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Book of abstracts

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Note: IC - Invited Conference
PC - Plenary Conference
OC - Oral Communication
P_I/P_{II} – poster session I/poster session II

IC-02. The Green Frontier: Cellulose Nanofibers Driving the Future of Bioelectronics

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The accelerating advancement of bioelectronics is transforming how technology integrates with living systems. Conventional electronic components often derived from rigid plastics or metallic conductors, fall short of these expectations, particularly when it comes to biocompatibility and ecological impact. This shortfall has spurred growing interest in renewable, bio-based materials, with cellulose nanofibers (CNFs) standing out as a leading candidate. These CNFs display exceptional tensile strength, large specific surface area, tunable surface chemistry, and optical clarity, making them versatile building blocks for a new generation of bioelectronic platforms. Beyond their mechanical robustness and green credentials, CNFs possess characteristics particularly suited for bioelectronics interface: their hydrophilic and porous structure fosters intimate contact with tissues, cells, and ionic media, ensuring stable signal transmission. Additionally, their surfaces can be chemically tailored or hybridized with conductive polymers, metallic nanoparticles, or carbon nanomaterials to impart electrical conductivity without sacrificing biocompatibility. Recent developments in flexible sensors, degradable electrodes, and ion-conducting membranes have demonstrated the remarkable potential of CNF-based materials in sustainable electronics. The emergence of CNFs marks a transformative convergence of biology and technology, turning a ubiquitous natural resource into a platform for advanced electronic functionality. This presentation explores our current achievements, remaining challenges, and future perspectives of cellulose nanofibers in bioelectronics, emphasizing their role in shaping a more sustainable technological future [1-2].

Acknowledgements

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IC-03. Plants bioactive compounds - sustainable solutions?Dinica Rodica Mihaela^{1*}

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Plants and phytochemical compounds constituted the human pharmacopoeia for thousands and thousands of years, until the first organic synthesis took place and the subsequent synthesis of other organic compounds existing in nature, for example aspirin, opened a new era dominated by the pharmaceutical industry. Organic compounds in plants are considered secondary metabolites, non-essential for the survival of plants, but they have an important role for them in signaling, protection or in attracting pollinators. Organic compounds found in plants are also significant for humans, their beneficial effects such as antioxidant, anti-inflammatory or antimicrobial being known and exploited.

This study presents the challenges encountered and the results obtained in the isolation of bioactive compounds from complex natural matrices. The importance of "green" extraction techniques such as microwave-assisted extraction or ultrasound and the use of cutting-edge techniques - such as chromatography and advanced spectroscopy (IR, NMR, MS), which are used to overcome these challenges and to accelerate the discovery and validation of these compounds are also highlighted. The possible therapeutic applications of bioactive compounds have been detailed through various biological studies such as antioxidant, anti-inflammatory, antimicrobial or antitumor. The obtained results can contribute to a better knowledge and understanding of the isolation and characterization of phytochemical compounds with importance in human health, to prevent or to treat various diseases but also for the development of new functional foods or for the practice of sustainable agriculture.

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IC-04. Exploring novel bonding motifs at the bottom of the periodic tableDumitru-Claudiu Sergentu^{1,2}¹"Alexandru Ioan Cuza" University of Iasi, Faculty of Chemistry, 700506 Iasi, Romania²"Alexandru Ioan Cuza" University of Iasi, ICI-RECENT AIR, 700506 Iasi, Romania*Correspondence to dumitru.sergentu@chem.uaic.ro

From Robert Boyle's 1661 departure of chemistry from alchemy in *The Sceptical Chymist*, to Gilbert N. Lewis's 1916 conceptualization of electron pairs in *The Atom and the Molecule*, to Robert Mulliken's 1928–1932 development of molecular orbital theory, and Linus Pauling's 1939 unification of chemical bonding principles in *The Nature of the Chemical Bond*, chemists have continuously sought to understand how atoms bind in molecules and materials. Yet, even today, chemical bonding defies simple description: from the debated quadruple bond in C₂, to the utterly complicated sextuple bonding in Cr₂, to the perplexing quintuple bonding in U₂ [1], and extending all the way to unconventional energy-degeneracy covalent bonding in actinide complexes [2], a unified theoretical framework remains elusive and the scientific community is actively calling for the need to rethink conventional bonding paradigms.

This talk explores new bonding motifs at the bottom of the periodic table and highlights research I have contributed over the past decade. I will present notable examples, potentially including novel bonds with curium and berkelium [3-4], the (non-)emergence of 5f- ϕ bonding in the sandwich complex thorocene [5], why energy-degeneracy covalency is not a sound theory to describe bonding in actinyl(VI) oxides and actinide(IV) hexachlorides [6-7], how cerium bonds to an aryl carbon [8], how cerium defies the concept of formal oxidation state, and how unusual bonds can be locked inside fullerene cages, remaining inaccessible otherwise.

Acknowledgements: DCS acknowledge support offered by the ICI-RECENT AIR research infrastructure.

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PC-01. Dual-functional photocatalysts for sustainable solar light-driven clean energy generation

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The growing demand for clean and renewable energy sources has highlighted the urgent need for efficient technologies capable of harnessing solar energy to drive sustainable solutions [1]. Considering the sustainability of solar energy, photocatalysis is a major advance for sustainable, nontoxic and economically viable technologies. As it makes use of sunlight, solar photocatalysis technology is inexpensive, environmentally friendly and universally applicable [2]. Nevertheless, dual-functional photocatalysis for O₂/H₂ evolution coupled with the oxidation/reduction of organic molecules in a single step is a relatively new field that has attracted radically increasing research interest over the past few years [3,4]. Currently, there are very few examples of dual-purpose photocatalytic systems in the literature that exhibit high apparent quantum yield (AQY) and O₂/H₂ evolution rates [5]. The desired characteristics of a dual-purpose photocatalytic system include those applied in general photocatalysis, comprising low cost, enhanced light absorbance in the visible region, prolonged excited-state lifetime, and high electron-hole separation efficiency [5]. To bring this field a step closer to real-world applications, future research endeavors should be directed toward the generation of abundant, chemically stable, and visible-light-responsive materials that can efficiently harvest solar irradiation. The aim of the present work is to explore the development of dual-functional photocatalysts aimed at addressing both energy production and environmental sustainability in the context of renewable energy technologies.

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PC-02. Controlled Electrodeposition of Ferromagnetic Nanomaterials for Multifunctional Applications

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The electrodeposition method allows the fabrication of ferromagnetic nanomaterials with precisely controlled magnetic, structural, and surface properties, supporting a wide range of applications, from biomedicine to catalysis. In this work, Ni, Co, NiFe, CoFe, CoPt, simple, multilayered, and/or core@shell nanomaterials were synthesized and tested for cancer detection and therapy, nanowarming, as well for catalysis. Optimization of electrodeposition parameters, including electrolyte composition, applied potential, pH, and the organic additives addition, allowed fine control over nanomaterials morphology, composition, and crystalline structure. Gold-coated CoFe nanomaterials (CoFe@Au) demonstrated excellent biocompatibility and theranostic properties. They acted as effective T₂ MRI contrast agents ($r_2 = 10.64$, $r_2/r_1 = 28$) while inducing up to 80% cell death in osteosarcoma cultures under alternating magnetic fields via magneto-mechanical actuation. Magnetic multilayered Au/Co₃₅Fe₆₅/Au nanomaterials were evaluated for magnetic heating and nanowarming applications. PEG-coated, Au-tipped nanomaterials achieved specific absorption rates (SAR) up to 2010 W g⁻¹ when aligned with an alternating magnetic field (20 kA*m⁻¹@190 kHz). When dispersed in vitrified VS55 cryoprotectant, they provided nanowarming rates up to 1000 °C*min⁻¹ (value 20 times higher than the critical warming rate), while maintaining minimal cytotoxicity in human fibroblasts. The shape, composition, and crystalline structure of CoPt nanoparticle were tuned by controlling the electrodeposition parameters. The as-prepared nanoparticles manifest enhanced methanol oxidation activity up to 85 mA cm⁻² at low Pt content. These results demonstrate that the electrodeposited ferromagnetic nanowires are highly versatile by combining tailored shape, magnetic and structural properties for applications crossing cancer therapy, MRI, cryopreservation, and electrocatalysis.

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**OC-01. DOEBNER REACTION PATHWAYS: WHERE CHEMISTRY
CRAFTS NEW COMPOUNDS**

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The Doebner reaction is a well-established synthetic route for producing substituted cinnamic acids through the condensation of aryl aldehydes with pyruvic acid under basic conditions. As a variant of the Knoevenagel condensation, it yields α,β -unsaturated carboxylic acids via carbon-carbon bond formation followed by decarboxylation. Owing to its efficiency in constructing conjugated systems, the reaction is widely utilized in the synthesis of bioactive and functionally substituted aromatic compounds. Incorporating amines into the reaction expands its scope, as imine formation can lead to alternative reaction pathways, including the formation of heterocycles such as carboxyquinolines, methylcarboxyquinolines, and pyrrol-2-one derivatives [1]. These products typically arise through intramolecular cyclization or *via* enamine intermediates. The reaction outcome is strongly influenced by the nature of the starting materials—particularly the type of amine (primary or secondary) and the electronic properties of the aldehyde [2].

The present study aims to explore new pathways and reaction conditions within the Doebner framework to generate novel compounds and enhance our understanding of its potential for complex heterocyclic synthesis. We optimized the reaction using various aniline derivatives and examined the influence of different aldehydic components, as well as the order of reagent addition, to better elucidate the underlying mechanism. Additionally, a closer investigation of a specific reaction pathway is currently underway and remains a central focus of our ongoing research.

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OC-02. Chemistry of lanthanide silicates for environmental barrier coating applications

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The development of new or improved materials is the basis for achieving a sustainable future and environmental durability. In order to achieve this, we look into lanthanide silicates as candidates for environmental barrier coating (EBC) for high temperature (exceeding 1400 °C) applications such as turbine engines¹, hypersonic vehicles, and energy systems [1,2].

The lanthanide silicates have a series of properties which are well suited to cover the role of EBC such as their thermal stability, low thermal conductivity, resistance to Calcium-Magnesium-Alumino-Silicate (CMAS) infiltration and water vapor corrosion. These properties not only extend the operational life of ceramic components but also reduce fuel consumption and emissions by enabling higher engine efficiencies.

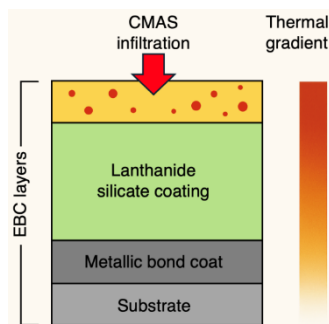


Figure 1. Section of the layers involved in lanthanide silicates as environmental barrier coating

This work focuses on the synthesis and optimization of the synthesis parameters, as well as structural studies, but also structural studies tested at high temperature for long periods of time. The results obtained were validated using different simulation methods.

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OC-03. Impact of SO₂ Replacement on Wine Quality: A Comparative Study of Traditional and Sulphite-Free Techniques

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Abstract

This study conducted a comparative evaluation of Fetească regală, Fetească regală frizzante, Cabernet Sauvignon, and Cabernet Sauvignon rosé wines, focusing on the technological and biochemical effects of sulphur dioxide (SO₂) substitution. Parallel vinifications under conventional and SO₂-free conditions were performed; the SO₂-free approach employed *Pichia kluyveri* inoculation and certified oenological antioxidant products. These alternatives maintained oxidative stability comparable to SO₂ [1-2]. Physico-chemical analyses confirmed stable fermentation and technological feasibility.

A metabolomic approach explored correlations between amino acids and biogenic amines under malolactic fermentation [2]. LC-MS/MS analyses revealed moderately higher biogenic amine levels in SO₂-free wines ($p < 0.05$). Anthocyanin content was assessed by HPLC, confirming their role in color retention and antioxidant potential [3]. Antioxidant kinetics were modelled via multi-order reaction curves with equilibrium phases estimated using a linear plateau response model. Color evolution was objectively quantified using a CIELab-based distance algorithm. GC-FID/MS analysis showed no significant differences ($p > 0.05$) in major volatile esters between treatments.

Overall, SO₂-free wines maintained comparable anthocyanin stability, color integrity, and aromatic balance. Phenolic compounds, especially tannins and flavonoids, contributed more to antioxidant protection than SO₂. SO₂ efficiently limited acetaldehyde accumulation without negatively affecting the volatile fraction [1-3].

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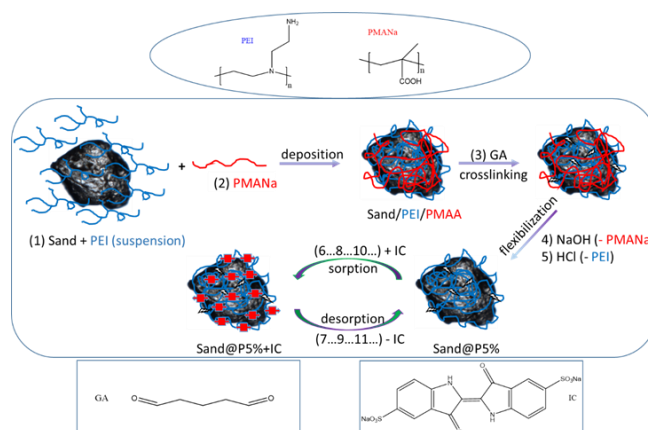
OC-04. Sand and Polyelectrolytes: A "hard/soft" combination for water cleaning

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The deposition of polyelectrolytes onto the surface of sand particles represents an interesting approach to obtain "hard/soft" composites with a high number of functional groups which can be used in pollutants removal from contaminated surface waters [1-3]. Herein, several polyelectrolytes [poly(ethyleneimine) (PEI), poly(acrylic acid) (PAA) and poly(sodium methacrylate) (PMANa)] were deposited through a non-stoichiometric interpolyelectrolyte precipitation method onto sand fractions of different sizes, followed by the cross-linking of polycation chains with glutaraldehyde (GA) (Scheme 1) [3].



Scheme 1. Fabrication of the "hard/soft" composites, subsequently used in Indigo Carmine (IC) multiple sorption/desorption cycles [3].

The sorbed amount of pollutants, for example the IC dye, in multiple column experiments, depended on the amount of organic material deposited on the sand particles. These composites, environmentally friendly, could be very promising sorbents in water treatment.

Acknowledgements

This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS-UEFISCDI, project number PN-IV-P1-PCE-2023-1545, within PNCDI IV.

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OC-05. Synthetic approach to a heterocyclic Schiff base as a precursor to Cu(II) complexes with potential anticancer activity

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Schiff bases are organic compounds containing an imine group ($-\text{CH}=\text{N}-$), formed by the condensation of amines with aldehydes or ketones. Their coordination through donor atoms (N, O, S) gives them structural versatility and valuable pharmacological potential. Heterocyclic variants with nitrogen-rich scaffolds, such as indole and benzimidazole, exhibit multiple biological activities: anticancer, antimicrobial, antioxidant, anti-inflammatory, and antiproliferative. Coordination with transition metals, particularly Cu(II), amplifies these effects [1,2].

Here, most of the steps in the development of a synthetic pathway toward a methoxy-substituted indolobenzazocine structure, designed as a precursor for Schiff base formation with 2-pyridinecarboxaldehyde, and subsequent coordination to Cu(II), are presented. The synthetic sequence was initiated from 4-methoxy-1H-indole-2-carboxylic acid and involved esterification, ethoxymethyl (EOM) protection, basic hydrolysis, amide coupling with 2-iodophenylethanamine (EDCI·HCl/DMAP), and subsequent Boc protection. An intramolecular Pd(II)-catalyzed Heck reaction ($\text{Pd}(\text{OAc})_2/\text{Ag}_2\text{CO}_3/\text{PPh}_3$) led to the formation of the tetracyclic indolobenzazocine core. This was followed by acidic deprotection and a thionation step to obtain the thiolactam intermediate. Two additional synthetic steps remain to complete the formation of the final metal complex. Preliminary molecular modeling suggested that methoxy substitution may enhance the biological profile of these derivatives.

The developed synthetic strategy provides access to a novel methoxy-substituted indolobenzazocine framework, offering a versatile precursor for Schiff base formation and subsequent Cu(II) coordination. This work establishes a foundation for the future exploration of their coordination chemistry and biological potential.

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OC-06. Antimicrobial coatings based on polysulfone for medical devices

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Polysulfones are part of a class of high-performance thermoplastic polymers with remarkable properties. They are distinguished by excellent thermal stability - essential for sterilization, outstanding chemical stability - ensuring the durability of the material in the presence of biological fluids or disinfectant solutions, superior mechanical strength and intrinsic biocompatibility. Due to these exceptional characteristics, polysulfones are frequently used in various fields of biomedical engineering [1]. Chemical modification of the polysulfone structure with quaternary ammonium salts provides it with antibacterial activity, hemocompatibility and hydrophilicity, improving the performance of this polymer in the biomedical field [2].

The aim of the present study was to chemically modify the structure of the polysulfone *via* quaternization reaction and to prepare coatings with superior antibacterial and antifungal properties by encapsulating norfloxacin, an antibiotic, and amphotericin B, an antifungal drug within the polymeric matrix. The rational design of this approach employed a multi-level strategy, namely: **(1)** the synergistic relationship between the antibiotic and the antifungal drug; **(2)** the occurrence of strong electrostatic interactions between the polymer and the antimicrobial agents in order to facilitate a sustained-release kinetic profile; **(3)** the complementary bioactivities of the incorporated drugs and **(4)** the intrinsic antimicrobial activity of the quaternized polysulfone.

The obtained coatings were structurally and supramolecularly characterized by FTIR spectroscopy and X-ray diffraction and polarized optical microscopy (POM), respectively. Their properties, such as wettability, antioxidant activity and antimicrobial efficiency, were also investigated, and the results revealed moderate hydrophilicity (70–90°), a DPPH radical scavenging capacity of up to 67.49% and a strong antimicrobial activity against *S. aureus*, *E. coli* and *C. albicans* microorganisms.

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OC-07. From Waste to Worth: Exploring Aroma Compounds in Grape Pomace for Sustainable Extraction Applications

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Grape pomace, the principal by-product of winemaking, represents a valuable yet underexploited source of aroma compounds with potential applications in the food, cosmetic, and fragrance industries. This review explores the composition, transformation, and recovery of these compounds, emphasizing the influence of grape variety, viticultural practices, and winemaking techniques on their concentration and sensory expression. The main volatile classes identified in grape pomace include terpenes, norisoprenoids, thiols, and esters, all contributing to its aromatic complexity. Winemaking parameters such as maceration time, fermentation temperature, yeast strain, and vineyard management practices significantly affect aroma profiles. For instance, leaf removal reduces thiols while increasing terpenes, and fermentation at lower temperatures enhances ester formation and floral notes. The introduction of non-Saccharomyces yeast strains has further expanded aromatic diversity, offering new possibilities for valorizing winemaking by-products [1].

Long-term maceration, especially in white winemaking, has emerged as a promising technique for producing pomace rich in distinctive aroma compounds [2]. Distillation and related extraction processes efficiently concentrate volatile compounds, enabling their use as natural flavoring agents or additives. Beyond sensory enhancement, many aroma compounds exhibit biological activities that improve product stability, sustainability, and health-related qualities [3]. Valorizing grape pomace through aroma recovery aligns with circular economy principles, transforming waste into a renewable source of high-value materials. Continued research on aroma formation, transformation, and extraction mechanisms will be essential to optimize recovery efficiency and broaden industrial applications, supporting both environmental responsibility and sensory innovation within the wine sector.

Acknowledgements

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OC-08. Synthesis of functionalized polyphenols with azaheterocycle skeleton

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Polyphenols are secondary metabolites widespread in the entire kingdom of plants, with excellent ability to protect against oxidative stress by removing free radicals, chelation of transition metals, and also inhibit various enzymes, that generate free radicals. Polyphenols have antioxidant, anti-inflammatory, anticancer and antibacterial activities and the ability to prevent degenerative diseases. They have extensive applications in food, beauty products, dietary supplements, medicine, the fields of household chemical products, agriculture and functional polymer materials [1, 2]. Our study presents a new ecologically friendly method of synthesis in the solid phase, of some polyphenolic derivatives, by protecting hydroxyl functionality. The ¹H- and ¹³C-NMR spectra as well as the single crystal X-ray diffraction studies proved unambiguously the structure of the compounds: two polymorphous of diacylated 3',4'-diacetoxy-acetophenone and a monoacylated 3',4'-diacetoxy-acetophenone [3].

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OC-09. Photocatalytic approach for ibuprofen advanced removal from aqueous solution in the presence of Zn-Co-Al-Fe layered double hydroxides derivatives

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The increased popularity of ibuprofen drug and the diversity of administration forms (oral, patches, intravenous, suppositories) led to its detection in water and accumulation trend in the environment [1]. Therefore, strategies to perform its advanced removal from wastewaters are developed. The photocatalytic reactions performed in the presence of visible light are efficient, green, and affordable costs solution in this respect.

In our work, a series of Zn, Co, Al and Fe layered double hydroxides (LDH) obtained by coprecipitation in aqueous solutions by using NaOH agent were used as photocatalysts or photocatalyst precursors for the advanced oxidation of ibuprofen by photocatalysis, under visible light irradiation [2, 3].

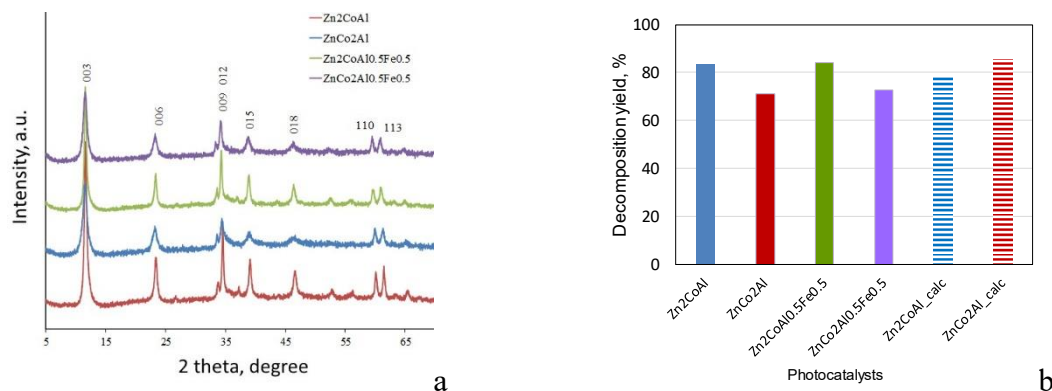


Figure 1. a. XRD patterns of the photocatalytic solids; **b.** decomposition yields after 360 minutes exposure under visible light irradiation

The synthesized LDH as well as the calcined forms were characterized by XRD, FT-IR spectroscopy, UV-DR spectroscopy, nitrogen adsorption at 77 K and thermal analysis, to confirm their crystalline structure, surface functional groups, porosity and thermal stabilities. The ibuprofen decomposition was monitored by UV-Vis spectroscopy.

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PI-1. Indigenous microflora as starter cultures during red wines production

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Fermentative yeasts are used industrially in the production of wine, having as their main characteristic the ability to assist the fermentation of simple carbohydrates in anaerobiosis, with the formation of ethyl alcohol and carbon dioxide. The purpose of the research consisted of applying microbiological methods and techniques to observe, isolate, and identify microorganisms in the examined products to establish the presence or absence of harmful microorganisms, especially the determination of the indigenous microflora.

The study evaluates the microflora of Cabernet Sauvignon and Merlot grapes from Javgur, Cimişlia district, during in the technological stages and aging of the wines. In the dynamics, a series of analyses on grapes, must and wine such as physico-chemical indices, microbiological testes and antioxidant capacity were performed.

Table 1. Physical-chemical indices of produced experimental wines

No.	Physical-chemical indices	Red dry wine Cabernet-Sauvignon	Red dry wine Merlot
1	Concentration of alcohol, % vol	12.63 ± 0.1	13.45 ± 0.1
2	Mass concentration of sugars, g/L	3.4 ± 0.1	4.5 ± 0.1
3	Mass concentration of titratable acids, g/L	7.7 ± 0.1	7.6 ± 0.1
4	Mass concentration of volatile acids, g/L	0.75 ± 0.05	0.68 ± 0.05
5	pH	3.65 ± 0.01	3.37 ± 0.01
6	Organoleptic quality, points	7.80 ± 0.05	7.85 ± 0.05

According to experimental results (table 1) the mass concentration of titratable acids in the wines obtained under micro winery conditions changed insignificantly, and the variation of the pH index values in the samples of dry wines obtained by spontaneous fermentation is within a limited range and constitutes 3.65 for Cabernet Sauvignon and 3.37 for Merlot.

The mass concentration of volatile acidity varies in both obtained wines (0.68–0.75 g/L), which can be attributed to differences in enzymatic activity and latent fermentation conditions. These results could be explained by the early development of *Kloeckera apiculata* during spontaneous fermentation, which is accompanied by an increase in volatile acidity and ethyl acetate content. Thus, especially due to the early and significant development of *Kloeckera apiculata*, spontaneous fermentation is accompanied by an increase in volatile acidity compared to induced fermentation.

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PI-2. Spectroscopic Characterization of Biomass Burning Composition: UV-VIS Investigations of Nitroaromatic Compounds

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Nitroaromatic compounds (NACs) are significant light absorption constituents found in atmospheric brown carbon (BrC). NACs from anthropogenic activities represent a major source of atmospheric pollution in urban areas. They can affect the Earth's climate, air quality, human health and can represent a major environmental hazard [1].

NACs in the atmosphere can result from biomass burning, released from waste water surface or might be formed from the oxidation of aromatic volatile organic compounds (VOCs) such as benzene, toluene and xylenes [2]. BrC is organic carbon found in aerosols which particularly can absorb light. The BrC can be found in the cloud condensation nuclei and the tropospheric particles and includes NACs as constituents, nitrophenols (NPs), nitroguaiacols (NGs) and nitrocatechols (NCs) [3].

The main objective of this study was to investigate NACs found in the atmosphere as precursors of BrC from anthropogenic sources such as biomass burning. Experimental studies were performed using a double-beam Jenway 6850 spectrophotometer (200-500 nm range, 0.1 nm resolution, at 0.1 s) using 10 mm quartz cuvettes. Three series of NACs with various functional groups were investigated for their UV properties. Differences in UV-VIS absorption spectra were evaluated based on functional groups attached to the aromatic ring and solvent polarity, with bathochromic and hypsochromic shifts of the absorption maxima. Also, Mass Absorption Coefficient (MAC) and Absorption Angström Exponent (AAE) were determined for a series of NACs that can act as precursors to BrC formation.

Acknowledgements

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PI-3. Functionalization of sodium alginate via Ugi multicomponent reaction and the self-associative behavior of the obtained derivative

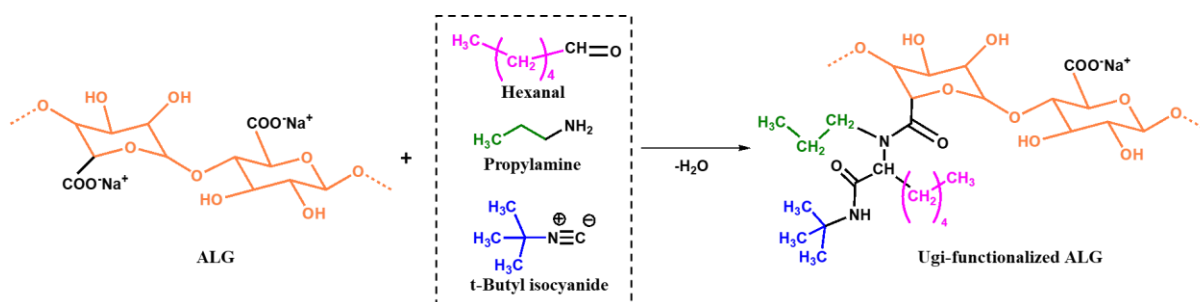
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Multicomponent reactions (MCRs) are chemical processes in which three, four, or more reactants combine in a single step to form a product with a complex molecular structure [1]. A notable example is the Ugi reaction, a four-component MCR that involves the condensation of an amine, a carbonyl compound (either an aldehyde or a ketone), a carboxylic acid, and an isocyanide. The final product is an α -acetamido carboxamide [2].

In this study, sodium alginate (ALG) was functionalized via the Ugi-MCR, employing propylamine, hexanal, and t-butyl isocyanide (**Scheme 1**).



Scheme 1. Functionalization of ALG via Ugi-MCR with hexanal, n-propylamine and tert-butyl isocyanide.

The successful functionalization of ALG was confirmed by ¹H NMR and FTIR spectroscopies. The degree of substitution—the percentage of carboxyl groups modified—was approximately 40% as determined by ¹H NMR, conductometry, and polyelectrolyte titration. The functionalized derivative exhibited self-associative behavior, forming micellar structures having a hydrodynamic diameter of about 320 nm.

Acknowledgements

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PI-4. Synthesis of pyrroloquinoline derivatives by conventional and unconventional methods

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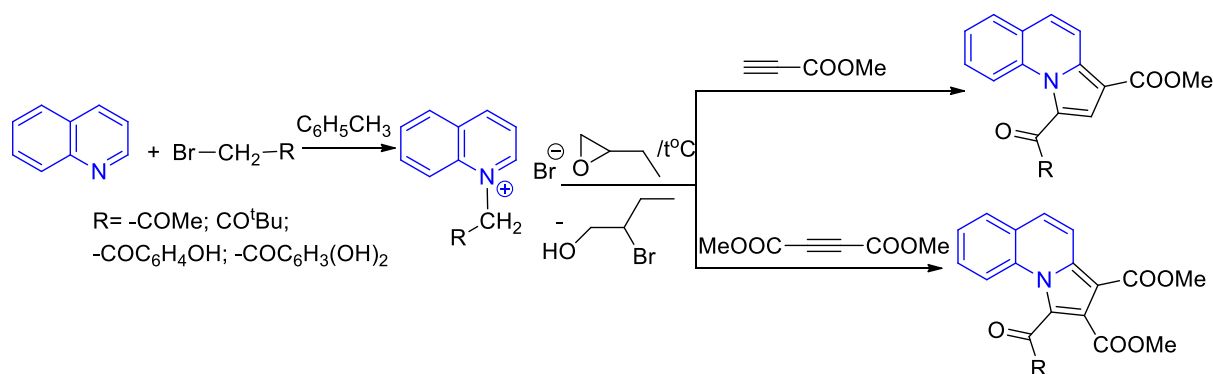
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Quinoline, also known as 1-aza-naphthalene or benzo[*b*]pyridine, is an aromatic heterocyclic compound frequently used as a structural core in the synthesis of derivatives with various biological properties, including anticancer, antibacterial, antifungal, antiviral, antiprotozoal, antihelminthic, antituberculous, anti-inflammatory, analgesic, anticonvulsant, and cardiotoxic effects [1, 2].

In this study, quaternary quinoline salts and substituted pyrrolo[1,2-*a*]quinoline derivatives were synthesized (Scheme 1) and characterized using both conventional (thermal heating) and unconventional (microwave heating) methods [3]. Structural confirmation was performed by IR and NMR spectroscopy (¹H, ¹³C, and two-dimensional 2D COSY, HMQC, and HMBC experiments).



Scheme 1. Chemical reaction equation for the synthesis of pyrroloquinoline derivatives.

The cycloaddition reactions were stereospecific, without the generation of regioisomers, leading to stable azaheterocyclic derivatives with promising pharmacological potential.

Acknowledgements

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PI-5. Physico-chemical characterisation of precipitation events in the Rarau Massif, north-eastern Romania

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Precipitations efficiently scavenge gaseous and aerosol pollutants from the atmosphere, providing a primary pathway for their entry into terrestrial and aquatic ecosystems [1,2]. In an unpolluted atmosphere, the equilibrium between rainwater and CO₂ leads to a theoretical pH of 5.6, values that fall below this threshold are indicative of acidic deposition [1-3]. The present study characterises the primary physico-chemical parameters, pH and electrical conductivity of wet deposition, from "Ion Gugiuman" Student Research and Practice Station (1572 m asl) in the Rarau Massif (Eastern Carpathians). This remote location is ideal for quantifying the impact of long-range pollutant transport. A total of 332 samples were collected over the period from December 2020 to May 2025 and subsequently analysed using a SevenDirect SD23 pH/Cond meter (METTLER TOLEDO). The analysis highlights a consistent acidic signature, with a pH Volume-Weighted Mean (VWM) of 5.09 ± 0.75 . The electrical conductivity VWM was found to be $17.36 \mu\text{S cm}^{-1}$ with a minimum of $3.2 \mu\text{S cm}^{-1}$ and a maximum of $295.8 \mu\text{S cm}^{-1}$. The observed pattern between [H⁺] and electrical conductivity suggests that acidity is a main contributor to the electrical conductivity. The results suggest that the site is subject to persistent acidic deposition, electrical conductivity indicating a response to both precipitation volume and acidity levels.

Acknowledgements: A.G.N acknowledge the support provided by the project "Integrated interdisciplinary system for the implementation of sustainable development activities in the North-East Region of Romania – SIDNER" (Cod SMIS: 337821), project cofunded through the Regional Program North-East 2021–2027, Investment priority: PRNE_P1, A more competitive, more innovative region, Call: RDI activities in collaboration with SMEs and investments in public RDI organizations and universities, oriented towards the needs identified in the regional entrepreneurial discovery process, Project call number: PR/NE/2024/P1/RSO1.1/1/2 – RDI INFRASTRUCTURES.

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PI-6. Toward reliable modeling of lanthanide absorption spectra: Benchmarking DFT and wavefunction methods for tetravalent cerium

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Among the lanthanides, cerium stands out for its ability to switch between the trivalent (Ce^{3+} ; $4f^1$) and tetravalent (Ce^{4+} ; $4f^0$) oxidation states, a redox process that underpins its diverse chemistry. However, while Ce^{3+} complexes are relatively well understood, Ce^{4+} complexes present a far greater challenge. This is because even deceptively simple systems such as $Ce(C_8H_8)_2$ (cerocene) display intermediate-valence electronic structures with strong static and dynamic correlation that are difficult to describe even with most advanced wavefunction theory (WFT) approaches [2]. Recent studies, however, have shown that the cerocene paradigm does not extend to all Ce^{4+} systems, and that the complex electronic structure in most of these cases may, in fact, be probed using single-configuration density functional theory (DFT) or post-Hartree–Fock perturbation theory methods [2].

In this contribution, we aim to establish a cost-effective computational protocol for accurately modeling the electronic structure of Ce^{4+} complexes, with a focus on their electronic absorption spectra. As part of this effort, we investigate the formally tetravalent $[CeX_6]^{2-}$ complexes ($X = F-Br$), which have been recently examined experimentally using UV–vis and X-ray absorption spectroscopy, alongside various correlated theoretical approaches [3,4]. Preliminary comparisons of WFT and DFT calculations indicate that DFT, particularly with the PBE0 exchange-correlation potential, can reproduce both the ground-state electronic structure in agreement with experiments and absorption features within 10 nm of experimental values.

Acknowledgements: DCS and IH acknowledge support offered by the "PHC Brancusi" Romania-France bilateral research program (code: PN-IV-P8-8.3-PM-RO-FR-2024-00-22), funded by the Romanian National Authority for Scientific Research and Innovation (UEFISCDI).

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PI-7. Synthesis and anticancer screening of new functionalized indolizines

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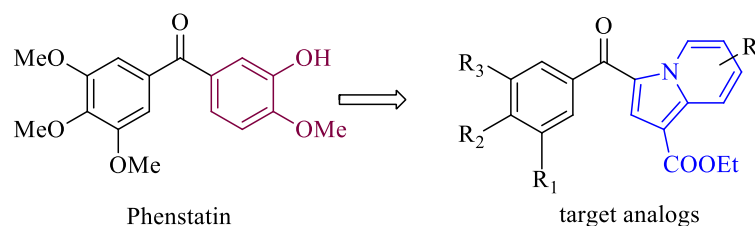
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Heterocyclic and especially azaheterocyclic compounds are essential in medicinal chemistry due to their presence in numerous bioactive molecules. Among them, indolizines exhibit diverse biological activities, particularly anticancer effects, through mechanisms such as tubulin inhibition, EGFR pathway disruption or apoptosis induction. Incorporation of bromine can further enhance molecular interactions and selectivity via halogen bonding, while ester substitution at C-1 has been shown to increase cytotoxic potency compared to acid or amide analogues. These structural features highlight indolizines as valuable scaffolds for developing new therapeutic agents.



In order to evaluate the anticancer potential, a series of new indolizine derivatives was synthesized via a [3+2] cycloaddition of monoquaternary salts derived from 3-bromopyridine and ethyl isonicotinate, respectively, to ethyl propiolate. The structures of the obtained compounds were confirmed by NMR and IR spectroscopy. Part of the compounds were tested at the National Cancer Institute (NCI, US), against a panel of 60 human cancer cell lines to assess their anticancer efficacy and the results are discussed herein.

Acknowledgements We acknowledge CERNESIM Research Centre at "Al. I. Cuza" University of Iasi for NMR experiments and the US National Cancer Institute (NCI) for anticancer testing of the compounds.

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PI-8. Kinetic investigations for the gas-phase reaction of carvacrol with OH radicals

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The troposphere contains a large amount of volatile organic compounds (VOCs) emitted in the gas-phase from both biogenic and anthropogenic sources [1]. Carvacrol (5-isopropyl-2-methylphenol) is emitted into the atmosphere by plants such as *Thymus* and *Origanum*. Together with thymol, they are potential gas-phase products from the OH radical-initiated oxidation of p-cymene. In the atmosphere, it can react with OH radicals to form gas-phase products that are precursors to photooxidants and secondary organic aerosol (SOA). Carvacrol has potential uses as an antimicrobial, antioxidant, antifungal, and anti-inflammatory agent due to its broad spectrum of biological activities while also contributing to the reduction of oxidative stress and the protection of tissues [2]. In this study, we report for the first time the gas-phase kinetic rate coefficient for the reaction between carvacrol and OH radicals. Kinetic measurements were performed in the ESC-Q-UAIC atmospheric reaction chamber, a cylindrical quartz reactor with a volume of 760 L, surrounded by 32 fluorescent lamps ($\lambda_{\max} = 365$ nm), connected to an FT-IR spectrometer via an White-type optical system to achieve a total optical path length of (492 ± 1) m [3]. 2-Methyl-2-butene and 1-methyl-1-cyclohexene were used as reference compounds in this relative rate kinetic study. Wall loss and photolysis of carvacrol were measured to perform the necessary corrections. The reactivity of carvacrol toward OH radicals will be compared with that of other aromatic compounds and with estimated Structure-Activity Relationship (SAR) values.

Acknowledgements

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PI-9. [2+2+1] Cycloaddition for the synthesis of unsymmetrical 7,7'-biindolizines

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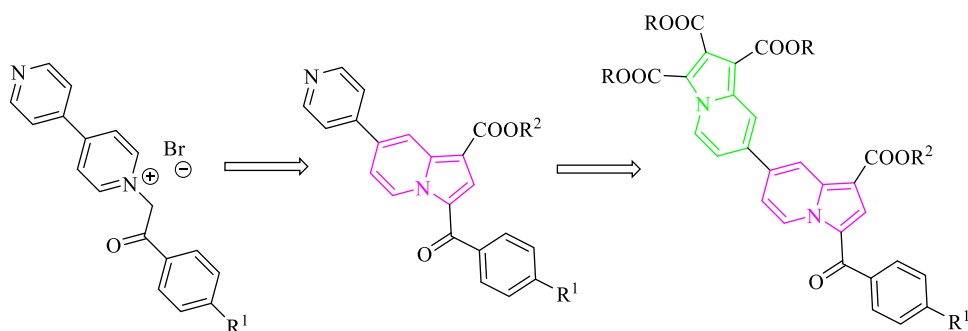
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Indolizines are aromatic nitrogen-containing heterocycles notable for their strong fluorescence and tunable electronic properties [1]. Among them, 7,7'-biindolizines stand out due to their extended π -conjugation, enhanced charge mobility, and tunable optical properties, rendering them promising candidates as organic semiconductors, light-emitting materials, and photodynamic systems [2].



In this work, we report an efficient, metal-free approach to unsymmetrical 7,7'-biindolizines via a [2+2+1] cycloaddition between ethyl 3-benzoyl-7-(pyridin-4-yl)indolizine-1-carboxylate and dimethyl acetylenedicarboxylate (DMAD). The transformation proceeds via selective C \equiv C bond cleavage, achieving direct formation of the second indolizine ring. The structures of the newly synthesized 7,7'-biindolizine compounds were proven by spectral (IR, NMR) methods [3].

Acknowledgements

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PI-10. Studies on Advancing Low-Cost Electrochemical Sensors for Air Quality Monitoring

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Atmospheric chemistry is highly influenced by the presence of air pollutants, as many of them affect the climate, ecosystems, and human health [1]. Air quality monitoring has become increasingly important as human activities have intensified in recent decades. People spend most of their time indoors, in homes and offices, and therefore a fast response to indoor air quality monitoring is essential [2-3].

In this study, an electrochemical sensor device was developed and tested for the purpose of self-exposure monitoring to several air pollutants, including O₃, NO, NO₂, and SO₂, with an emphasis on ozone (O₃) monitoring. The prototype instrument was built using low-cost electrochemical sensors and a few affordable electronic components, all assembled on a perfboard. A series of preliminary tests were conducted under varying humidity conditions and in the presence of gas-phase chemical interferences from volatile organic compounds (VOCs) to evaluate the prototype's response.

Preliminary features of the device were evaluated using an experimental setup specifically designed for the needs of this study. Additionally, a robust ozone monitor was employed to validate the data collected by the newly developed device. The sensors were used to monitor the exposure to ozone in real urban environments, particularly in areas with heavy traffic and various weather conditions. Sensor data were compared with measurements from the IS-2 monitoring station, with reference data retrieved online for the corresponding measurement period.

Acknowledgements

The grants support offered by *PN-IV-P8- 8.3-PM-ROFR-2024- 0178 (NaOH)* from UEFISCDI project and the SIDNER project (Cod SMIS: 337821), project PR/NE/2024/P1/RSO1.1/1/2 – RDI INFRASTRUCTURES were acknowledged.

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PI-11. Modern analytical approaches in prospecting ecological solutions for pharmaceutical waste management

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Pollution is one of the most discussed topics worldwide due to its implications in all aspects of life. One of the most critical issue is the presence of expired medicines entering landfills or water systems. This contributes to the development of antibiotic resistance which nowadays has drawn scientific attention. Antibiotic resistance has the potential to affect people at any stage of life, as well as the healthcare, veterinary, and agricultural sectors. *Hermetia illucens*, a saprophagous insect feeding with decaying organic matter, can reduce the concentration of antibiotics and heavy metals under specific environmental conditions [1]. The research in the present work aims to use the larval stage of *Hermetia illucens* to reduce antibiotic concentrations in selected landfills and identify optimal environmental conditions enhancing larval degradation efficiency. To achieve the proposed objectives, a multidisciplinary analytical approach, through sample preparation and advanced instrumental analysis, is envisaged [2]. Residual compounds analysis is employed to determine whether bioaccumulation occurs at any larvae's development stages. Absence of harmful amounts of residual compounds or antibiotics will allow use of larvae in various applications such as chitin extraction, protein-rich animal or aquaculture feed, biofertilizer production, biogas generation, and soil amendment. If proven effective, this approach could represent an initial step toward reducing the spread of antibiotic resistance in the environment while promoting an environmentally sustainable strategy.

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PI-12. Mansorine – A Natural Coumarin with Neuroprotective Potential in an Okadaic Acid-Induced Alzheimer's Disease Zebrafish Model

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The search for bioactive natural compounds capable of addressing complex neurodegenerative disorders represents a growing field of sustainable chemical and biomedical research [1]. Alzheimer's disease (AD), a major neurodegenerative pathology characterized by progressive memory loss and cognitive impairment, poses an urgent need for safer and more effective therapeutic options. Mansorine (MA), a coumarin compound isolated from *Mansonia gagei*, has been reported to exhibit strong antioxidant and anti-inflammatory activities, suggesting potential neuroprotective properties. In this study, we investigated the effects of mansorine on cognitive performance using *Danio rerio* (zebrafish) as a preclinical model of AD [2,3]. An Alzheimer-like condition was induced by exposure to okadaic acid (OKA, 10 nM) for four days. The experiment included six groups (n = 10): Control (DMSO), Galantamine (1 mg/L, positive control), OKA (10 nM, DMSO vehicle), and OKA combined with mansorine at 1, 3, or 6 µg/L. Mansorine was administered for seven days, with medium renewal every three days. Cognitive function was evaluated through Y-maze (spatial memory, locomotor activity) and Novel Object Recognition (NOR) tests. Data were analyzed using one-way ANOVA followed by Tukey's post hoc test (GraphPad Prism 9, p < 0.05). Exposure to OKA caused significant impairments in both spatial and recognition memory (p < 0.0001 vs. control), while galantamine treatment reversed these effects. Mansorine at 3 and 6 µg/L significantly improved cognitive performance (p < 0.001), increasing exploration of the novel arm and preference for the novel object, alongside enhanced locomotor activity. The lowest concentration (1 µg/L) showed no significant improvement. These results demonstrate that mansorine effectively counteracts OKA-induced memory deficits, supporting its neuroprotective and cholinergic modulatory properties. From a chemical perspective, the study highlights the relevance of naturally derived coumarin scaffolds as promising leads for sustainable drug discovery targeting neurodegenerative diseases.

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**PI-13. DEVELOPMENT AND CHARACTERIZATION OF
NITROGEN-HETEROCYCLIC SULFONAMIDES**

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Because of their broad variety of pharmacological uses and variable reactivity, sulfonamide derivatives are essential to the fields of organic and medicinal chemistry [1]. The incorporation of the sulfonamide group ($-\text{SO}_2\text{NH}_2$) into heterocyclic structures contributes to improving the chemical stability, bioavailability, and biological activity of the resulting molecules [2].

In the present study, a sulfonamide group ($-\text{SO}_2\text{NH}_2$) was introduced to a variety of heterocycles, including (iso)quinoline, pyridine, benzimidazole, phthalazine, phenanthroline, and others, employing a quaternization procedure resulting in novel nitrogen heterocyclic derivatives [3].

A combination of spectroscopic methods, including nuclear magnetic resonance (NMR), Fourier transform infrared spectroscopy (FTIR), and mass spectrometry (MS), were used to thoroughly characterize the obtained compounds. As a result, the presence of the sulfonamide group in the molecular structure was confirmed.

This reaction represents the first step toward obtaining new and innovative compounds possessing nitrogen heterocyclic structures and sulfonamide moieties, enabling subsequent functionalization, facilitating the introduction of the sulfonamide group into the heterocyclic framework.

Acknowledgements This work was supported by a grant of the Romanian National Authority for Scientific Research, CNCS – UEFISCDI, project PN-IV-P7-7.1-PED-2024-1008. (76PED/05.05.2025).

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PI-14. Antioxidant activity of new molecular hybrid based on homodrimane, thiosemicarbazone and oxadiazole unit

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The synthesis of molecular hybrids combining distinct pharmacophores is a key direction in modern chemistry, often yielding new bioactive compounds. Significant progress has been made in developing terpeno-heterocyclic hybrids, particularly those based on the homodrimane skeleton, known for diverse pharmaceutical and biological activities. Numerous hybrids incorporating benzothiazole, benzimidazole, thiadiazole, and other heterocyclic units have been reported, exhibiting notable biological properties [1]. The current study was focused on synthesis and evaluation of the antioxidant activity for a novel homodrimane derivative bearing thiosemicarbazone and oxadiazole core **2** and its precursor **1**, both derived from commercially available (+)-sclareolide. The structures of the synthesized compounds were established by modern spectral methods of analysis: ATR-FTIR, ¹H, ¹³C and ¹⁵N NMR.

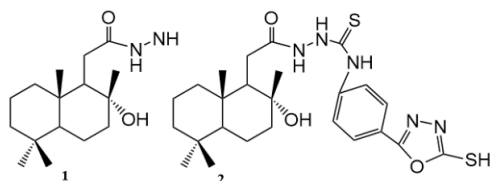


Figure 1. Chemical structure of molecular compounds.

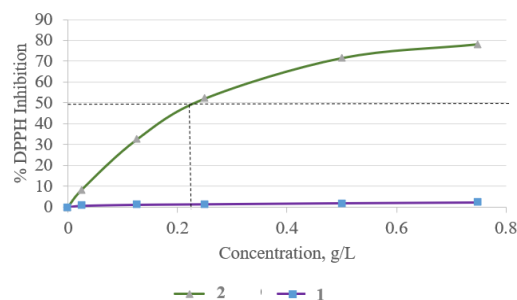


Figure 2. DPPH radical scavenging activity of compounds **2** and **1** at various concentrations.

The antioxidant activity of the synthesized compounds **1** and **2** was evaluated using the DPPH assay. Compound **2** exhibited a concentration-dependent antioxidant activity. At the highest tested concentration (0.75 g/L), **2** achieved approximately 80% inhibition indicating substantial radical scavenging potential. The IC₅₀ value, defined as the concentration required to inhibit 50% of the DPPH radicals, was calculated to be approximately 0.23 g/L. In contrast, **1** demonstrated negligible DPPH inhibition across all tested concentrations, with values remaining below 5%. Since **2** is structurally derived from **1**, the observed activity suggests that the structural modifications introduced were essential in conferring antioxidant activity.

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PI-15. Synthesis of new hybrid-chimeric compounds *via* Cu(I)-catalyzed Huisgen azide-alkyne 1,3-dipolar cycloaddition

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The cycloaddition reactions represent powerful tools in organic synthesis for the construction of heterocyclic compounds. Among them, 1,3-dipolar cycloadditions continue to receive considerable attention from the scientific community, even though the concept was introduced by Rolf Huisgen decades ago. In particular, the Cu(I)-catalyzed 1,3-dipolar cycloaddition of azide and alkynes (CuAAC) provides an efficient route to 1,2,3-triazoles-1,4-disubstituted [1, 2].

This study reports the synthesis of new hybrid-chimeric compounds with triazole structure using one terminal alkyne derivative and a series of alkyl/acyl azides *via* 1,3-dipolar cycloaddition approach, in line with click chemistry strategies (Figure 1).

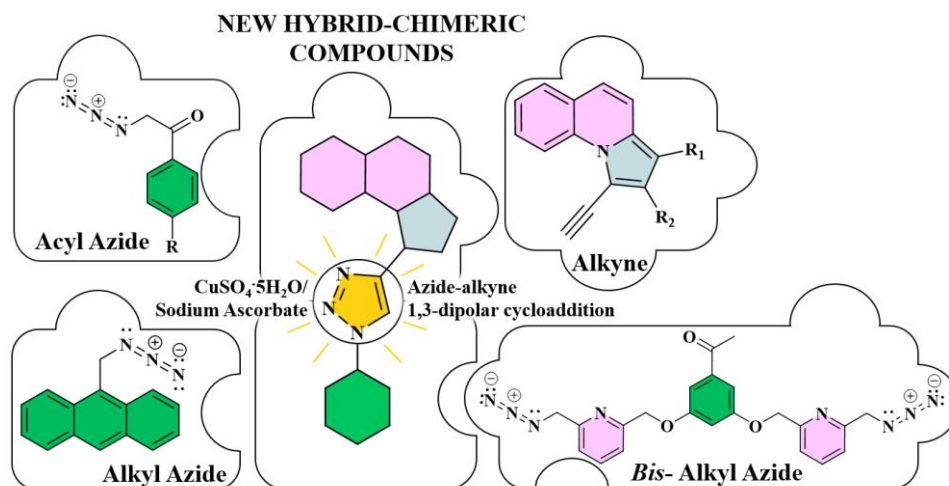


Figure 1. Design in the class of new hybrid-chimeric compounds

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PI-16. New products obtained from the cycloaddition of benzimidazolium ylides to activated alkynes

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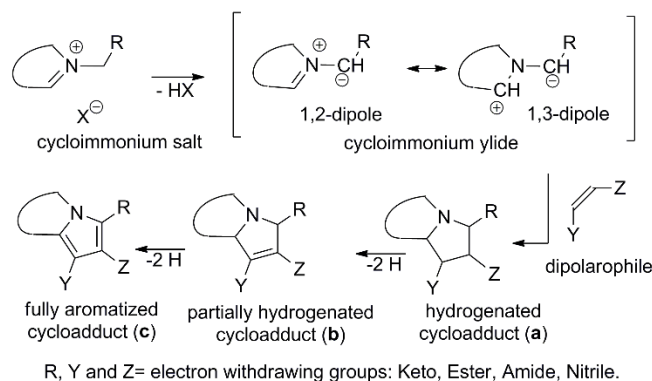
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A widely used, but also disputed method for the synthesis of the pyrrolo[1,2-*a*]quinoxalinone derivatives, an important class of heterocyclic compounds due to their biological activities, is the cycloaddition reaction of the benzimidazolium ylides to dipolarophiles [1, 2].

The cycloaddition reaction of cycloimmonium ylides involves three stages: (i) generation of the ylide from the corresponding salt; (ii) a Huisgen 3+2 cycloaddition of ylide to dipolarophile, and formation of a cycloadduct; (iii) total or partial dehydrogenation of the intermediary cycloadduct, with the final formation of a more stable aromatized adduct (**Scheme 1**).



Scheme 1. Reaction pathway for the cycloaddition of cycloimmonium salts to olefinic dipolarophiles. The first two stages have been thoroughly investigated and described in literature [1-5], while the intermediate's dehydrogenation in the third stage leads to a large variety of products including total or partial hydrogenated [3, 4], fully aromatized cycloadducts [2, 3, 4] or even with an altered structure of the cycloadduct [2, 5]. It is the latter case we focus in this study.

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PI-17. Phytochemical study and antioxidant activity of *Eclipta alba* L (Hassk.) from Burkina Faso

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Today, the use of medicinal plants in traditional therapy is increasing and diversifying. *Eclipta alba* L. is a member of the Asteraceae family, commonly referred to as false daisy or bhringaraj. The plant contains multiple classes of bioactive constituents: glycosides, triterpenoids, alkaloids, and flavonoids. The diversity of chemical classes suggests a complex pharmacodynamic profile, with possible synergistic or pleiotropic effects contributing to the observed pharmacological activities. In Burkina Faso, in the central plateau region, the species are used in the treatment of various diseases, including microbial infections, childhood mycoses, and childhood convulsions [1-3]. This study aimed to determine the phytochemical profile and the evaluation of the biological activity of *Eclipta alba*. Three methods, namely DPPH, TAC, and ABTS, were used to evaluate the ability of the extract to neutralize free radicals. This plant could be used in the treatment of diseases related to oxidative stress.

Acknowledgements

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PI-18. Matrix-Assisted Laser Desorption/Ionization Imaging Mass Spectrometry for Lipid Distribution Analysis in Biological Tissues

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Matrix-Assisted Laser Desorption/Ionization Imaging Mass Spectrometry (MALDI-IMS) enables spatially resolved molecular mapping of biological tissues with a spatial resolution of approximately 50 μm . This study investigates the optimization of MALDI imaging protocols for mouse and human heart tissues sections, emphasizing sample preparation, method adjustment and a qualitative oriented approach involving lipid signal interpretation. Sample preparation represents a critical step in the experimental workflow, ensuring optimal sensitivity and spatial resolution for the specific analytes of interest [1]. Mouse tissue sections were affixed with optimal cutting temperature (OCT), cryosectioned at -25°C and mounted on indium–tin oxide (ITO) coated slides to ensure conductivity and minimize charging effects during MALDI analysis [1]. The matrix deposition for both, mouse tissue sections and human formalin-fixed paraffin-embedded (FFPE) heart sections used α -cyano-4-hydroxycinnamic acid (CHCA), applied via an optimized TM sprayer, while calibration employed red phosphorus clusters. Spectra were acquired using a MALDI-ToF mass spectrometer and processed with flexControl and flexImaging to produce ion distribution maps. Distinct lipid species, including a lipid putatively assigned as plasmalogen-type phosphatidylcholine (PC O - 40:5), were observed in mouse heart tissue. Human heart sections exhibited strong paraffin-derived interferences, however tissue-specific signal distributions were still observed, which may aid in heart tissue characterization. In mouse tissue, spatial intensity variations closely reflected morphology, highlighting the importance of careful sample handling, matrix application, and section integrity for reliable imaging. MALDI-ToF IMS effectively revealed distinct lipid distributions, demonstrating its potential for biomedical research while emphasizing the need for optimized protocols to ensure accurate molecular insights.

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PI-19. Quality Control and Assay of Ascorbic Acid in Pharmaceutical Dosage Forms using Chemical and Instrumental Analysis

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Vitamin C is one of the most widely used bioactive compounds in the pharmaceutical and food supplement industries due to its essential roles in protecting against oxidative stress, maintaining immune system functions, and supporting normal metabolic processes. In this context, the present study aimed to quantitatively determine the ascorbic acid content in two types of chewable tablets using two complementary analytical techniques: the volumetric (iodometric) and the UV-VIS spectrophotometric methods [1]. The main objective was to validate these approaches as simple, accurate, and cost-effective procedures for the quality control of pharmaceutical formulations containing vitamin C. The volumetric method was based on iodometric titration, in which ascorbic acid acts as a reducing agent and is oxidized to dehydroascorbic acid in the presence of I₂. In parallel, the spectrophotometric UV-VIS analysis was performed and absorbance measurements were carried out at the wavelength of 262 nm, corresponding to the maximum absorbance of ascorbic acid [2-4]. The calibration curve, plotted as absorbance versus concentration expressed in mg/mL within the range 20-100 mg/mL, showed excellent linearity ($R^2 = 0.998$), confirming the accuracy and reliability of the method according to the Beer-Lambert law. The results obtained from both the volumetric and spectrophotometric determinations were highly consistent and closely matched the concentrations declared by the manufacturers, demonstrating that both analytical techniques are suitable for precise and reproducible quantification of vitamin C in chewable tablet formulations. These findings support the use of iodometric titration and UV-VIS spectrophotometry as complementary, rapid, and inexpensive analytical tools for the routine quality control of ascorbic acid in solid pharmaceutical products. Furthermore, this study provides a methodological basis for extending these techniques to other pharmaceutical forms or fortified food matrices, as well as for their potential application in bioavailability and stability studies of vitamin C-containing preparations.

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PII-1. DES-AQRES: A green and efficient aluminium oxide nanoparticle system based on deep eutectic solvents with enhanced safety and performance

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Alumina nanoparticles (Al_2O_3 NPs), commonly referred to as Al-NPs, have attracted considerable interest in numerous scientific and industrial fields due to their unique biological and physicochemical characteristics. Their nanoscale size (1–100 nm) and exceptionally high surface area-to-volume ratio make them highly suitable for diverse applications [1], including catalysis, electronics, energy storage, biomedicine, and abrasives [2].

Conventional synthesis techniques typically involve the use of hazardous solvents, aggressive surfactants, and significant energy input, posing environmental and safety concerns. Recently, deep eutectic solvents (DESs) - formed through the combination of a hydrogen bond donor (HBD) and acceptor (HBA) - have gained attention as eco-friendly alternatives due to their low toxicity, biodegradability, and non-volatile nature [3].

In this study, the synthesis of Al_2O_3 nanoparticles from aluminium waste, was achieved using a **Quick, Reduced cost, Efficient and Simple** choline chloride - based DES system (DES-AQRES), under mild thermal conditions. The synthesized nanoparticles were characterized using XRD, SEM, confirming the phase purity and nanoscale dimensions.

The results show that the multifunctional role of DESs as environmentally friendly biobased solvents, not only facilitates precise control over particle size, phase, and morphology, but also strongly aligns with the principles of green chemistry, offering a scalable and sustainable route for the fabrication of nanomaterials that integrate environmental responsibility with technological advancement.

Acknowledgements

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PII-2. Insights into the mechano-chemical behaviour of the kinesin-like protein Tea2

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Tea2 (kinesin-like protein Tea2) belongs to the kinesin-like protein family and contains one kinesin-motor domain. It is originary from *Schizosaccharomyces pombe* (Fission yeast), having a molecular weight of 70 kDa and a sequence length of 628 amino acids [1]. This molecular motor promotes microtubules growth, possibly through the interactions with the microtubule ends. Also, Tea2 is required for proper localization of tea1 and tip1 to the cell and interacts with Mal3 and Tip1, being thus stimulated the ATPase activity of this kinesin molecular motor [2]. In this paper, we have developed a mechano-chemical study of Tea2 motor protein processivity to investigate the dynamics and force generation of the Tea2 using an optical tweezers set-up with force-feedback system [3]. The analysis of processivity parameters kinesin Tea2 consisted of the stall force, velocity and run length measurements both in the absence and presence of the two end-binding proteins, Mal3 and Tip1 by varying the concentration values of molecular motors. The presence of these two proteins in the Tea2 motor protein solution resulted in a doubling of average run length, helping the motor protein to move over a longer distance with the same average velocity. Compared to the single conventional kinesin, single Tea2 motor protein moves with an average velocity of 5 times lower and the maximum load carried is 4 times lower. These low values of average velocity and stall force are due to the presence of the second MT-binding region, known as interacting region with Mal3. Meanwhile, in case of a high concentration of Tea2, the processivity of this motor protein is reduced, being characterized by a low average velocity and a high run length. In conclusion, the analysis of the mechano-chemical behavior of Tea2 kinesin can be a suitable model for the development of biomimetic transporters with features of kinesin molecular motors with various applications in nanomedicine.

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PII-3. Morphological and compositional characterization of microplastics as a transport vector

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Microplastics (MPs) are globally recognized as emerging pollutants that are ubiquitous in the environment [1]. The toxic potential of MPs is also due to the fact that they are considered a vector for the transport of other inorganic, organic, and microbiological pollutants. The mechanisms that promote the adsorption of pollutants on the microplastic surfaces are hydrophobic action, electrostatic action, pore filling, van der Waals force, hydrogen bonding, and π - π interaction [2]. In this paper, the detailed morphological structure of different MPs particles and their elemental composition were analyzed to characterize them as a transport vector. Morphological and elemental analysis was performed using the combined SEM - EDX (Scanning Electron Microscope - Energy Dispersive X-ray) technique, and the polymer composition using the FTIR (Fourier Transform Infrared Spectroscopy) method. From the images obtained at different magnifications, porous structures were observed that provide a favorable environment for the fixing of contaminants. Also, various fractures were highlighted that favor the fragmentation of microplastics and the formation of new micro or even nano-sized particles. EDX analysis revealed trace amounts of toxic metals in the microplastics, such as Fe, Cu, Zn, Cd, Ni, and Hg. A particle was identified as containing approximately 26% titanium, which, following FTIR analysis, was confirmed to be a paint fragment, also considered to be a microplastic.

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PII-4. UV- C degradation of some pharmaceuticals in aqueous solution

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Industrial and municipal wastewater represents a major source of aquatic ecosystems contamination with pharmaceutical compounds. Conventional wastewater treatment plants are not effective in removing pharmaceutical substances, so they are discharged into receiving water bodies. The increasing presence of this class of emerging pollutants in the environment requires the development of new techniques for their removal at treatment plants [1]. This study aims to test the effectiveness of eliminating two non-steroidal anti-inflammatory drugs (NSAIDs), namely diclofenac and ketoprofen, in aqueous solutions subjected to UV-C irradiation. This class of pharmaceutical substances is widely used in pain relief and inflammation treatment. Specialized studies have highlighted the presence of NSAIDs in wastewater, surface water, groundwater, sediments and even snow, which may be a cause for concern for the biotic components of ecosystems. [2].

The main objective of this study was to perform photolysis at 254 nm wavelength of diclofenac and ketoprofen in aqueous solutions at concentrations of 100 ng/mL, similar to those found in wastewater. Advanced wastewater treatment plants use UV-C lamps as an effective disinfection method. For this reason, the present study aims to capitalize on this technology by investigating its ability to achieve photolysis of various pharmaceutical substances. The results of this experiment highlighted the total photolysis of the drugs ketoprofen and diclofenac but also of their main degradation products identified following analyses performed with a liquid chromatograph coupled with a high-resolution mass spectrometer.

Acknowledgements The experimental results have been obtained within the REXDAN Research Infrastructure developed within the project An Integrated System for Research and Monitoring of the Complex Environment in the Danube River Area, REXDAN, SMIS code 127065, co-financed by the European Regional Development Fund through the Competitiveness Operational Program 2014-2020, contract no. 309/10.07.2021.

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P11-5. Quantification and use of the indigenous microbiome of grapes from the area with the Protected Geographical Indication "Ștefan Vodă"

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Abstract: The chemical and sensory qualities of wine are greatly influenced by the variety of the yeast microbiota [1]. The importance of the microbiome of grape berries from various geographic locations and varieties, as well as winemaking techniques and climate conditions, has recently been recognized. The microbial terroir was proposed as a result of all of these investigations, as well as metabolic research and a sensory assessment of the wines that were produced. This study is reflecting that using selected cultures, complete fermentation takes place quickly, and as a result more alcohol is formed compared to spontaneous fermentation (1 to 1,5 %vol), the sensorial characteristics emphasize the grape variety and terroir characteristics, also is less sensitive to microbial alterations [2].

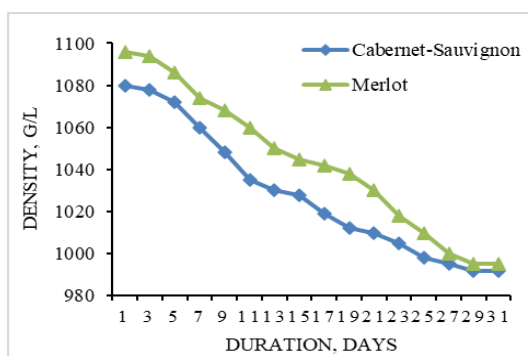


Figure 1. Kinetics of spontaneous fermentation of musts

The data from monitoring the fermentation (figure 1) processes pointed out that the selected flora produced a minimal degree of foaming in pre-fermentation stage, the active stage started after 24-48 hours from inoculation of starter culture, the tumultuous stage started after 48 hours and continued for 8-10 days. Thus, the use of selected starter cultures can ensure a balanced wine and it also may develop wines according to wine market tendencies and to support wine's geographical authenticity.

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P11-6. Where rivers meet, pollutants move - understanding the heavy metals' dynamics at the Argeş–Danube confluence

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This study monitored the behavior of heavy metals of major ecotoxicological importance such as Pb, Cd, Cu, Zn, Ni, and Cr [1] at the water–sediment interface, in the confluence area of the Argeş River with the Danube, between river km 431-432. Metal concentration determinations were performed by TXRF. Based on the analytical results, solid–liquid distribution coefficients (K_d) were calculated, essential parameters for describing the tendency of each metal to remain retained in the sediment or to pass into the water [2,3]. The results highlighted differences in some heavy metals between upstream and downstream, suggesting a direct influence of the Argeş River input, but also of nearby agricultural and urban activities on the total content of heavy metals in the Danube River [4]. Comparative analysis of K_d values indicated a higher sorption of Ni and Pb, while Cd showed the lowest retention, suggesting significant differences in metal mobility between the downstream and upstream environment. This study represents an integrated approach which provides a complex picture of the interaction between local physico-chemical processes and the distribution of heavy metals at the water–sediment interface, contributing to the understanding of the transport and accumulation mechanisms in the Argeş–Danube confluence area and to the substantiation of the ecological risk assessment in the transboundary sectors of the river.

Acknowledgements

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PII-7. Tracing the Hidden Threat: Heavy Metals in Agricultural and Protected Soils

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Soil contamination with heavy metals represents a serious threat to both human health and ecological stability, primarily through crop ingestion, dermal exposure, and bioaccumulation along the food chain [1]. This study examined eleven composite soil samples collected in triplicate from various sites in Iași County, including four Natura 2000 protected areas: Mârzești Forest, Plopi Lake—Belcești, Moldova Delta, and Valea lui David. Soil humidity (gravimetric method), pH, and organic matter content were determined to explore their interdependence with heavy metal concentrations. Heavy metals were analysed using energy-dispersive X-ray spectroscopy (EDS, EDAX system, AMETEK Inc.) and X-ray fluorescence spectrometry (XRFS, Vanta 4, Olympus), while scanning electron microscopy (SEM, Quanta 450, FEI) provided complementary structural insights. Chromium exceeded permissible limits in 45.45% of samples, with values ranging from 106 to 186 mg/kg—nearly twice the alert threshold. Elevated mercury, arsenic, and lead levels were detected in the Mârzești Forest site, surpassing national alert values (Hg - 1 mg/kg, As - 15 mg/kg, Pb - 50 mg/kg) [2,3]. The influence of past military activities during World War I, together with the area's classification as a protected site, may have contributed to the contamination observed. Nevertheless, the status of "protected area" should not be equated with low environmental risk. These findings highlight the necessity of continuous monitoring and responsible land management, even within officially protected ecosystems.

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PII-8. Advanced multi-residue analysis of PAHs, PCBs and pesticides in Danube River sediments (Romania)

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Considered a storage space for contaminants in the aquatic ecosystem, sediment is a real reservoir for water-insoluble pollutants, which also can bind to suspended or bottom solid particles. Because they do not break down easily, these pollutants are very persistent, and they can remain in the environment for very long periods. In this study, the sediment samples collected from the Danube territory between Galati and Corabia were analyzed in terms of semi-volatile contaminants, such as pesticides, polychlorinated biphenyls, and polyaromatic hydrocarbons. The extraction of the target analytes was made by using an improved, well-optimized QuEChERS method, and the evaluation of the previously mentioned compounds was carried out with a gas chromatograph combined with a triple quadrupole mass spectrometer (GC-MS/MS). The obtained results show that the first sediment sample - S1 - collected from kilometer 168, in the Smardan-Macin region, presented the highest pollution in terms of variety and concentration. In order to evaluate the quality of aquatic ecosystems, identify the sources of pollution, and better understand the processes of bioaccumulation and biomagnification, it is crucial to monitor the presence of contaminants and measure their concentration in the river sediment.

Acknowledgements

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PII-9. Influence of thermal treatment on the structural, magnetic and transport properties of $\text{La}_{0.54}\text{Nd}_{0.11}\text{Sr}_{0.35}\text{Mn}_{0.85}\text{Co}_{0.15}\text{O}_{3\pm\delta}$ manganite

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The effect of sintering treatment on the structural, magnetic, and transport properties of the $\text{La}_{0.54}\text{Nd}_{0.11}\text{Sr}_{0.35}\text{Mn}_{0.85}\text{Co}_{0.15}\text{O}_{3\pm\delta}$ compound has been investigated in this study. The sample obtained by the sol–gel method was sintered at 1473 K and 1523 K, respectively. X-ray diffraction (XRD) analysis shows that both samples crystallize in a rhombohedral perovskite-type structure with an R-3c space group. Rietveld refinement indicates a slight decrease in the unit cell volume and an increase in the average crystallite size, suggesting different concentrations of various cations ($\text{Co}^{2+/3+}$, $\text{Mn}^{3+/4+}$), as confirmed by X-ray photoelectron spectroscopy (XPS) data. Magnetization measurements reveal that both samples undergo a paramagnetic–ferromagnetic (PM–FM) phase transition and exhibit a significant decrease as the sintering temperature increases, the Mn^{4+} - Co^{2+} double-exchange interaction responsible for ferromagnetic ordering [1] being replaced by the less effective Co^{2+} - Co^{3+} and Mn^{4+} - Co^{3+} interactions in sample treated at 1523 K. Consequently, the magnetic moment and Curie temperature (T_C) decrease (Tab. 1). Both samples show the insulator-metal (IM) transition temperatures below to T_C .

Table 1. Variation of unit cell volume (V), average of crystalline size (D), microstrain (ϵ), $\text{Mn}^{3+}/\text{Mn}^{4+}$ ratio, molar magnetization (p), Curie temperature (T_C) and insulator-metal transition temperature (T_{IM}) for $\text{La}_{0.54}\text{Nd}_{0.11}\text{Sr}_{0.35}\text{Mn}_{0.85}\text{Co}_{0.15}\text{O}_{3\pm\delta}$ manganite.

T, K	V (Å^3)	D (nm)	$\epsilon \cdot 10^3$	$\text{Mn}^{4+}/\text{Mn}^{3+}$	p ($\mu_B/\text{f.u.}$)	T_C (K)	T_{IM} (K)
1473	347.173	55.5	2.86	0.20	3.45	317	265
1523	344.286	58.01	2.88	0.58	1.75	302	94/265

The resistivity curve of the sample sintered at the higher temperature displays two distinct maxima. We consider that the insulator-metal transitions reflect the spin-dependent interfacial tunneling due to the difference in magnetic order between surface and core as the temperature increases [2].

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P11-10. Comparative thermal and surface characterization of activated carbons obtained from peach stones

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Activated carbons derived from biomass waste represent a promising approach due to their wide availability, cost-effectiveness, and favourable properties as adsorbents. The production of activated carbon (AC) can serve as a sustainable strategy with multifunctional applications, including energy storage, resource recovery, and environmental remediation [1-3].

Activated carbons CAP-25 and CAPO-25 were synthesized from peach stones via high-temperature steam activation (900 °C). Despite their similar textural origins, the samples exhibit distinct surface chemistries. CAP-25 possesses a basic surface dominated by phenolic groups and a high degree of carbonization, whereas CAPO-25, obtained by post-synthesis oxidation, is enriched in acidic oxygen functionalities (carboxylic, lactonic, anhydride).

Thermogravimetric analysis revealed significant differences in their thermal behavior. CAP-25 shows limited mass loss (~5%) below 150 °C due to desorption of physisorbed water, while CAPO-25 exhibits higher loss (~14%), consistent with increased hydrophilicity. The oxidized sample presents a pronounced DTG peak at 180–300 °C, corresponding to decomposition of carboxylic and lactonic groups, followed by a less intense feature at 400–550 °C. In contrast, CAP-25 remains largely stable up to 500 °C, with the main degradation event (phenolic and carbonyl decomposition) centered around 600 °C. Both carbons stabilize above 700 °C, although CAPO-25 demonstrates slightly reduced thermal stability due to its higher oxygen content. Overall, post-synthesis oxidation significantly modifies the surface chemistry and stability of activated carbons.

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PII-11. Building a science-based framework for sustainable sediment management in the Danube–Black Sea System

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The Danube-Black Sea system faces a major challenge in sediment management due to hydromorphological changes and pollutant loads that affect not only sediment quantity and quality but also water quality and ecosystem resilience.

This paper presents the concept of an integrated sediment management framework, which could serve as a basis for sustainable decision-making on sediment dredging, transport, reuse, and remediation. This framework is based on a combination of sediment chemical characterization and physical and biological indicators to assess their quality, mobility, and reuse potential, and is in line with the objectives of the "Restoring Waters and Oceans" and our national research initiatives. The scientific framework presented in this study provides a practical basis for the implementation of European directives on water and sediment governance, contributing to the long-term ecological resilience of the Danube-Black Sea corridor and transforming sediments into a valuable resource for sustainable development.

Data obtained from laboratory analyses focusing on trace toxic metals, microorganic pollutants, and the presence of microplastics are correlated with real-world bathymetric and hydrological measurements in the field and help to model sediment transport and deposition processes under different scenarios. This approach allows the identification of potential ecological risks and hotspots that are experiencing excessive sedimentation, excessive erosion, or both. By exploring opportunities for the safe reuse of dredged sediments in construction, agriculture, and habitat restoration, the numerical sediment transport model helps to promote the principles of the circular economy. This contribution highlights the potential of science-based strategies to transform sediments from a waste management problem into a valuable component of sustainable river basin management.

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PII-12. Synthesis, Characterization, and Tunability of Substituted Benzimidazolium Precursors for Ionic Liquid Development

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The search for environmentally friendly and versatile solvents has led to the development of ionic liquids, which offer a sustainable alternative to traditional volatile organic compounds. Ionic liquids (ILs) are defined as a class of organic salts with melting points below 100 °C [1]. This class of compounds has gained significant interest due to their intrinsic properties, such as a negligible vapor pressure, wide electrochemical window, thermal stability and structural tunability, properties that endorse ionic liquids for diverse applications in a multitude of chemical and industrial fields [2].

This study reports the synthesis and characterization of a new series of precursors designed for the development of ionic liquids based on substituted benzimidazolium cations. A set of benzimidazolium salts was synthesized through quaternization reactions involving an iodophenyl-substituted benzimidazole. By systematically varying the alkylating agent, the melting points, viscosities, electronic properties, and hydrophobicity profiles of the resulting compounds can be tuned.

The synthesized compounds were characterized by NMR spectroscopy, Mass Spectrometry, FT-IR, TGA/DSC, and Single Crystal X-ray Diffraction. Selected molecules were also tested for antimicrobial activity.

Furthermore, the structural diversity of the cations enables exploring correlations between molecular architecture and physicochemical behavior. These insights will guide future design strategies for task-specific ionic liquids. The versatility of the ionic liquids underscores their potential as next-generation materials for multiple technological fields.

Acknowledgements

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PII-13. Zn_{10%}:Fe₃O₄ Nanoparticles as Dual-Function Systems for Controlled Doxorubicin Release and Magnetic Hyperthermia

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The integration of magnetic hyperthermia with controlled drug delivery provides a promising strategy for improving therapeutic selectivity and efficacy in aggressive malignancies. Magnetic nanoparticles (MNPs) function as dual-purpose platforms, enabling localized thermal energy generation and controlled drug delivery under external magnetic stimulation. In this study, zinc-doped magnetite nanoparticles (Zn_{10%}:Fe₃O₄) were synthesized via the coprecipitation method and stabilized using the non-ionic surfactant Pluronic F127 to enhance colloidal stability and biocompatibility. Structural characterization by X-ray diffraction confirmed the formation of a single-phase cubic spinel structure, while dynamic light scattering revealed a hydrodynamic diameter of approximately 244 nm. The measured zeta potential is of -16 mV showing stability under aqueous conditions suitable for biomedical applications.

Doxorubicin was successfully loaded onto the MNPs, achieving an encapsulation efficiency of 34% and a drug loading capacity of 5.7%. The release profile obtained by dialysis method at constant volume demonstrated controlled and pH-dependent release without a burst effect, achieving cumulative release of ~80% at pH 7.4 and ~52% at pH 6.4 after 240 h. *In vitro* cytotoxicity of Zn_{10%}:Fe₃O₄ nanoparticles was evaluated in MDA-MB-231 triple-negative breast cancer cells under five treatment conditions, both in the presence and absence of hyperthermia (HT). Under hyperthermia, Zn_{10%}:Fe₃O₄@DOX decreased viability to 64%, showing only marginal improvement over non-HT conditions. Physical mixtures and individual therapeutic agents exhibited limited effects (73-79%), suggesting that the cytotoxic response is primarily governed by nanoparticle-mediated drug delivery rather than thermal synergy.

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PII-14. NMR and GC-based evaluation of essential oils: developing safe, skin-friendly alternatives for onychomycosis management

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Onychomycosis, a common nail fungal infection, causes nail discoloration and thickening. Conventional oral antifungal treatments pose drawbacks, including rising resistance from overuse and adverse side effects, emphasizing the need for safer, more effective alternatives. [1]. These limitations emphasize the need for alternative antifungal strategies. Essential oils show promise due to bioactive compounds like linalool, terpinen-4-ol, and eucalyptol, which disrupt fungal membranes and inhibit growth. Ensuring efficacy and safety requires thorough assessment of each oil's chemical composition and purity before formulation [2].

In this study, essential oils from various commercial suppliers were analyzed using Nuclear Magnetic Resonance (NMR) spectroscopy and Gas Chromatography (GC). These techniques enabled identification and quantification of key constituents, allowing selection of oils with optimal antifungal potential for bath bomb formulations. All formulation ingredients were chosen for their non-toxic, skin-friendly properties, providing a safer alternative to conventional bath products containing synthetic or harmful chemicals. Combining analytical characterization with safe formulation practices establishes a foundation for developing effective, non-toxic interventions for onychomycosis and underscores essential oils as promising candidates for future antifungal therapy.

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PII-15. Design, synthesis and characterization of novel hybrid compounds based on phthalazino-acetophenone scaffolds

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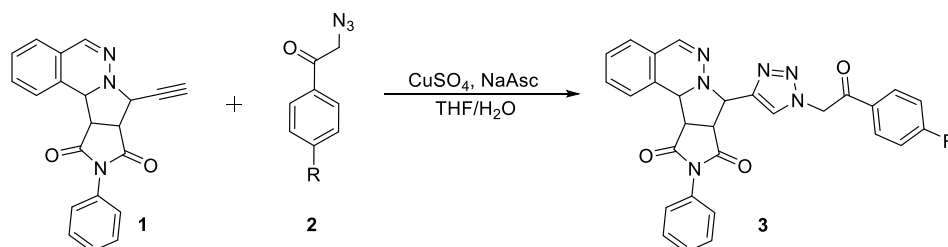
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Hybrid compounds with phthalazine scaffold are of a particular interest due to their diverse biological properties, such as: anticancer, antimicrobial, anti-inflammatory [1]. The acetophenone scaffold is another extremely versatile organic fragment widely used in various fields due to its unique properties. It represents a key component in the production of perfumes, flavors, pharmaceutical products and is frequently used in organic chemistry as a precursor in the manufacturing of dyes, plastics, agrochemicals and drugs [2,3].

The main objective of our work was to use click chemistry to obtain hybrid molecules in which two distinct pharmacophores - the cycloadduct with a phthalazine core **1** and a diversely substituted phenacyl fragment containing an azide functional group **2** are connected via a 1,2,3-triazole unit. Following this direction we obtained novel phthalazine-acetophenone based hybrids **3**, and their structures were confirmed by spectral analysis (FT-IR, NMR and X-Ray diffraction).



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P11-16. AI-Guided QSAR, Docking and MD for Designing Next-Generation GLP-1/GIP Agonists with Extended Action

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Obesity remains a major public health challenge, with rising prevalence and more than 200 comorbidities. Incretin-based pharmacotherapy — particularly GLP-1 receptor (GLP-1R) agonists and dual GLP-1R/GIPR agonists — has transformed clinical management. The dual agonist tirzepatide has shown superior weight loss and glycemic control versus semaglutide in head-to-head trials [1,2]. However, current peptide therapies typically require weekly injections, cold-chain stability, and complex manufacturing, which may limit accessibility and adherence. There is a clear need for molecules with prolonged half-life (ideally monthly), improved oral bioavailability, and reduced cost.

This work proposes an AI-integrated pipeline to discover next-generation GLP-1R/GIPR agonists (including dual and, prospectively, triple agonists) with optimized potency and pharmacokinetics. We will (i) mine structure–activity determinants from known GLP-1, GIP and dual agonists; (ii) develop QSAR models to quantify contributions of N-terminal substitutions that confer DPP-4 resistance (e.g., α -aminoisobutyric acid at position 8 in GLP-1 analogs) and albumin-binding lipidation to extend half-life [3,4]; (iii) generate de novo peptide variants via generative chemistry constrained by ADMET filters; (iv) evaluate receptor engagement through ensemble docking; and (v) prioritize finalists using short molecular dynamics simulations to verify binding stability and the exposure of lipidation handles for albumin association [3,4]. Expected outcomes include candidates with extended plasma half-life, reduced effective dose, and improved tolerability suitable for less-frequent administration. Beyond dual agonism, recent clinical data suggest that unimolecular triple agonists may further amplify metabolic benefits, motivating this as a future direction for our workflow [5].

By coupling QSAR, docking, and MD with machine-learning-guided design, the pipeline aims to compress design–make–test cycles, lower discovery costs, and deliver clinically relevant GLP-1/GIP agonists with superior profiles.

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PII-17. Phenolic content and antioxidant activities of *Uvaria chamae* leaf fractions

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Uvaria chamae is a tropical plant widely used in traditional Togolese medicine to treat several metabolic diseases and whose antioxidant and anti-inflammatory properties are known. Its leaves are notably used to treat diabetes and high blood pressure [1]. Ultrasonic fractionation, on the other hand, is a method that allows the extraction, separation and characterization of bioactive compounds from complex plant mixtures [2]. The objective of the present work was to evaluate the phytochemical content and antioxidant activity of some extracts of *Uvaria chamae* obtained by ultrasound assisted extraction and to study their antioxidant potential. The phytochemical characterization consisted of determinations of total phenolic compounds (TPC) by the Folin-Ciocalteu method and total flavonoids (TFC) with the aluminum chloride method, as well as the determination of antioxidant properties on plant extracts fractionated in solvents of increasing polarities, respectively hexane, chloroform, ethyl acetate, butanol and distilled water. Different methods (DPPH[•], ABTS^{•+}, total antioxidant capacity, ferrous ion chelation) were used to evaluate the antioxidant capacity of the fractions [3]. The free polyphenol content varied from 6.75 to 254.37 mg EAG/ g DW and the flavonoid content from 4.14 to 186.13 mg EQ / g DW. The identification of remarkable concentrations of this class of compounds in the analyzed extracts suggests a possible use of this plant in diseases generated by free radical species. Butanol fraction showed the highest DPPH (IC₅₀=48.05 μg/mL) and ABTS (IC₅₀=24.37 μg/mL) radical scavenging activity. These results constitute a promising avenue for the discovery of new natural compounds.

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PII-18. Extraction and study of biologically active molecules from Piper Nigrum

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Black pepper (*Piper nigrum*) is one of the most widely used spices in the world, with a long history in food and traditional medicine. Its main active ingredient, piperine, is an alkaloid with diverse pharmacological properties, including anti-inflammatory, analgesic, and antibacterial properties, and capable of increasing the bioavailability of some drugs [1]. However, its chemical structure offers the possibility of obtaining derivatives with improved biological properties, a topic of current interest in pharmaceutical research [2-3]. The work aimed to extract piperine from two commercial types of pepper, using conventional methods (Soxhlet with ethanol and chloroform) and green methods (ultrasound-assisted extraction with natural eutectic solvents – NADES). The extracts with piperine were evaluated for their chemical composition and then evaluated for their biological activities. The extracts with piperine were used further in semi-synthetic reactions, allowing the production of new derivatives. The lowest extraction yield (6.11%) was obtained from ground pepper using the Soxhlet method with chloroform as solvent, and is also close to the yield (6.31%) of the same extraction method with ethanol as solvent. It can be concluded that the system is less efficient for obtaining the compounds of interest. In comparison, extractions carried out with NADES are more efficient, both from an ecological point of view. The analysis of the compounds was carried out by thin-layer chromatography and FTIR spectroscopy, confirming the desired chemical transformations. The study demonstrates that green chemistry-based approaches can provide efficient and sustainable methods to obtain molecules with high therapeutic value, thus opening up avenues for further research on the biological activity of piperine derivatives.

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Co-organizers



Partener



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