 1.4 fold compared to conventional extraction without enzymes. Moreover, enzymatic treatment improved solubility of isolated protein for 41%, water holding capacity for 30%, while oil holding capacity remained approximately the same. Our findings indicated that white protein fraction can be prepared in larger quantities and with improved functional properties from cellulose-aided extraction of pumpkin leaves as green and environmental-friendly protocol.

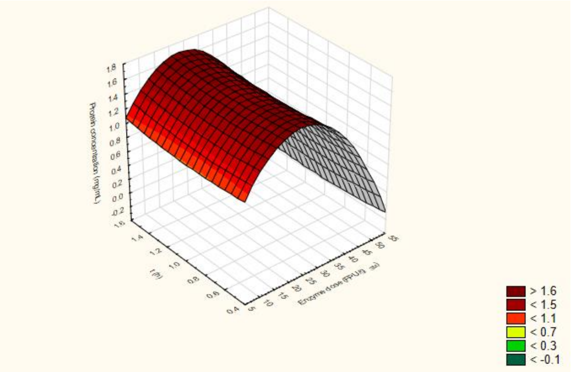

Figure 1. Results of optimization of protein concentration extracted from pumpkin leaves with Cellulase complex

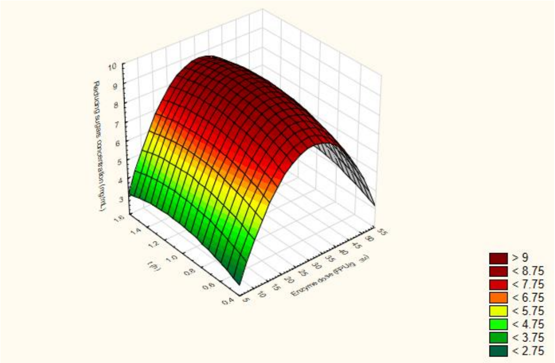

Figure 2. Results of optimization of reducing sugars concentration extracted from pumpkin leaves with Cellulase complex

Acknowledgement. The financial support by the Science Fund, Republic of Serbia, Project MultiPromis, Grant No.7751519 is greatly acknowledged.

CHAMOMILE TEA RESIDUES AS AN ALTERNATIVE (LOW-COST) ADSORBENT IN LEAD REMOVAL FROM SOLUTIONS

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Heavy metal pollution refers to excessive amounts of heavy metals in the environment, which can negatively impact human health and the natural environment. Because these elements might be present in food samples and can stay in the environment for decades, it is crucial to maintain the ongoing transmission of these components in the environment.

This study aims to examine the effectiveness of a low-cost waste adsorbent for removing heavy metals from aqueous solutions. We chose lead as a metal and chamomile residues as a biosorbent for this study.

To determine the ideal operating conditions, we experimented with various adsorbent masses, metal solution concentrations, pH levels, contact time between the metal and absorbent, etc. To measure the amount of metal, we used inductively coupled plasma-optical emission spectrometry (ICP OES), to examine the morphology of the residues scanning electron microscope (SEM), and infrared spectra (FTIR) were used.

The results demonstrated that chamomile tea has a significant adsorption capacity for Pb^{2+} removal from water. The adsorption process reached equilibrium within a short contact time, indicating its potential for rapid treatment.

To conclude, we have highly promising low-cost biosorbents that are simple to use in environmental remediation.

Keywords: heavy metal remediation, agricultural waste, ICP-OES, SEM, pollution

ENZYMATIC MODIFICATION OF PECTIC FIBER EXTRACTED FROM SOY HULL BY DIFFERENT PROTOCOLS

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Pectic fiber was extracted from soy hull, a by-product of soybean processing, by three different protocols involving diluted HCl to produce APF (pectic fiber extracted with hot acid), USPF (pectic fiber extracted with acid and ultrasound) and RTPF (pectic fiber extracted with acid at room temperature). These fibers were subjected to modification with enzymes - endo-polygalacturonase and pectin-methylesterase, and modified m-APF, m-USPF and m-RTPF were produced. Unmodified pectic fibers had high molecular weights - M_w of dominant fraction was 3550 kDa for APF, 1815 kDa for USPF and 2020 kDa for RTPF. Weight average molecular weight of dominant fraction of modified pectic fiber was 1780 kDa for m-APF, 1460 kDa for m-USPF and 1930 kDa for m-RTPF (Figure 1). *In vitro* antioxidant activity of modified and unmodified pectic fiber was analyzed using ABTS test and results showed increased values for modified pectic fiber. Flow curves of modified and unmodified pectic fibers were investigated and dramatic decrease in viscosity was observed for m-USPF and m-RTPF comparing to corresponding unmodified pectic fibers (Figure 2). Applied modification procedure led to considerable changes in their characteristics and properties, such as decrease in molecular weight, viscosity reduction, and increased antioxidant activity. Enzymatic modification of pectic fiber from soy hull could be further directed to influence certain desired characteristics that allow production of pectic fiber with properties suited for particular food applications.

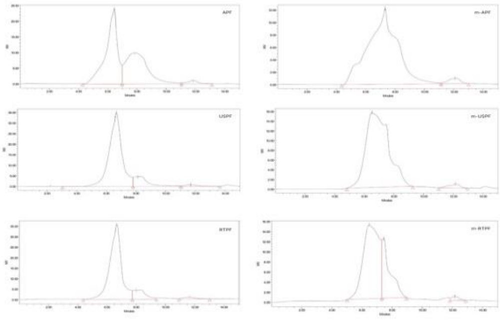

Figure 1. HPSEC profiles of unmodified and modified soy hull pectic fibers

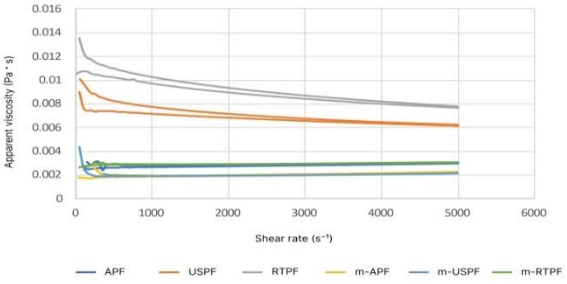

Figure 2. Flow curves of modified and unmodified soy hull pectic fibers

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POLYMERS OF VINYLPHOSPHONIC ACID WITH DIALKYLVINYL PHOSPHONATES AND THEIR ANTICORROSION PROPERTY

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Vinylphosphonic acid homopolymer and its copolymers with different comonomers or oligomers like diacrylates, dialkylvinylphosphonates etc gained applications in diverse domains: as polymer electrolytes membranes for fuel cells, as ion exchange membranes, in water treatment processes, in controlling steel corrosion, as adhesives for metallic surfaces, in the composition of products for bone reconstruction and tissue engineering in medical field and in dental cement. The functional synthetic copolymers based on vinylphosphonic acid (VPA) with different monomers have great importance in polymer chemistry due to their special properties given by the presence of phosphonic group.

The aim of this paper is to study the properties in aqueous solution of copolymers of vinylphosphonic acid with dimethylvinylphosphonate and to investigate the possibility to apply these copolymers in surface protection against corrosion.

Homopolymer of vinylphosphonic acid (PVPA) and copolymers of vinylphosphonic acid (VPA) with dimethylvinylphosphonate (DMVP) at different molar ratio were obtained by radical polymerization using UV light and photoinitiator.

The polymers were tested as corrosion inhibitors for iron and their presence in aqueous solution decreased the corrosion current density by the formation of protective film on iron surface. The presence of phosphonate groups from dimethylvinylphosphonate monomer in copolymers was beneficial and at a molar ratio VPA:DMVP 4:1 and 3:1 enhanced the anticorrosion property in comparison with homopolymer of vinylphosphonic acid.

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A FINGERPRINT-BASED APPROACH TO IDENTIFY AND REPURPOSE DRUGS WITH SIMILAR SIDE EFFECTS

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Drugs work by interacting with specific biological targets in the body. However, they can also affect other targets that are not intended, causing unwanted side effects. These side effects pose significant challenges in drug discovery, emphasizing the need for predicting them before human testing. In this study, we looked at how the chemical structures of about 1200 approved drugs [1,2] relate to their side effects. We mapped the drugs based on their chemical structure with the side effects collected from FDA's platform [3] obtaining over 2,000,000 chemical structure-side effect pairs. Only drug-side effect pairs that were statistically significant [4] were further used to create a fingerprint profile, where each bit indicates whether a drug has a certain side effect or not. By applying hierarchical clusterization to the data, we identified 75 distinct drug clusters based on similar side-effect profiles. Interestingly, we observed that chemical similarity within these clusters is considerably lower. This approach can help to find drugs based on their clinical side effects, in addition to their chemical and biological properties.

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PLSDA MODELING OF BLOOD BRAIN BARRIER PENETRATION BY SMALL MOLECULES

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The blood-brain barrier (BBB) function is to restraint the passive diffusion of polar compounds from the blood to the brain, to permit the transport of nutrients to the brain, to restricts neurotoxic compounds which are present in blood from traversing into the fluid existing in the central nervous system (CNS), etc. Therefore, the BBB play a pivotal role in CNS related diseases and its modeling represent one of the main challenges of drug discovery programs. The forecast of ability of a small molecule to pass through the BBB is a crucial issue in early drug discovery, especially for CNS related diseases such as Alzheimer and dementia. PLSDA represent an advantageous scenario for predicting the BBB permeability, which can process large datasets of small molecules integrating substantial chemical diversity and a high number of physico-chemical descriptors. We compiled a reasonably extensive standard validation dataset of experimentally determined BBB permeability values, curated and annotated with literature references (84 molecules with BBB+ and 256 molecules showing BBB) which display reduced analogue bias in active and inactive set, whereas inactives are experimentally validated negative compounds. The physico – chemical descriptors were calculated with QickProp and FILTER softwares and further analyzed with PLSDA algorithm, resulting a good overall classification accuracy, underlying the main physiochemical descriptors which differentiate the compounds which penetrate BBB (BBB+) with reference to the one which cannot pass BBB (BBB-).

MODIFICATIONS IN PLANTS POLYPHENOLS PROFILE DUE TO BIOTIC STRESS AND CLIMATE CHANGE

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Polyphenols are a vast class of secondary metabolite-derived chemicals found throughout plant life. Their concentration and profile could be modified due to different plant conditions as physiological stages and abiotic and biotic stress. Biotic stress as herbivory or fungi, influence not only the total phenols concentration but also the profile of different polyphenols. Even more, the carbon dioxide concentration in the air increased in the last year to 421 ppm which represents a 1% changing compare with 2022.

We used plant species from the *Brassicaceae* family (*Brassica oleracea* variety *capitate*, *Brassica oleracea*, variety *botrytis*, grown at high carbon dioxide (800 and 1200 ppm) to test the influence of elevated carbon dioxide on plants polyphenols. At the same time, biotic stress has been induced using cabbage moth *(Mamestra brassicae)*, cabbage white *(Pieris brassicae)*, and Greenhouse whitefly *(Trialeurodes vaporariorum).*

It has been shown that the polyphenols (as syringic or cumaric acid) concentration decrease for plants grown at high carbon dioxide concentrations but the presence of insects determines an increase in polyphenols concentration probably due to their involvement in defence strategy.

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CARBONIZATION OF TREE OF HEAVEN FOR BIOCHAR PRODUCTION: A PROMISING UTILIZATION OF INVASIVE SPECIES FOR PESTICIDE ADSORPTION

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The increasing presence of pesticides in soil and water systems has raised concerns about their adverse effects on ecosystems and human health. To address this issue, biochar has emerged as a sustainable solution due to its high adsorption capacity [1]. This study focuses on utilizing tree of heaven (Ailanthus altissima) biomass as a feedstock for biochar production [2], aiming to develop an efficient and environmentally friendly approach for pesticide adsorption.

Tree of Heaven, a fast-growing and invasive species, poses a significant challenge to ecosystems. By converting this biomass into biochar through carbonization, we can simultaneously address the issue of invasive species while creating a valuable resource for environmental remediation. The carbonization process involves pyrolysis under controlled conditions to transform the biomass into a stable carbon-rich material with a high surface area and porosity. In this study, we investigate the influence of carbonization parameters, such as temperature, and $ZnCl_2$ activation on the physicochemical properties and adsorption capacity of prepared biochar samples. Characterization techniques, including Scanning Electron Microscopy, Fourier-Transform Infrared, and Raman spectroscopy, were employed to evaluate the biochar's morphology and functional groups.

Batch adsorption experiments are conducted to assess the performance of the Tree of Heaven biochar in removing neonicotinoid pesticides from aqueous solutions. The effects of initial pesticide concentration, contact time, and suspension composition (single components or pesticide mixtures) on the adsorption process are investigated. Adsorption isotherms were employed to analyze the adsorption behavior and understand the mechanisms involved.

Preliminary results demonstrate that the activated tree of heaven-derived biochar exhibits a remarkable adsorption capacity for neonicotinoids. Tested biochar samples present promising adsorbents due to their porous structure and abundance of functional groups, enabling hydrogen bonding with investigated pesticides. Furthermore, the invasive species-derived biochar shows promising stability and reusability, making it a sustainable alternative for long-term pesticide removal applications. These findings contribute to the development of efficient and sustainable solutions for environmental remediation, addressing both the issue of invasive species and pesticide contamination.

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PHOSPHONATE METAL-ORGANIC FRAMEWORKS AS ENVIRONMENTALLY FRIENDLY ADSORBENT MATERIALS

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At the present time, due to the growth and development of the industry, many toxic substances are found in the water resources, affecting the quality of life and the environment. It is necessary that those substances are removed from the water, to improve human and environmental health. The aim of the study is the synthesis of different solid materials, taking into account the 12 principles of green chemistry, and obtaining materials with high phenol adsorption capacities. The materials, phosphonate metal-organic frameworks (MOF) are obtained from the reaction between phosphonoacetic acid (CP) - the organic component, and a divalent metal salt (Co^{2+} and Mg^{2+}) - the inorganic component, in hydrothermal conditions[1]. As a second step in materials synthesis, the obtained phosphonate MOFs were impregnated with ammonium or imidazolium based ionic liquids[2], namely 1-ethyl-3-methylimidazolium chloride and N-methyl-N, N, N-trioctylammonium chloride (Aliquat 336) to increase the adsorption capacity and verify the physical and chemical properties. The phenol adsorption was tested for both materials, and the best results were obtained in the case of materials impregnated with ionic liquids, which revealed adsorption capacities increased by 20% comparing with initial phosponate MOFs.

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COLOUR DETERMINATION USING CIELab SPACE OF A NEW DIRECT DYE DRIVED FROM 4,4'-DIAMINOSTILBENE-2,2'-DISULPHONIC ACID

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CIE L*a*b* (CIELAB) is the most complete color model used conventionally to describe all the colors visible to the human eye. The colour of a new direct eco-friendly dye with disazoic structure obtained using 4,4'-diaminostilbene-2,2'-disulfonic acid as diazocomponent and 2,7-didroxynaphtalene as middle component was evaluated in terms of CIELAB parameters: lightness (L*), redness (a*), yellowness (b*), chroma or saturation (C*) and hue angle (h°) 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 ΔECMC were calculated against a standard namely Pigment White 6 (C.I. 77 891). In this way an objective analysis of the colour has been made, the trichromatic coordinates being intrinsic properties that do not depend on the application concentration and that identify precisely the shade.

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BIODEGRADABLE CHITOSAN-BASED FILMS: CHARACTERIZATION, PROPERTIES AND APPLICATIONS

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Widely found in nature, chitosan, a cationic polymer possesses numerous beneficial properties such as antimicrobial and wound healing properties, biocompatibility, biodegradability and low toxicity, advantages that make this polysaccharide useful in biomedical application [1]. The objective of this study was to design chitosan-based films with enhanced antibacterial, using nisin as a potential antimicrobial compound. Due to its film-forming capacity, chitosan is suitable for polymeric wound dressing development, while nisin is an antimicrobial peptide with a GRAS (Generally Recognized As Safe) status, approved for use, mainly in food industry [2], but recent approaches indicate its use biomedical fields. Blend solutions of chitosan with medium molecular weight and nisin were used to prepare polymeric films via solvent casting method [3]. Several physico-chemical properties, as well as microbiological analysis and biodegradability assays were performed in order to characterize chitosan-based films and their use in biomedical applications. The results showed that chitosan materials are suitable for sustained release of nisin, and their physico-chemical properties are similar to those of the most common wound dressings on the market. Moreover, the microbiological analysis showed that the addition of nisin increases the antibacterial effect of the films, and the biodegradability assays showed that the materials tested are safe for the environment.

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Zn GRAFTED ORDERED MESOPOROUS SILICA KIT-6 for CO_2 ADSORPTION

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In the present study, composites containing Zn were prepared by impregnating the hydrothermally prepared mesoporous KIT-6 support with 30 wt% metal oxide content, followed by functionalization with aminopropyl trietoxisilane (APTES) in ratios of 20-40 % [1-4]. The well-ordered three-dimensional mesoporous structure of the KIT-6 support was confirmed by small angle X-ray diffraction (SAXRD) patterns. N_2 adsorption-desorption analysis results showed that the mesoporous structure of KIT-6 was preserved after oxide loading. The adsorption of CO_2 and its temperature programmed desorption using thermogravimetry were studied for amino-functionalized composites at different temperature. The CO_2 adsorption/desorption of KIT-6 Sil showed that both the adsorption capacity (mmoleCO_2/g adsorbent) and the efficiency of amino groups (moleCO_2/mole NH_2) depend on the temperatures. In order to investigate the regenerability and cyclic stability of KIT-6 sil and Zn/KIT-6 sil, multistage CO_2 adsorption–desorption cycles were performed by DTA/TG at 40-120ºC.

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ENHANCED RECOVERY AND PROPERTIES OF PROTEIN ISOLATE FROM PUMPKIN LEAVES FROM ENZYME ASSISTED EXTRACTIONS

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Food proteins are known to have important role in human diet and are recognized as the most valuable functional ingredients in food production. According to it, research in food science and technology is focused on the exploration of alternative protein sources that will provide adequate human nutrition and have a lower environmental impact [1]. Large amounts of leaves that are left after the manufacturing of some crops in food industry are not utilized. RuBisCO (ribulose-1,5-bisphosphate carboxylase/oxygenase) is the main protein in green leaves and the most abundant protein in nature [2]. The aim of this study was to explore the effect of commercial enzymes Viscozyme and Enzyme complex on the efficiency of extraction and functional and biological properties of RuBisCO protein from pumpkin leaves. According to the obtained results, recovery of RuBisCO protein with the assistance of Viscozyme and Enzyme complex was about 4 and 10 times more efficient than recovery in conventional extraction process. Moreover, enzyme-assisted extractions enable production of protein isolates with superior functional properties in comparison to isolate from extraction without enzymes. Proteins extracted with the assistance of Viscozyme and Enzyme complex showed improved solubility by 4 and 3 folds, respectively. Protein from extraction with Viscozyme expressed improved water and oil holding capacities while protein obtained with the assistence of Enzyme complex exhibited comparable antioxidant activity to the isolate from the conventional extraction. The presence of the RuBisCO protein was confirmed by SDS PAGE electrophoresis and the subunits ~20 and ~50 kDa were read. These results highlight high potential of green enzyme-assisted protocol in preparation of protein isolates from pumpkin leaves as a nutritious and functional food ingredient in context of global food security and protein supply.

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DETERMINATION OF HEAVY METAL CONCENTRATIONS IN DAIRY PRODUCTS NEAR POWER PLANTS IN KOSOVA

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Trace metals pollution has detrimental consequences on the ecosystem and environment in general. Heavy metals can contaminate the environment in direct or indirect ways. Some of the most known paths of polluting the environment today are mining, agriculture, industrial operations, improper waste disposal, etc. Industrial activities are also one of the main sources of pollution. Therefore, in addition to their existence in water and the environment, these trace elements must also be tested in food samples.

This experimental investigation offers data of heavy metal concentration in dairy products near the power plants of Kosova, Kastriot. To do the determination ot these metals, we used the inductively coupled plasma optical emission spectroscopy (ICP-OES) technique. Particularly, arsenic, cadmium, chromium, copper, iron, mercury, lead, and zinc were among the heavy metals examined.

It is never sufficient to supply information about the worst pollution but is is a fact that pollution should always be continuously monitored to prevent both human and environmental catastrophic events. Because of this, we can state that the contamination that we are dealing with is average, and ongoing analysis is necessary to keep this region under control.

Keywords: heavy metal pollution, dairy products, ICP OES technique, power plants

THEORETICAL AND SURFACE/ELECTROCHEMICAL INVESTIGATIONS OF PHOSPHONIC ACIDS AS EFFECTIVE INHIBITOR FOR CARBON STEEL CORROSION IN SALINE ELECTROLYTE

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Iron corrosion is effectively inhibited by organic compounds containing heteroatoms such as N, P, O and/or p-electrons or non-bonding electrons. The order in which the inhibitory efficiency of heteroatoms decreases is P > N > O. Phosphonates and phosphonic acids are widely known for their inhibitor ability, with low environmental impact. This group of substances can quickly produce an imperceptible. but strong protective layer on metal surfaces. This binding capacity reduces the exposure of the active metal to the corrosive environment. Vinyl phosphonic acid (VPA) and N,N′-phosphonomethylglycine (PMG) were tested as corrosion inhibitors for iron in saline environment. Polarization (CP) investigations show that PMG and VPA act in NaCl as mixed-type inhibitors. Values for charge transfer resistance (Rct) and double layer capacitance (Cdl) were estimated from impedance spectroscopy (EIS) data. The CP and EIS data show that these compounds could slow down the corrosion process. VPA ensures an efficiency (IE) of inhibiting the corrosion process of over 90% and the chloride ion can interfere beneficially in the corrosion mechanism. The 50% mixture of these compounds give IE higher than 96% (Figure1). The calculated values of ELUMO, EHOMO, energy gap, dipole moment, electronic hardness, global softness, electrophilic index and electronic potential map for the compounds under study agree with the experimental results.

Carbon steel 1:1 VPA:PMG

Figure 1. Unprotected (carbon steel)-left and protected (by the phosphonate additives)-right, carbon steel specimens immersed in saline solution at room temperature.

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TRANSITION METAL-DOPED HETEROPOLY COMPOUNDS FOR THE ETHANOL CONVERSION

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Heteropoly compounds with the general formula $Cs_xMH_{3-x}PW_{12}O_{40}$ (x=2, 2.25, 2.5 and M = Pd or Ni) were prepared and used as catalysts for the ethanol dehydration reaction. Ethanol conversion to ethylene and other organic compounds used as starting materials for organic industry of synthesis present a major interest because the ethanol is obtained from renewable starting materials [1, 2]. The effects of the Pd and Ni on the structure and catalytic activity of the catalysts were investigated.

The thermal decomposition was evaluated using simultaneous thermogravimetric analysis (TG) and differential thermal analysis **(**DTA**)** and consists of water release: physically adsorbed water, hydrogen-bonded water and constitutive water (the water formed of the protons and the oxygen of the $(PW_{12}O_{40})^{3-}$). The release of constitutive water causes the destroying of Keggin units with formation of corresponding oxides and the loss of acidic catalytic activity. FTIR spectra showed that the transition metal-doped catalysts maintained the specific bands to Keggin unit $[PW_{12}O_{40}]^{3-}$X-ray diffraction results indicated that all synthesized compounds exhibit the reflections corresponding to cubic crystalline structure. Catalytic activity of catalysts in ethanol conversion was studied by continuous flow reaction technique (CFRT) and the products were analyzed on gas- chromatography with FID detector. The introduction of large counters cation, such as Cs into acid, lead to an increase of surface area and enhanced the catalytic activity. The palladium doping prevents the coke formation and improves the burning of coke. Coke formation during ethanol dehydration does not affect the Keggin structure that led us to conclude that such catalysts can be regenerated.

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FUNCTIONALIZED POLYMERIC SUPPORTS WITH AMINO-PHOSPHONATED AND AMINOACID-PHOSPHONATED GROUPS FOR REMOVAL OF AROMATIC AMINES FROM AQUEOUS SOLUTIONS

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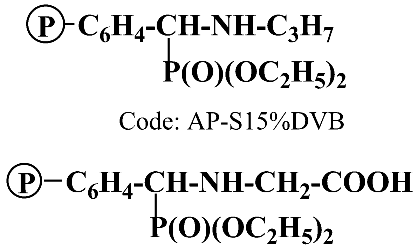
Aromatic amines are the important compounds used as intermediate or precursor in the manufacture of organic synthesis such as azo dyes, antioxidants, fuel additives, corrosion inhibitors, pesticides, antiseptic agents, medicines for poultry and the synthesis of pharmaceuticals [1]. However, the presence of aromatic amines in water, even at very low concentrations, is extremely harmful to aquatic life and human health [2-4]. The aim of this work was to obtain new adsorbents for using in removal of aromatic amines from aqueous solutions. Styrene-15% divinylbenzene copolymers grafted with aminophosphonated groups (code: AP-S15%DVB) and aminoacid-phosphonated groups (code: AM-S15%DVB) (see Scheme 1) were used to remove pollutants such as: aniline, 2-methyl-aniline and 4-methyl-aniline. The structure of the copolymers is as follows:



$$\text{Ⓟ}-C_6H_4-\underset{\displaystyle P(O)(OC_2H_5)_2}{\underset{|}{CH}}-NH-C_3H_7$$

Code: AP-S15%DVB

$$\text{Ⓟ}-C_6H_4-\underset{\displaystyle P(O)(OC_2H_5)_2}{\underset{|}{CH}}-NH-CH_2-COOH$$

Code: AM-S15%DVB

Scheme 1. The structure of the tested copolymers.

It was found that the speed of the adsorption process was high at the beginning, in each case. After 30 min, more than 90% of the total adsorption capacity was adsorbed. After 240 min, during which the adsorption equilibrium was established, the amount of adsorbed 4-methyl-aniline (AP:0.374 mmol/g, AM:0.376 mmol/g) was in each case greater than the amount of 2-methyl-aniline (AP:0.370 mmol/g, AM:0.367 mmol/g) and aniline (AP:0.232 mmol/g, AM:0.157 mmol/g). Among the aromatic amino-derivatives used for the adsorption process, 4-methyl-aniline was the best adsorbed and aniline the least. The adsorbent with the best adsorption capacity was AP-S15%DVB. The alkyl substituted anilines were better adsorbed most probably due to the inductive effects (-I) of the alkyl substituents affecting the substrate polarity. It was found that the sorption mechanism of 4-methyl-aniline from aqueous solutions was chemisorption.

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GLYCOLIPIDOMICS OF HUMAN TEMPORAL LOBE EPILEPSY: A HIGH RESOLUTION TANDEM MASS SPECTROMETRIC STUDY

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In this study, we have developed a high-resolution tandem mass spectrometry (MS) approach to assess presumed changes in gangliosidome of human hippocampal tissue affected by temporal lobe epilepsy (TLE) in comparison with the healthy hippocampus. The most common form of epilepsy in humans is Temporal lobe epilepsy (TLE). The molecular events underlying seizures involve changes in membrane ion homeostasis leading to altered neuronal excitability [1,2]. Numerous (patho)physiological effects of glycoconjugate have been confirmed, including regulation of membrane ion transport, but the potential role in the molecular pathogenesis of TLE has not been explored in detail.

In the current research, an approach based on HR MS and MS/MS, using a nanoESI Orbitrap platform operating in the negative ion mode was for the first time developed, optimized and applied for the determination of ganglioside expression in human brain tissue samples. Our research was focused on the assessment of the changes in the ganglioside pattern in adult hippocampus affected by TLE vs. normal hippocampus, on the detection of specific TLE structures and the comprehensive characterization of the TLE-associated gangliosidome. The mixtures analyzed in this study were purified from human hippocampus affected by TLE (sample HipE) and age-matched normal hippocampus tissue (sample Hip), used as the control. The MS experiments were conducted in the negative ion mode on a LTQ Orbitrap Velos equipped with nanoESI source. The optimized nanoESI HR MS parameters allowed the multicharging of gangliosides, enhanced the ionization of long-chain polysialylated GT1 and GQ1 structures and provided a fair ionization/detection of minor components. In the comparative assay, the accurate mass measurement allowed the discrimination of 72 different species in HipE, with no less than 20 of GQ1 type discovered for the first time as associated to TLE [3]. Multistage mass spectrometry (MS^n) was carried out by higher energy collision dissociation (HCD) at variable collision energies within 35-80 eV range to enhance a high coverage of fragment ions. The results show marked differences in the ganglioside expression in TLE vs. control, particularly with respect to the sialylation degree of components, discovered as a general marker of TLE.

Since HR MS screening has indicated that the structures in the GQ1 class dominate numerically the HipE and may represent markers of TLE, a detailed structural analysis by HCD MS^n using as the precursor ion the $[M-4H^+]^{4-}$ detected at m/z 603.7844, which, corresponds to GQ1(d18:1/18:0) was carried out. GQ1b(d18:1/18:0) was found as a specific TLE biomarker.

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METAL-ENHANCED ANTIOXIDANT ACTIVITY OF A NATURAL PRODUCT PROMOTES NEUROPROTECTION

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Folk medicine has over the eons provided therapeutics to a number of diseases, with variable albeit definitive healing potency. That practice was based on natural products, emanating from different sources of the plant kingdom, with key molecular components exhibiting antioxidant, anti-carcinogenic, anti-inflammatory, and antidiabetic activity. Among such components, polyphenols are a family of natural compounds, the chemical structure of which is linked to beneficial effects in human physiology. Flavonoids belonging to that family have been well known for their avidity to combat Reactive Oxygen Species (ROS), thus counteracting oxidative stress. This biological property has drawn keen interest as means to provide protection from neurodegeneration and diseases, such as Alzheimer's and Parkinson's.

In an effort to exploit nature's potency against neurodegeneration, a) extracts of the plant Cronus mas L. were obtained through green chemistry employing β-cyclodextrin, b) the toxicity profile of aqueous extracts from Cronus mas L. was investigated to affirm the atoxic character, and c) the influence of a soluble and bioavailable complex metal ion forms on the extracts was examined to establish the extent of antioxidant power against neurodegenerative processes associated with cellular oxidative stress.[1] In that respect, the aqueous soluble extracts have been investigated in the presence of a hybrid metal-(α-hydroxycarboxylato) compound, i.e. zinc-citrate, in neuronal cell cultures (N2a, SH-SY5Y). The choice of neuronal cell lines was based on their sensitivity toward oxidative stress, thereby acting as reliable model systems of neuroprotection vs neurodegeneration.

The experimental results suggest that the a) plant extracts are atoxic to the neuronal cells over 24, 48 and 72 hours (viability, morphology, migration, proliferation) in a concentration (up to 1 mM) and time-dependent manner, b) antioxidant activity of the cells against oxidative stress, induced by H_2O_2, avails itself in a concentration-dependent fashion, and c) activity of the cells is enhanced in the presence of zinc-citrate. The experiments were carried out in a manner reflecting both the a) protective effect of the hybrid metal-organic species, and b) recovery of cell physiology from oxidative stress.[2]

The effect of zinc-citrate, as a well-defined and characterized form of an indigenous physiological metal ion, suggests that its concurrent interactions with the plant extract components and cytosolic targets of the neuronal cells either avert or revert oxidative stress-induced aberrations, essentially proffering effective neuroprotection.[3] The ensuing investigation of the influence of the genetic machinery of the cells under the influence of both the extracts and zinc-citrate is expected to reveal how these two factors exemplify the ultimately observed phenotype, thus reflecting merit to developing appropriately formulated pharmaceutical preparations serving as neuroprotectants in human physiology.

Acknowledgements: This research has been conducted in the framework of the Regional Operational Programme Central Macedonia 2014-2020 ("Development of natural product with neuroprotective action based on the plant Cornelian cherry", action code: KMP6-0079229) that was co-financed by Greek national funds and the European Union (European Regional Development Fund).

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METAL-ORGANIC SYNTHETIC CHEMISTRY OF Co(II,III) WITH O,N-TERMINAL SUBSTRATES. MAGNETIC AND ELECTRONIC PROPERTIES

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Oligonuclear and polynuclear transition metal clusters (with organic ligands bound to several metal atoms) have been the basis of advanced materials due to their potential in catalysis, nanoscience, optoelectronics, and magneto-optics.[1,2] Of particular importance in the field of sensors, molecular-based magnetic materials have attracted considerable attention in recent years because of their physical properties in low-dimensional magnetic systems (single-molecule magnets (SMMs) and single-chain magnets (SCMs)).[3] Poised to pursue the development of such metal-organic materials capable of exerting magnetic behavior, synthetic research was undertaken in the lab. Among the metal ions investigated, cobalt attracted considerable attention due to its chemical reactivity with appropriately configured (O,N,O)-terminal containing amino alcohol ligands.

Optimization of the specific metal-organic systems in this study has been investigated synthetically based on the a) reaction mixture composition, involving ternary aromatic chelators, such as 2,2'-bipy and 1,10-phen, b) molecular stoichiometry, c) reactivity temperature, d) solvent system, and e) temperature of isolation (4-25 °C). Successful isolation of six variable nuclearity ternary clusters, based on Co(II) and iminodipropanol in methanol, reveals that there is a temperature-specific trend in the chemistry employed, when it comes to the assembly of cluster species isolated in crystalline form and discrete phase. The isolated crystalline materials were characterized physicochemically by elemental analysis, FT-IR, UV-Visible, Photoluminescence, TGA, X-ray crystallography, EPR, magnetics (Fig. 1), and Hirshfeld analysis.

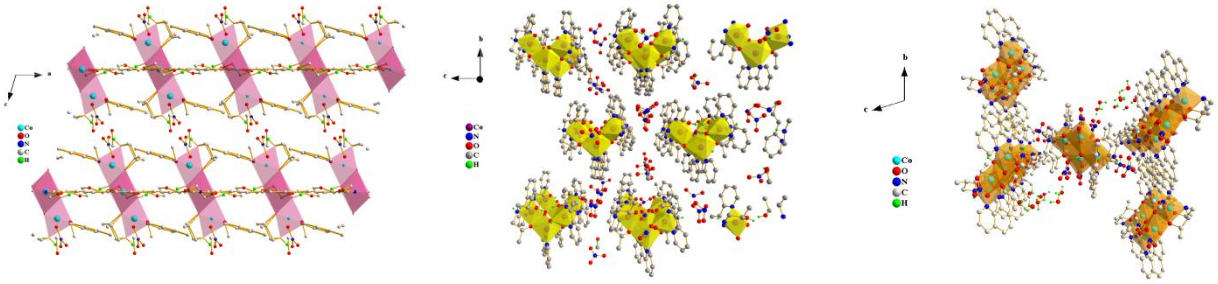

Figure 1. Lattice clusters of tetranuclear Co(II,III) assemblies

The collective physicochemical data on the investigated systems formulate structure-lattice, structure-electronic and magnetic behavioral profiles, thereby setting the parameterization for the design and synthesis of new materials with specified optical and magnetostructural properties.

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ION MOBILITY TANDEM MASS SPECTROMETRY OF HUMAN CEREBROSPINAL FLUID GANGLIOSIDOME

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The proximity of cerebrospinal fluid (CSF) with the brain, its permanent renewal, and better availability for research than tissue biopsies, as well as ganglioside (GG) shedding from brain to CSF, impelled lately the development of protocols for the characterization of GGs and discovery of central nervous system (CNS) biomarkers expressed in CSF [1]. Although CSF sampling is more difficult than urine or blood, as CSF is in direct contact with the brain and spine, CSF testing is more effective in diagnosing a variety of CNS conditions. In this context, we have implemented ion mobility separation mass spectrometry (IMS MS) and tandem mass spectrometry (MS/MS) for the exploration of human CSF gangliosidome and the characterization of rare human CSF glycoforms, with potential biomarker role [2,3]. The normal lumbar CSFs investigated here were obtained from adult individuals exhibiting no signs of tumors, intracranial haemorrhage or acute inflammatory process of the central nervous system (CNS). The extracted GG sample of 5 pmol/µL in methanol was infused into a Synapt G2S and the signal was acquired in the negative ion mode at 1.6 kV ESI voltage and 45 V for cone, respectively. IMS MS separation and screening revealed 113 distinct GG species in CSF; of these, more than 76% were found polysialylated, which is similar with the percentage of the polysialylated GG species (over 78%) detected in human brain using the same approach. In comparison with the brain tissue, we have discovered in CSF several components containing fatty acids with odd number of carbon atoms and/or short glycan chains. Further, the structural confirmation of GD3(d18:1/18:0) and GD2(d18:1/18:0), exhibiting shorter carbohydrate chain, a feature of CSF, was achieved by collision-induced dissociation (CID) MS/MS. The detailed evaluation of the GG profile in CSF revealed also the incidence of some new and biologically relevant species. The doubly charged ions at *m/z* 1018.004 and *m/z* 1019.008 assigned, according to mass calculation, to GalNAc-GD1(d18:1/18:1) and GalNAc-GD1(d18:1/18:0) were further submitted to CID MS/MS for detailed investigation of the oligosaccharide and ceramide structures. The incidence of only one mobility feature for each of the investigated species, together with the diagnostic fragment ions allowed the unequivocal identification, among the six possible structures for each of the fragmented structures, of the exact isomers in the CSF. Hence, by IMS MS/MS, GalNAc-GD1c(d18:1/18:1) and GalNAc-GD1c(d18:1/18:0) having both Neu5Ac residues and GalNAc attached to the external galactose were for the first time discovered in CSF and structurally characterized. The current data substantiate the high potential of IMS MS and CID MS/MS technique in revealing rare GG components and deciphering structural isomers in body fluids, where such species have a few times lower expression than in neural tissue. Moreover, human CSF and brain display a similar GG pattern, a finding that might be useful in clinical analyses targeting early diagnosis of CNS diseases, based on discovery of biomarkers in CSF or blood/serum.

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A BLACK BUT BRIGHT POLYMER: POLYANILINE WITH BORONIC GROUPS ITS PREPARATION, PROPERTIES AND ADSORPTION APPLICATION

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Due to their unique characteristics and the exciting potential of their practical applications, conducting polymers have received particular attention in recent years [1]. A member of this group of conductive polymers is polyaniline (PANI). Due to the multiple forms of oxidation and protonation that polyaniline presents, it can be more suggestively represented by a sequence of benzoid nuclei - B, and quinoid nuclei - Q, according to the general formula below (eq.1):

$$-[(B\text{-}NH\text{-}B\text{-}NH)_y(B\text{-}N=Q=N)_{1-y}]_n- \quad (1)$$

Leucoemeraldine (y=1), a pale yellow, emeraldine (y=0.5), a green and conductive substance, and pernigraniline (y=0), a dark violet substance-all of which are polyanilines-combine to produce the polymer [2]. Poly(3-aminophenylboronic acid) (PABA) si similar with PANI but has the advantage of a high density of boronic acid groups and hence to a better sensitivity than PANI. This paper reports our attempt to use electrochemical impedance spectroscopy (EIS) to investigate the nature of adsorption of azo dye on the PABA surface. To obtain high exposed surface area to improve the adsorbent properties of the PABA was electrochemically deposited on electrode (Pt) as we reported. Different isotherms were chosen to fit the EIS experimental data. The highest correlation coefficient gives the best fit for Langmuir kinetic model. The change of free energy of adsorption (ΔG^o_{ads}) and the adsorption constant (K_{ads}) evaluated for the adsorption of dye onto PABA/Pt electrode were found to be -33.61 $kJ\cdot mol^{-1}$ and 32.71 $kmol^{-1}$, respectively. These indicate that adsorption process is spontaneous, takes place via a combination of physical and chemical adsorption but mainly due to physical adsorption with the formation of a stable adsorbed dye layer on the PABA surface.

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PHOTOCATALYTIC PROPERTIES OF COORDINATION POLYMERS BASED ON COPPER(II): PRELIMINARY STUDIES

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Water pollution, a consequence of rapid industrialization and urbanization, has become a global problem. Organic compounds generated from various industries produce problematic pollutants in water. Among them, residual textile dyes are the main source of pollution worldwide [1]. Various techniques have been applied to remove dyes from waste water: physical, chemical or biological, among these methods photocatalysis gaining attention, since it is an efficient and ecological method [2].

In this paper three copper(II) coordination polymers: $^{1}_{\infty}[Cu_3L_2(N_3)]CH_3COO$ (**CP1**) $^{1}_{\infty}[Cu_3L_2(NO_3)]NO_3\cdot 2MeOH\cdot 2H_2O$ (**CP2**), and $^{1}_{\infty}[Cu_3L_2(H_2O)](ClO_4)_2$ (**CP3**), based on the Schiff base H_2L (N,N'-bis[(2-hydroxybenzilideneamino)propyl]piperazine), were applied as photocatalysts for degradation of three industrial dyes. Acid Orange 7 (AO7), Methyl Orange (MO), and Direct Green 8 (DG8) dyes were selected as potential colored pollutants.

Photocatalytic experiments were carried out under visible irradiation at 546 nm, and room temperature using 1 g/L compound (**CP1 ÷ CP3**).

The investigated coordination polymers exhibited efficient photocatalytic performance for the degradation of AO7, MO, and DG8 dyes under Vis irradiation (Fig. 1a), among which, **CP1** exhibited the best photocatalytic activity with a percentage degradation higher 60%.

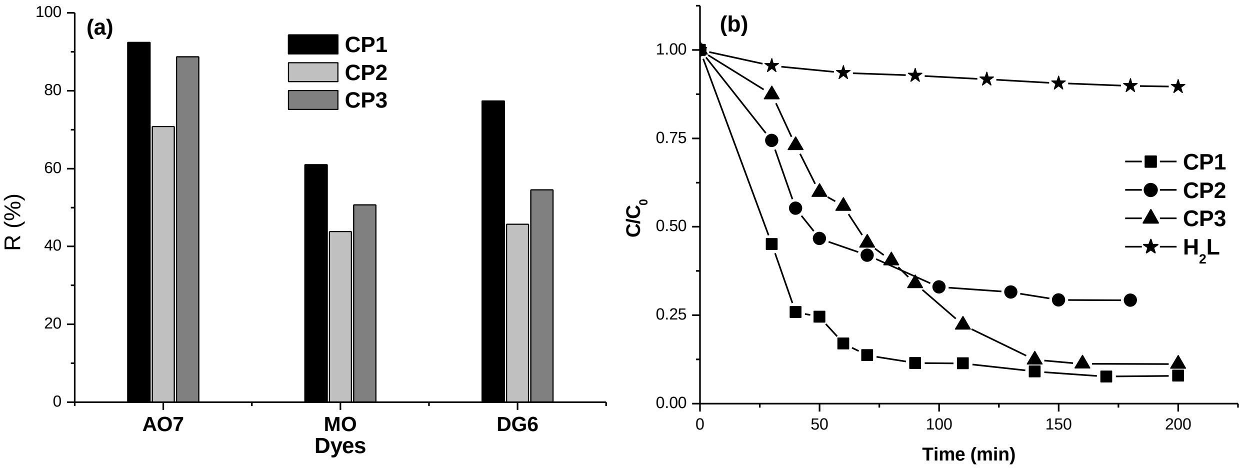

Figure 1. (a) Photodegradation efficiency of **CP** for AO7, MO, and DG8 dyes, under visible irradiation (545 nm), (b) Photodegradation of Acid Orange 7 in time, under visible light (545 nm), in the presence of the ligand (H_2L), and with **CP** complexes.

For all investigated dyes the photocatalytic degradation efficiency increased in order: **CP2** < **CP3** < **CP1**. The kinetic studies showed that the degradation process followed pseudo-first-order kinetic.

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PERSPECTIVES ON THE STRUCTURAL DESIGN OF COPPER(II) LIQUID CRYSTALLINE COMPLEX BASED ON SCHIFF BASE LIGAND

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Liquid crystalline (LC) phases are considered to have promising prospects for the progress of new high-performance components with potential applications as optical data storage [1] thermoplastics [2], sensors [3], high-performance fibres [4], etc. In order to achieve the right properties for device applications a key role is the understanding of structure-activity relationships. The most well-known strategy to obtain LC phases in organic compounds is by combining flexible alkyl tails with rigid cores such as aromatic or heteroaromatic rings through linking groups. These molecules present various layered smectic phases or non-layered nematic phases [5]. Structural diversity and unique properties can be induced by incorporating metal ions into organic liquid crystals [6].
Here we present the synthesis of a new rod-like Schiff base 3,4,5-tris(dodecyloxy)benzyl 4-((2-hydroxybenzylidene)amino)benzoate (H_2L) and its copper(II) complex CuL_2 (Figure 1).

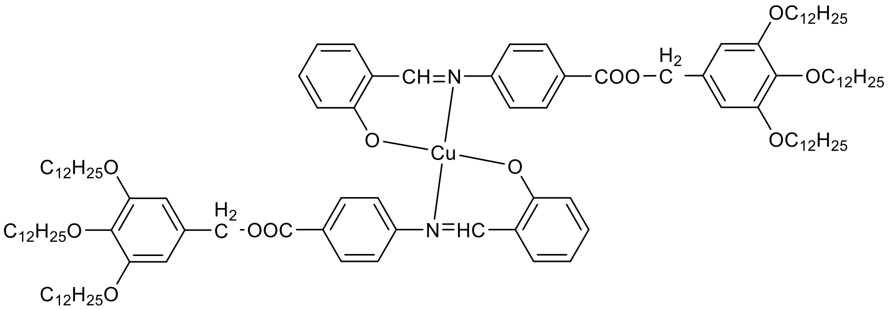

Figure 1. Proposed structure of CuL_2 complex

The obtaining and the purity of the Schiff base was confirmed by electronic, IR, and NMR spectroscopy. The copper(II) complex was characterized by atomic absorption spectrometry, IR and UV-Vis spectroscopy. The mesomorphic nature of both compounds was investigated by Polarized Optical Microscopy and Differential Scanning Calorimetry techniques.

Acknowledgements. This work was supported by a grant of the Romanian Ministry of Education and Research, CNCS - UEFISCDI, project number PN-III-P4-ID-PCE-2020-1958, within PNCDI III.

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MAO-B SELECTIVITY: *IN SILICO* INVESTIGATION

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A dataset of 126 MAO-B inhibitors compiled from literature published resources was used to develop a comprehensive computational approach, including a pharmacophore atom-based 3D quantitative structure–activity relationship (QSAR) model, activity cliffs, fingerprint, molecular docking, and MM-GBSA analysis. The best pharmacophoric hypothesis, AAHR.2, including two hydrogen bond acceptors (A), one hydrophobic (H), and one aromatic ring (R) provided a statistically significant 3D QSAR model, as shown by statistical parameters: $R^2 = 0.900$ (training set); $Q^2 = 0.774$ and Pearson's $R = 0.884$ (test set), stability $s = 0.736$. Crucial structural features such as hydrophobic and electron-withdrawing fields illustrated the relationships between molecular properties and inhibitory activity. ECFP4 analysis pointed out that the quinolin-2-one moiety plays an essential role for selectivity towards MAO-B with an area under curve (AUC) of 0.962. Significant potency disparities in the MAO-B chemical space were identified as two main activity cliffs. Key interactions of MAO-B inhibitors with essential residues such as TYR:435, TYR:326, CYS:172, and GLN:206 were consistently identified by a docking algorithm as responsible for MAO-B activity. The outcomes provided by molecular docking are consistent and adjunctive to pharmacophore 3D QSAR, ECFP4, and MM-GBSA methodology.

The computational outline drawn here may support biological chemists to model and forecast new potentially selective small-molecule inhibitors for MAO-B.

Acknowledgements. This work was supported by Project No. 1.2, from the "Coriolan Dragulescu" Institute of Chemistry Timisoara, Romania.

DEEP INSIGHTS INTO THE H_2, CO_2, AND CH_4 ADSORPTION ABILITY OF DISCARDED CIGARETTE BUTTS

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Discarded cigarette butts pose a significant waste disposal and environmental pollution hazard, primarily because they mainly contain cellulose acetate, which is non-biodegradable. In addition to contributing to litter, they also contain contaminants, such as toxic heavy metals, that can leach into waterways, potentially causing detrimental effects on living creatures. The survey scrutinizes the possibility of valorizing discarded smoked cigarette butts to create carbon nanostructures with high specific surface area in an effort to convert hazardous waste into high-value products. In general, porous carbons made from cigarette butts have a specific surface area of up to around 1600 m^2/g, a total pore volume of 0.82 cm^3/g, and a percentage of microporosity (2nm) up to 71%. These characteristics are achieved through pyrolysis and activation treatment by adjusting synthesis conditions. The ability of these materials to hold gas molecules only depends on their textural features, which were precisely and carefully assessed by nitrogen adsorption measurement utilizing an ASAP 2460 (Micromeritics Inc.). For precise and trustworthy gas adsorption measurements, the f-PcT handmade, optimized Sievert-type (volumetric) equipment was used to assess the adsorption properties of H_2, CO_2, and CH_4. Different gas adsorption isotherms showed that 5.2 and 1.03 Wt% of Hydrogen were adsorbed for the best sample at about 77K and 298K, respectively. Further, 13.9 and 14.4 Wt% of CH_4 and CO_2 were adsorbed by this sample. Before adsorption experiments, each sample was subjected to Helium (He) picnometry measurement to determine the value of the bone density [3]. To improve adsorbent-adsorbate interaction, the proposed synthesis technique aims to increase surface area and optimize pore diameter. Comparing the produced carbons to other porous materials based on carbon, they show an unusual potential to store hydrogen and methane.

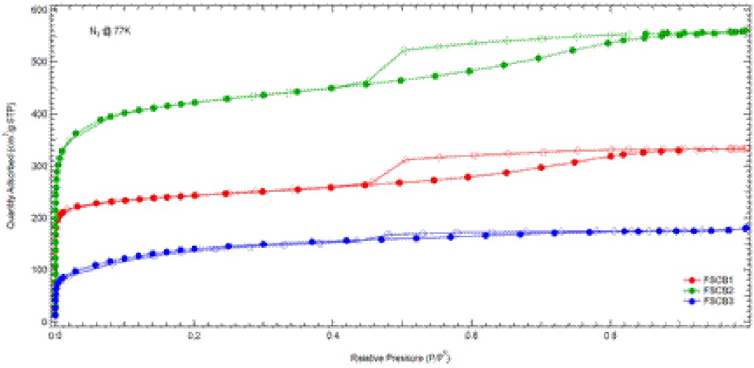

Figure: N_2 adsorption-desorption isotherms at 77K

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AGGREGATION INDUCED EMISSION FOR A HETERO POLYNUCLEAR COMPLEX IN DIFFERENT SOLVENTS

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Transition metal complexes have received increased attention due to their interesting photophysical and redox properties,[1] making them promising materials to be used as optoelectronic devices (e.g., optical storage and OLEDs) and biomedical tools. For this type of applications, the luminescent materials are used as solids and/or aggregates,[2] thus many advances in this area have been restricted by the issue of aggregation-caused quenching (ACQ), which usually turns off the emission of many luminophores in solid and aggregated state.[3] This phenomenon can be overcome by aggregation induced emission (AIE), thus enabling the systems to achieve significant solid-state emission.[4] The AIE effect can enhance the fluorescence quantum yields of aggregates with respect to the single molecules.[5]

On this background, we present the synthesis and characterization of a hetero-polynuclear penta-coordinated Zn(II) complex based on a ligand which contains two terpyridine moieties. As ancillary ligand a gallate derivative decorated with two long alkyl chains and one ferrocene moiety was used. The photophysical properties of the ligands and the complex were investigated in solvents of different polarities. To envisage the effect of hydrophilicity and hydrophobicity of the solvents on the self-assembly behavior, the photophysical properties of the Zn(II) complex have also been investigated in solvent/non-solvent systems.

Acknowledgements. This work was supported by a grant of the Romanian Ministry of Education and Research, CNCS - UEFISCDI, project number PN-III-P1-1.1-PD-2021-0427, within PNCDI III.

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ZR-BASED METAL-ORGANIC FRAMEWORKS AS DRUG DELIVERY SYSTEMS FOR THE ORAL ADMINISTRATION OF CAPTOPRIL AND IBUPROFEN

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Herein, we report the preparation of some Zr-MOFs materials using chemical and solvothermal methods and investigation as drug delivery systems. Their structure was investigated by FT-IR spectroscopy, TGA, SANS, PXRD and SEM methods. The materials showed two linkers deficiencies per Zr_6 formula unit presenting well-crystallized similar features specific for the UIO-66 type materials. The nitrogen porosimetry and SANS data reveal the presence of pores with average dimension of ~4 nm and the average sizes of the Zr-MOF nanocrystals are suggested to be around 30 nm. The obtaining materials were investigated as drug carriers envisaged for controlled drug release. Thus, Captopril and Ibuprofen loading and release experiments in different buffered solutions have been performed, resulting in enhanced drug loading capacity and good results in drug delivery. The cumulative percent of drug release in phosphate buffered solution was higher at pH 7.4 compared with pH 1.2. The release rate could be controlled by changing the pH of the releasing solution. A different Captopril release behaviour has been obtained when the experiments were performed using a permeable dialysis membrane.

AGGREGATION STUDIES ON A HETERO-BIMETALLIC COORDINATION COMPLEX

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Emissive materials in solid states are proposed to bring huge developments in the area of electro-optics or biomedicine.[1] Zn(II) complexes are widely studied examples of *d*^{10} luminescent coordination complexes. Due to the metal closed-shell nature, the general strategy to obtain luminescent Zn(II) coordination complexes is to use a luminescent ligand whose excited states should be stabilized after complexation implying a red shift of the spectrum. Moreover, the bulky coordination environment around the metal center blocks excimer formation when passing from solution to the condensed states that may quench the emission. Herein, we present the photophysical properties of a hetero-bimetallic penta-coordinated Zn(II) complex based on a terpyridine ligand and two monodentate gallate units decorated with several long alkyl chains and ferrocene moieties.[2] The molecular structure is presented in Figure 1a.

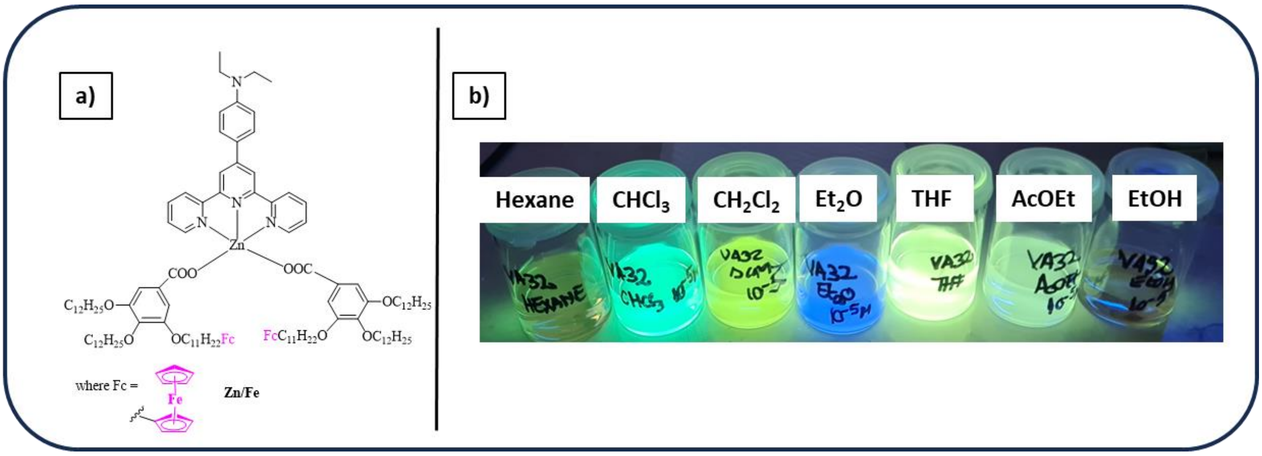

Figure 1. Molecular structure (a) and emission in solvents of varying polarities under UV lamp at 365 nm (b) of Zn(II) complex

Moreover, the photophysical properties in different solvents were investigated, the complex presenting aggregation properties as a function of the solvent polarity. (Figure 1b)

Acknowledgements. This work was supported by a grant of the Romanian Ministry of Education and Research, CNCS - UEFISCDI, project number PN-III-P4-ID-PCE-2020-1958, within PNCDI III.

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MERCAPTOPROPYL FUNCTIONALIZED MESOPOROUS SILICA AS CARRIERS FOR CLOTRIMAZOLE

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Mesoporous silica particles were synthesized by sol-gel method in order to be tested for their drug loading and release properties, starting from mixed silica precursors, tetraethoxysilane and mercaptopropyltriethoxysilane using the co-condensation method. The carriers demonstrated enhanced drug loading capacity of 99.87% and also showed good results in drug delivery. The cumulative percent of drug release in acidic buffered solution was 45.07% after 3 hours of release. The in vitro release data were applied to various kinetics models to predict the drug release mechanism and kinetics. A good coefficient of determination was obtained for Higuchi model. The drug release mechanism in acidic obeyed the Fickian diffusion mechanism. Considering the material characterisation N_2 adsorption-desorption isotherms were determined by N_2-physisorption measurements at 77 K for simple material as well for the material after functionalization with mercaptopropyl. After functionalization, the specific surface area decreases from 1213 m^2/g to 69.34 m^2/g and the pore diameter, from 3.54 to 2.4 nm but the total pore volume increases slightly from 0.8 to 1.05 cm^3.

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EU-OPENSCREEN DRIVE - ROMANIAN PARTNER ACTIVITIES AND A SHORT HISTORY OF EU-OPENSCREEN IN ROMANIA

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EU-OPENSCREEN is the European Research Infrastructure Consortium (ERIC) covering chemical biology research and early drug discovery activities such as assay adaptation, high-throughput screening, and structural optimization of the 'hit' compounds. Romania participated as a member in the preparatory and transition phase of the EU-OPENSCREEN project, whereas in operational phase was accepted as a candidate member for extension of membership by working with Ministry of Research, Innovation and Digitization in order to join the EU-PENSCREEN ERIC as specified in the project "Ensuring long-term sustainability of excellence in chemical biology within Europe and beyond", acronym EU-OEPNSCREEN DRIVE. Romanian partner activities consist in organization of annual workshops aimed at dissemination of project activities, mainly compound donation in European Academic Compound Library (EACL) and strengthening the interaction inside national chemical biology network RoChemBioNet. EU-OPENSCREEN was prioritized in two consecutive Romanian Infrastructure Roadmaps in 2017 and 2021. Following 2017 roadmap, "Coriolan Dragulescu" Institute of Chemistry received 9.1 mil euros funding through Competitiveness Operational Program for the implementation of the infrastructure project RO-OPENSCREEN.

EXPLORING THE CHEMICAL SPACE OF NATURAL COMPOUNDS FOR TYPE 2 DIABETES: PRELIMINARY *IN SILICO* STUDY

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Type 2 mellitus diabetes (T2MD) is a chronic disease which affects adults, young people, and even children. The reduced efficacy over time and various adverse effects (*e.g.* weight gain, hypoglycemia, fluid retention, and gastrointestinal symptoms) of the conventional agents used to treat T2MD, require the search for alternative therapies that overcome these limitations. In this light, gliptins (FDA approved drugs: sitagliptin, saxagliptin, vildagliptin, linagliptin, alogliptin, etc.) have become a research area of intense focus and a promising solution to fight T2MD. In the present study, a dataset of 406,747 unique natural compounds (NPs) from COCONUT database was screened against the gliptins (query molecules) to identify NPs as possible anti-diabetic candidates. Based on 1) the Tanimoto similarity coefficient (85%) which detected 90 similar NPs, and 2) the drug-likeness distribution probability (the RandomForest method) which detected 11 out of 90 NPs, we identified the top 4 candidates that obey the QED (Quantitative Estimate of Drug-likeness) and NPscore (Natural Product-Likeness Score) criteria and could potentially act as anti-diabetic candidates. Moreover, the results are supported by a good model performance with a classification accuracy (ACC) of 0.801, Area Under Curve (AUC) score of 0.870, sensitivity (SE) of 0.718, and specificity (SP) of 0.869. Overall, our findings are a promising starting point for other T2DM medication alternatives.

Acknowledgements. This work was supported by Project No. 1.2, from the "Coriolan Dragulescu" Institute of Chemistry Timisoara, Romania.

IDENTIFY NEW BIOLOGICAL ACTIVITIES OF YOUR COMPOUNDS (EU-OPENSCREEN ERIC)

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As the European Research Infrastructure for Chemical Biology and early Drug Discovery, EU-OPENSCREEN (*www.eu-openscreen.eu*) supports researchers with the aim to accelerate drug discovery efforts in an open-access setting through collaborations with international researchers from academia and industry.[1,2]

The consortium brings together 33 scientific partners from universities and public research institutions in 10 European countries. Under the coordination of the Institute of Chemistry Timisoara, Romania is progressing towards EU-OPENSCREEN full membership.

EU-OPENSCREEN offers to external researchers the possibility to screen at EU-OPENSCREEN partner sites our Academic Compound Library submitted by chemist. This offers the possibility to the submitters, to expose their compounds to a variety of biological targets. The submitted compounds are tested in suitable bioassays, which are developed by the biology community in EU-OPENSCREEN screening campaigns. Once a compound has been identified as an active hit compound, a research collaboration between the chemist (who submitted the compound) and the biologist (who developed the bioassay) can be initiated.

In EU-OPENSCREEN, we have collected over 5,000 compounds from chemists around the world, which will now be screened for novel bioactivities and characterised in a panel of bioprofiling assays (https://www.eu-openscreen.eu/services/bioprofiling-assays.html). The primary screening data will be made available to the scientific community in EUOPENSCREEN's open-access European Chemical Biology Database (www.ecbd.eu).

Here we will present how academic compounds including those received from the Polytechnic University of Timisoara are made accessible through EU-OPENSCREEN and explain the procedure and benefits for chemists that submit their compounds to uncover the hidden bioactivities of their compounds.

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ANTIOXIDANT ACTIVITY AND HALOCHROMIC BEHAVIOR OF NEW SYNTHETIC BENZOPYRYLIUM DERIVATIVES

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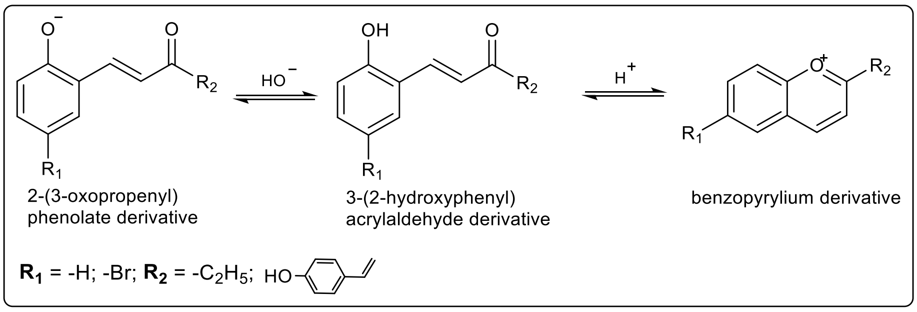
In the last years, benzopyrylium salts were reported as important and unexplored class of compounds with potential applications as therapeutical agents [1]. Moreover, the compounds containing benzopyrylium subunits showed halochromic behavior capable of existing in more than two forms when subjected to different pH values indicating their importance in dye applications and optical pH sensors [2-4].

As a continuous work of our research group in the frame of halochromic systems, new benzopyrylium derivatives were synthesized by introducing alkyl, bromo and vinylphenol substituents to understand their effect on the antioxidant activity and halochromic properties. The compounds were characterized for confirmation of the structure via FT-IR and NMR spectroscopy. The equilibrium between the multistate of the different chemical species considering the changes in color due to the pH shift has been studied. This ability can be attributed to the various species involved in the interconversion of the compound in acidic or basic conditions (Scheme 1). Antioxidant studies indicated a good free radical scavenging properties of studied compounds by DPPH method.



Scheme 1. Proposed network of chemical reactions

Acknoledgements. This work was supported by Project 4.1.1 of the "Coriolan Drăgulescu" Institute of Chemistry.

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ICT - INTERDISCIPLINARY CENTER FOR SMART SPECIALIZATION IN CHEMICAL BIOLOGY, RO-OPENSCREEN

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General information

- *Beneficiary*: "Coriolan Dragulescu" Institute of Chemistry - ICT, Timișoara
- Project co-financed by European Regional Development Fund under the Competitiveness Operational Program 2014-2020
- *Priority Axis 1* – Research, Technological Development and Innovation to Support Economic Competitiveness and Business Development
- *Investment priority 1a* – Improving research and innovation infrastructures and capacities to develop excellence in RDI and promoting centers of expertise, especially those of European interest
- *Action 1.1.1.* Large research and development infrastructures
- *Period*: 20.07.2020 – 31.12.2023
- *MySMIS Code*: 127952
- *Investment Value*: 42,587,899.61 RON

General objective

The aim of the **RO-OPENSCREEN** project implemented by "Coriolan Dragulescu" Institute of Chemistry is to create an *Interdisciplinary Center for Smart Specialization in Chemical Biology, RO-OPENSCREEN* with high-level academic research, addressed to the Romanian and European scientific community. The Center will carry out integrative research by applying advanced technologies of automated management of compound libraries, chemical synthesis, structural analysis, determination of biological activities and chemoinformatics.

Description of the investment

The implementation of the project consists of two main components:

I. Modernization/consolidation of two of our own buildings under conservation, namely C20-Materials warehouse and C21- Laboratory. These two buildings considered for development of the new ICT interdisciplinary research center are located in Timișoara, 22 Cornelia Salceanu Street. The modernization/consolidation works include: design and technical assistance, obtaining approvals and authorizations and the actual works: site organization and modernization/consolidation works of the two buildings.

II. The provision of research tools and equipment for three laboratories with specific interdisciplinary biological chemistry, united in the new ICT research center, will ensure the functionality of the following laboratories: (*i*) - Chemoinformatics laboratory; (*ii*) - Chemical bookstore laboratory; (*iii*) - Chemical synthesis, characterization and analysis laboratories. The thermal power plant, reagent transfer station, IT and communication systems are located in the C20-Materials warehouse.

The laboratoratories will be set up with high-performance equipment including automated imagining and multimode microplate reader, automated liquid handling and acoustic transfer of nanovolumes platforms, SAXS/WAXS diffractometer with GISAXS module, polarized and fluorescence optical microscope with hot stage, benchtop NMR spectrometer, ultra-performance liquid chromatography–high-resolution mass spectrometry, thermogravimetric analysis/ FTIR-Raman, circular dichroism coupled with chiral liquid chromatography, high-performance computing and communication system, etc., will place the Center within a rich national and European scientific networks.

The new Center will offer an integrated research infrastructure, unique in Romania, that allows extensive physico-chemical investigations and complete analytical services on the structure of chemical compounds following approved European procedures. Moreover, the center's interdisciplinary research infrastructure developed by combining chemical screening and *in vitro* bioassays will accelerate the process of discovering new compounds with biological activity. These compounds will form the *National Library of Biological Activity Compounds (LNCB).*

Description and valorization of the results

The research infrastructure provided by the project will facilitate the collection and quality management of LNCB's chemical compounds. This library will be connected with the EU-OPENSCREEN's compounds collection through the RoChemBioNet national network. High-capacity, systematic and automatic biological screening workflow of chemical compounds in LNCB, will be implemented. The LNCB will enable the scientific community to explore chemical space with the goal of developing new molecular structures transferable to the clinic and the drug industry.

The complex and high-performance equipment, mandatory to organize an integrated system of research laboratories dedicated to synthesis, structural characterization and primary biological evaluation, will facilitate the increase of ICT competitiveness and attractiveness for new cooperation initiatives at national, regional and European levels. Moreover, the infrastructure will afford to continue the current topic research to a superior level and allow new research directions by developing complex drug discovery projects, agricultural agents, cosmetics, etc.

The training programs through the project implementation will provide a framework to develop strengths, encourage innovation and will boost adherence to high research standards of human resource.

Overall, it is RO-OPENSCREEN's focus on a high-quality compound library and modern research infrastructure that strengthens our attractiveness as a location that facilitates the research scientific community with knowledge exchanges, access to perform tests, determinations and analysis on state-of-the-art equipment and exploring the chemical space through a unique compound collection.

ICT - Interdisciplinary Center for Smart
Specialization in the Field of Chemical Biology,
RO-OPENSCREEN

ENZYMATIC ROUTE FOR SYNTHESIS OF ESTOLIDES FROM NATURAL HYDROXY FATTY ACIDS

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Hydroxy-fatty acids synthesis has been intensively studied in the recent years due to their potentials applications in different fields including cosmetics, food industry, inks. Their corresponding polyesters known as estolides have been detected in plants and secretions from the granular hairs of the capillary and their applicability has already been proved. Estolides are branched polyester derived from oils and fats and are mainly industrially produced by energy intensive chemocatalytic processes that usually occur at T>200°C. In our previous studies we demonstrated that enzymatic synthesis is a viable alternative for the synthesis of various saturated estolides [1]. Their properties such as high viscosity, good oxidative stabilities place them as promising candidates for applications in cosmetic ingredients or as biodegradable lubricants [2]. Enzymatic synthesis by using lipases of these compounds could represent overcome to the high temperature and metal catalyst used by chemical route. Up to now there are a few reports about the enzymatic synthesis of these polyesters completed with a detailed characterization of the product [2].

In this work the synthesis of ricinoleic acid based estolide by using lipases from different sources sources have been screened as biocatalyst at temperatures up to 75ºC. The substrate conversions were calculated based on GC-MS analysis and the reaction products mono-, di-, poli-estolides, or different size macrolactones have been characterized by MALDI-TOF MS, NMR, TG and DSC techniques.

Acknoledgements. This work was supported by Politehnica University Timisoara, Romania, through the program "Supporting research activity by financing an internal grant competition – SACER 2023", Competition 2022, Contract no. 31/03.01.2023.

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SUPRAMOLECULAR SYSTEMS OF 2-CHLORO-5-NITROBENZOIC ACID WITH ANTIBACTERIAL ACTIVITY

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Human infections caused by Gram+ or Gram- bacteria are a public health problem, causing severe health problems and an economic burden on the healthcare system. Therefore, finding new compounds with antibacterial effects, either as standalone treatments or combined with existing antibiotics, has become a constant focus in scientific research. Herein, an alkanolammonium salt (HMMEA)(2Cl5NB) and a 2D coordination polymer $[K(2Cl5NB)(H_2O)]_n$ (MMEA - methylethanolamine; 2Cl5NBH - 2-chloro-5-nitrobenzoic acid) has been synthesized and characterized by single crystal X-ray diffraction and IR spectroscopy and then compared with 2Cl5NBH. Both compounds generate supramolecular systems assembled by hydrogen bonds and π-π stacking interactions in the organic salt, and weak H-bonds in the coordination polymer. Their antibacterial activities were screened against Gram+ (*Staphylococcus aureus, S. aureus MRSA)* and Gram- bacteria (*Salmonella typhimurium, Escherichia coli*) as standardized strains and strains isolated from hospitalized patients. The minimum inhibitory concentration, bacterial cell viability and inhibition rate of biofilm formation were determined. The results revealed that the new compounds exhibited a bacteriolytic or bacteriostatic effect depending on the tested concentration and the bacterial strain under study, with the highest sensitivity recorded in Gram+ bacteria compared to Gram- ones. The decrease in the concentration of the tested compounds leads to a decrease in the antibacterial effect.

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