ROMANIAN ACADEMY
„CORIOLAN DRĂGULESCU" INSTITUTE OF CHEMISTRY
24 Mihai Viteazu Av., RO-300223,
Timişoara, Romania, fax: 0256-491824

The 18th Edition of the Conference

NEW TRENDS IN CHEMISTRY RESEARCH

NOI TENDINȚE DE CERCETARE IN DOMENIUL CHIMIEI

BOOK OF ABSTRACTS

NewChemRes $2^{0}_{2}6$

September 2-4, 2026
TIMIŞOARA

Dear colleagues,

It is our great pleasure to warmly welcome you to **the 18th edition** of **the International Conference "New Trends in Chemistry Research"** / "**Noi tendințe de cercetare în domeniul chimiei**" (**NewChemRes 2026**), held in Timișoara on 2-4 September 2026. This traditional scientific event is organized by the "Coriolan Dragulescu" Institute of Chemistry of the Romanian Academy, in partnership with the Romanian Chemical Society and Politehnica University Timișoara.

Continuing its tradition, the conference provides an international platform for dialogue and collaboration, bringing together researchers from more than **11** countries, doctoral students from Romania and abroad, as well as professionals from the industrial sector. Participants will have the opportunity to exchange ideas, present research findings, share recent discoveries, and put forward innovative visions, thereby contributing to shaping new directions for a more sustainable and innovative future for chemistry.
The conference is not only a venue for showcasing the latest achievements, but also an occasion for collaboration, networking, and the initiation of joint projects, opening pathways towards scientific and technological partnerships at both national and international levels.

The scientific program includes plenary lectures, oral presentations, poster sessions, research equipment promotion, and a visit to the **RO-OPENSCREEN Interdisciplinary Center** (https://ro-openscreen.ro/). Moreover, two special sessions dedicated to **the CERSUS (6CoEx/2026)** and **SusBioGly (87PED/2025) projects** will highlight the central role of chemistry in promoting sustainability and advancing the Sustainable Development Goals.
We would like to express our sincere gratitude to all *speakers, members of the Scientific and Organizing Committees, chairpersons, sponsors, and everyone* who contributed to the organization and success of this event.

We wish you an inspiring, engaging, and professionally rewarding conference!

The "Coriolan Drăgulescu" Institute of Chemistry

Scan for conference details

NewChemRes

ORGANIZERS

"CORIOLAN DRĂGULESCU" INSTITUTE OF CHEMISTRY

ROMANIAN ACADEMY – TIMIȘOARA BRANCH

ROMANIAN CHEMICAL SOCIETY – TIMIȘOARA BRANCH

POLITEHNICA UNIVERSITY OF TIMIȘOARA

With financial support from:

Project Center of Excellence
PN-IV-P6-6.1-CoEx-2024-0056

Societatea de Chimie din ROMANIA

ProAnalysis®

ABL&E–JASCO România S.R.L.

printtech
dpar@printtech.ro

Laboratorium
Together. A Step Forward™

Filtration Group®
Industrial

Altium

Timisoara City tour:
Prof. Marius Crisan

With publication opportunity from:

sustainability

molecules

International Journal of *Molecular Sciences*

CHAIRPERSONS

Dr. Liliana CSEH	"Coriolan Dragulescu" Institute of Chemistry
Dr. Alina BORA	"Coriolan Dragulescu" Institute of Chemistry

ORGANIZING COMMITTEE

Dr. Carmen CRETU	"Coriolan Dragulescu" Institute of Chemistry
Dr. Ildiko BUTĂ	"Coriolan Dragulescu" Institute of Chemistry
Dr. Orsina VERDEȘ	"Coriolan Dragulescu" Institute of Chemistry
Dr. Luminița CRIȘAN	"Coriolan Dragulescu" Institute of Chemistry
Dr. Ionela FRÎNGU	"Coriolan Dragulescu" Institute of Chemistry
Dr. Andreea NISTOR	"Coriolan Dragulescu" Institute of Chemistry
Dr. Roxana NICOLA	"Coriolan Dragulescu" Institute of Chemistry
Chim. Nicoleta STOIAN	"Coriolan Dragulescu" Institute of Chemistry
Dr. Cristian NEANU	"Coriolan Dragulescu" Institute of Chemistry
Dr. Sorin MARINESCU	"Coriolan Dragulescu" Institute of Chemistry

With the valuable support of the Accounting and Administrative Departments

SCIENTIFIC COMMITTEE

Acad. Maria ZAHARESCU	Romanian Academy
Dr. Yann SARAZIN	Université de Renee, France
Prof. Evamarie HEY-HAWKINS	Leipzig University, Germany
Dr. Livius COTARCĂ	LC Consulting, Italy
Prof. Gary HIX	Middlesex University, United Kingdom
Assoc. Prof. Alessandro PELLIS	University of Genova, Genova, Italy
Prof. Fabio ARICÒ	Università Ca' Foscari, Venezia, Italy
Dr. Dan PANTOȘ	University of Bath, United Kingdom
Conf. Dr. Ioana Luiza GĂINĂ	Babes-Bolyai University, Cluj Napoca
Prof. Francisc PÉTER	Politehnica University Timişoara
Dr. Ramona CURPĂN	"Coriolan Dragulescu" Institute of Chemistry
Dr. Sorin AVRAM	"Coriolan Dragulescu" Institute of Chemistry
Dr. Aurelia VIȘA	"Coriolan Dragulescu" Institute of Chemistry
Dr. Nicoleta PLEȘU	"Coriolan Dragulescu" Institute of Chemistry
Dr. Elisabeta I. SZERB	"Coriolan Dragulescu" Institute of Chemistry
Dr. Ana-Maria LACRĂMĂ	"Coriolan Dragulescu" Institute of Chemistry

CONTENTS

DESIGN OF SMART AMPHIPHILIC NANOPARTICLES FOR PRECISION & SUSTAINED DRUG-RELEASE

Edouard BADARAU

Institute of Chemistry & Biology of Membranes & Nanoobjects (CBMN), University of Bordeaux
Geoffroy St Hilaire Alley, Building B14, 33600 Pessac, France
edouard.badarau@u-bordeaux.fr

Mimicking the cellular environment on a nano-scale, the phospholipid (PL)-derived carriers (*e.g.* liposomes) are today the most successful clinically-approved drug delivery systems (DDS). [1] Although liposomes enhance the shelf-life of a free drug, however, the drug generally escapes from the carrier (*via* passive diffusion), without any temporal or regional control. Several approaches are described in literature to regulate the liposomal permeability, and thus the cargo release. A highlight on **stimuli-controlled DDS** and **sustained-release DDS** developed by our group will be detailed during this presentation. Both offer a great potential for clinical disease management, as they feature many benefits over the classical DDS currently on the market: for example, externally activated DDS enable a precise drug delivery to specific target sites **where** and **when** external stimuli are applied. Several proofs of concepts were validated in literature for a variety of external stimuli: ultrasounds-, magnetic-, thermo-, electric- or light-energy. [2] They require natural products (*e.g.* phospholipids) but also the use of additives that induce the carrier's decay in the presence of an external stimulus.
Our proposal is different: our group develops additive-free approaches based on analogues of natural phospholipids either in classical phospholipid series [3, 4] or having a bola-amphiphilic pattern. [5] For example, diazirine-conjugated phospholipids can be used to formulate liposomes able to release their cargo by light stimulation. In the case of slow-release DDS, we developed a new class of tripolar bola-amphiphiles by connecting two natural phospholipids through a polar moiety: such compounds are able to generate more stable and less permeable liposomes than the classical generations of liposomes (Figure).

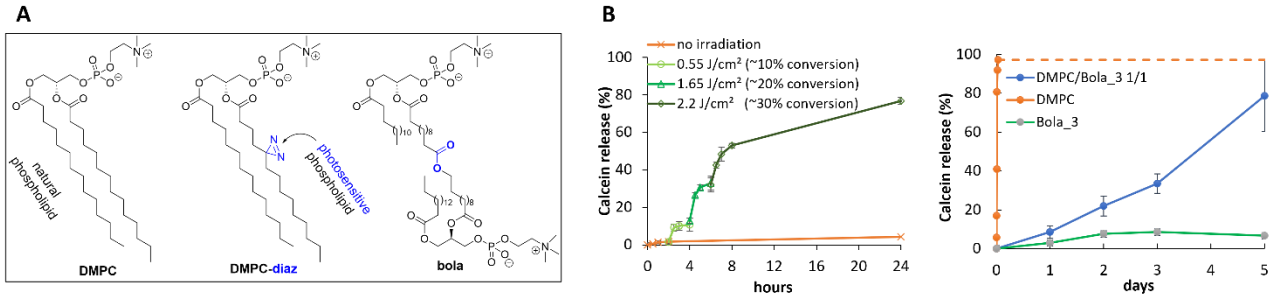


Figure (A) Example of a natural (DMPC), photosensitive (DMPC-diaz) and bola-lipid (bola); (B) Cargo release profiles of photosensitive or bola-induced liposomes

Acknowledgements
Financial supports from Initiative d'Excelence (IdEx) – Emergence Call (LiRLi Project), Ligue contre le Cancer (PhotoSENSEI & PhotoBOLASOMES projects) and from Aquitaine Science Transfert (SATT) are gratefully acknowledged.

References
1. EMA/20989/**2025** (https://www.ema.europa.eu).
2. Hu H., et al., Smart Mater. Med. 2024, 5:386.
3. Saryeddine L., et al., J. Colloid Interface Sci. 2024, 653:1792.
4. Badarau E., et al., 2024, WO2024084096A1.
5. Al Yaman K., et al., Bioconjugate Chem. 2024, 35:1900.

ADVANCING GREEN CHEMISTRY IN BIO-BASED PLATFORM CHEMICAL SYNTHESIS

Fabio ARICÒ

Ca' Foscari University of Venice, Department of Environmental Sciences, Informatics and Statistics, Campus Scientifico, Via Torino 155, 30172 Mestre, Italy.
Fabio.arico@unive.it

The development of green synthetic methodologies is a fundamental challenge in replacing fossil-based chemical production with renewable alternatives. In this context, bio-derived platform molecules obtained from lignocellulosic biomass—such as furan derivatives, isosorbide, levulinic acid derivatives, sugar alcohols, and other oxygen-rich building blocks—have emerged as valuable precursors for the synthesis of advanced polymers, pharmaceuticals, fine chemicals, and functional materials. Despite their potential, the conversion of these renewable substrates frequently depends on hazardous reagents, toxic solvents, and labor-intensive multistep procedures that compromise the overall environmental performance of the process.

Our research addresses these limitations through the development of green synthetic strategies based on the use of organic carbonates as both reaction media and sustainable reagents. Among these, dialkyl carbonates—and especially dimethyl carbonate (DMC)—have proven to be highly effective for the selective transformation of biomass-derived substrates, including D-sorbitol, D-fructose, galactaric acid, and other renewable feedstocks. Acting simultaneously as solvent and reagent, DMC enables chlorine-free, highly selective transformations under relatively mild conditions while replacing more hazardous conventional reagents.

Beyond the selection of renewable raw materials and benign reaction media, the proposed methodologies are designed according to the principles of green chemistry, with the aim of reducing waste generation, lowering energy requirements, simplifying purification steps, and improving overall process efficiency. These synthetic approaches provide access to high-value platform molecules and functional intermediates that are relevant for the production of bio-based polymers, pharmaceutical ingredients, green solvents, and specialty chemicals.

To assess the environmental performance of the developed methodologies, established green chemistry metrics were systematically applied. These quantitative tools supported process optimization, enabled objective comparison between alternative synthetic routes, and provided valuable guidance for future scale-up and potential industrial implementation.

BIOMASS-DERIVED TEREPHTHALIC ACID THROUGH SELECTIVE OXIDATION OF RENEWABLE P-CYMENE OVER EARTH-ABUNDANT CATALYTIC MATERIALS

Iuliana M. CHIRICA, Florentina NEATU, Mihaela M. Trandafir, Stefan NEATU, Mihaela FLOREA*

Catalytic Materials and Catalysis, National Institute of Material Physics, Atomistilor 405A, Magurele, Ilfov, Romania
mihaela.florea@infim.ro

The transition from fossil-based chemical manufacturing to renewable carbon utilization is a central challenge in the development of sustainable polymer industries. Terephthalic acid (TPA), the principal monomer employed in the production of polyethylene terephthalate (PET), is currently synthesized almost exclusively from petroleum-derived p-xylene. Developing alternative routes based on renewable feedstocks is therefore essential for reducing the environmental footprint of PET production and advancing circular and bio-based economies. Among the various biomass-derived aromatic platforms, *p*-cymene has emerged as a particularly attractive precursor because it can be readily obtained from naturally abundant terpenes such as limonene, α-pinene, and eucalyptol. The selective oxidation of *p*-cymene to terephthalic acid, however, remains a demanding transformation due to the complexity of the consecutive oxidation steps and the need to control the formation of partially oxidized intermediates.

This contribution presents recent progress in the catalytic aerobic oxidation of bio-based *p*-cymene to terephthalic acid using heterogeneous catalysts composed exclusively of earth-abundant elements. Particular attention is devoted to mixed manganese-based oxide systems, including Mn–Fe and Mn–Co materials, [1, 2] as well as novel MAX-phase-derived catalytic platforms. The influence of catalyst composition, redox properties, surface acidity, oxygen pressure, reaction temperature, reaction time, and catalyst loading on the conversion of *p*-cymene and the selectivity toward terephthalic acid is analyzed in detail. Mechanistic aspects associated with the activation of molecular oxygen and the sequential oxidation of methyl and isopropyl substituents are discussed to identify the key factors governing catalyst performance. Among the investigated materials, Mn–Fe mixed oxides exhibited outstanding catalytic behavior, enabling the production of bio-based terephthalic acid in yields reaching 51% under molecular oxygen, one of the highest values reported for heterogeneous catalytic systems operating without noble metals. [1] The enhanced activity is attributed to the synergistic interaction between redox-active manganese species and iron centers, which promote efficient oxygen activation and facilitate the deep oxidation pathway toward terephthalic acid. Furthermore, catalyst synthesis through co-precipitation generates highly dispersed active phases with a favorable distribution of acid sites and surface Co^{3+} species, resulting in improved oxidation efficiency and product selectivity.

These findings demonstrate the potential of low-cost, non-toxic, and earth-abundant catalytic materials for the sustainable production of renewable terephthalic acid. The study provides valuable design principles for next-generation oxidation catalysts and contributes to the development of viable biomass-to-PET value chains based on terpene-derived feedstocks.

Acknowledgments
This work was supported by the Romanian Ministry of Education and Research through the Core Program 2023–2026 (contract PC3-PN23080303) and CCCDI-UEFISCDI for project number PN-IV-P7-7.1-PED-2024-2346 (84/2025).

References
1. Neațu F., Culică G., Florea M., Pârvulescu V.I., Cavani F., ChemSusChem. 2016, 9:3102–3112
2. Trandafir M.-M., Neațu S., Bocîrnea A., Counsell J., Cavani F., Florea M., Neațu F., ChemCatChem. 2020, 12:6248–6258.

MECHANISM OF SELF-ASSEMBLY OF COMPLEX MESOPHASES AND STAGES IN DEVELOPMENT OF SPONTANEOUS CHIRALITY

Goran UNGAR

Xi'an Jiaotong University and University of Sheffield
g.ungar@xjtu.edu.cn

New 3D ordered phases were discovered in alkyl-ended rod-like molecules either free or attached as side-groups to polymer backbone. One of them turns out to be ubiquitous. Its unit cell contains 8 counter-twisted ribbons in small molecules. [1, 2] In the polymers the side-groups describe double-helices wound around 8 bundles of siloxane main chains, see Figure (left). [3] High-resolution electron density (ED) maps show that the helices have non-uniform twist, consisting of alternating high-splay and high-twist segments. Even more intriguing is the gyroid cubic structure displayed by polymers with shorter end-chains, see Figure (right). [4] We also found that often 90-95% of the self-assemly of thes and other complex structures actually occurs continuously in the melt. A statistical theory is developed reproducing the experimental data quantitatively. [5] It also explains the second-order transition between normal and chiral melt preceeding the transition to the ordered phase in these systems of nonchiral molecules.

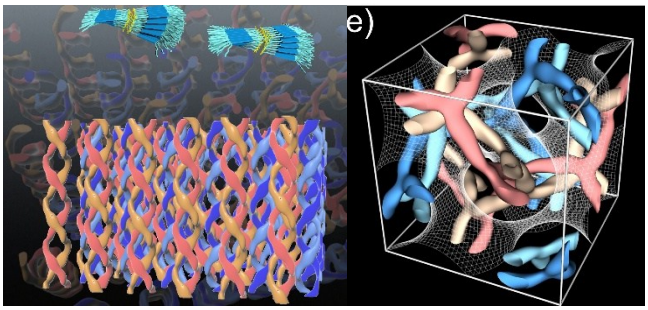


Figure: ED maps of the complex new LC structures. Left: Fddd orthorhombic LC phase of polymer with longer end-chains (3x3 unit cells). [3] Right: polymer with shorter chains in its side groups displaying the first 4-network gyroid cubic phase. [4]

References
1. Li Y.X., Gao H.F., Zhang R.B., Gabana K., Chang Q., Gehring G.A., Cheng X.H., Zeng X.B., Ungar G., Nature Commun. 2022, 13: 384.
2. Wang Y., Li Y.X., Cseh L., Chen Y.X., Yang S.G., Zeng X.B., Zhang R.B, Liu F., Hu W.B., Ungar G., J. Am. Chem. Soc. 2023, 145: 17443.
3. Xue Y.N., Li Y.X., Tang Y.M., Yang S.G., Jia R.Y., Cseh L., Liu F., Zeng X.B., Ungar G., J. Am. Chem. Soc. 2025, 147: 19711.
4. Tang Y.M., Xue Y.N., Yang S.G., Zeng X.B., Ungar G., Angew. Chem. Int. Ed. 2025, 65: 22314.
5. Xue Y.N., Zeng X.B., Wu B.W., Li Y.X., Cseh L., Liu J., Yang S.G., Gehring G.A., Liu F., Ungar G., Angew. Chem. Int. Ed. 2025, 64: e202505548.

THE PREFORMULATION TOOLBOX: HOW INSTRUMENTAL TECHNIQUES DRIVE RATIONAL DRUG DEVELOPMENT

Ionuţ LEDEŢI, Adriana LEDEŢI

University of Medicine and Pharmacy Victor Babeş Timişoara, Faculty of Pharmacy, Advanced Instrumental Screening Center, 2 Eftimie Murgu Square, Timişoara, Romania
ionut.ledeti@umft.ro

The development of safe and effective pharmaceutical dosage forms relies critically on a thorough understanding of the physicochemical properties of active pharmaceutical ingredients (APIs) prior to formulation. Preformulation - the science of characterizing a drug substance in its pure form and in combination with excipients - constitutes the essential first step in rational drug product design. This lecture presents a systematic overview of the instrumental techniques that form the modern preformulation toolbox, with emphasis on their complementary roles and the mechanistic insights they collectively provide. Spectroscopic methods, including attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR), enable the identification of functional group interactions and the detection of chemical incompatibilities between APIs and excipients. Powder X-ray diffraction (PXRD) provides definitive information on solid-state phase composition, polymorphic transitions and the amorphous or crystalline character of drug substances and their binary mixtures. Thermal analysis techniques - thermogravimetry (TG), differential thermogravimetry (DTG) and differential scanning calorimetry (DSC) - reveal the thermal behavior of APIs, including melting, desolvation, polymorphic transitions and degradation onset, and are indispensable for compatibility screening under thermal stress conditions. [1-3]
Beyond static characterization, this lecture highlights the growing importance of kinetic analysis in preformulation, with particular focus on non-isothermal isoconversional methods, including the Friedman, Kissinger-Akahira-Sunose (KAS) and Flynn-Wall-Ozawa (FWO) approaches, as well as non-parametric kinetics (NPK), as tools for elucidating solid-state degradation mechanisms and predicting long-term stability. Representative case studies drawn from the preformulation of steroid-based APIs used in gynecological and hormonal therapies illustrate how the integration of these techniques enables the rational selection of excipients, the identification of incompatibilities at technologically relevant temperatures and the establishment of safe processing and storage conditions. The lecture further discusses the use of statistical tools, including Pearson correlation analysis of spectral data, as a means of reducing subjective interpretation in compatibility assessments. [4-6] Collectively, the presented data demonstrate that a rigorous, multi-technique preformulation strategy is not merely a regulatory formality, but a genuine decision-making framework that underpins the development of stable, reproducible and therapeutically effective pharmaceutical products.

References

1. Bengescu C., Ledeți A., Olariu T., Cîrcioban D., Muntean C., Vlase G., et al., J. Therm. Anal. Calorim. 2023, 148:4641–4649.
2. Ledeti I., Romanescu M., Cîrcioban D., Ledeti A., Vlase G., Vlase T., et al., Pharmaceutics 2020, 12:58.
3. Ridichie A., Bengescu C., Ledeți A., Sbârcea L., Bertici R.-A., Rusu G., et al., J. Therm. Anal. Calorim. 2025.
4. Ledeți A., Baul B., Ridichie A., Ivan D., Vlase T., Tomoroga C., et al., Molecules 2024, 29:5527.
5. Ledeți I., Ledeți A., Vlase G., Vlase T., Matusz P., Bercean V., et al., J. Pharm. Biomed. Anal. 2016, 125:33–40.
6. Ridichie A., Ledeți A., Sbârcea L., et al., J. Therm. Anal. Calorim. 2025, 150:6717–6730.

LEVOGLUCOSENONE: A VERSATILE PLATFORM MOLECULE FOR THE PREPARATION OF HIGH-BOILING SOLVENTS AND BUILDING BLOCKS FOR POLYMER SYNTHESIS

Alessandro PELLIS,[1*] Francesco Maria RABONI[1], Maria Jose CALANDRI[1], Cicely May WARNE[2], Con Robert MCELROY[3]

[a] *University of Genova, Department of Chemistry and Industrial Chemistry, via Dodecaneso 31, 16146, Genova (GE), Italy*
[b] *BOKU University, Department of Agricultural Sciences, Institute of Environmental Biotechnology, Konrad-Lorenz-Strasse 20, 3430 Tulln an der Donau, Austria.*
[c] *University of Lincoln, School of Chemistry, LN6 7DL, Lincoln, UK*
alessandro.pellis@unige.it

Most commercial solvents and polymers are synthesized from the seven base chemicals derived from the petrochemical industry via the distillation of crude oil. In recent years there has been a strong drive to move away from non-renewable feedstock and to develop chemicals, solvents and materials derived from renewable resources using more sustainable synthetic procedures and considering the end of life of these products.
One promising platform molecule is levoglucosenone (LGO), a chiral compound that can be easily obtained via pyrolysis of materials containing cellulose, such as wood chips and bagasse. The chirality at C1 and C5 in LGO gives it advantages in stereoselective synthesis when compared to achiral biomass derivatives while the reduced number of chiral centers simplifies its use when compared to monosaccharides. Enantio-, stereo-, regio- and chemo selective reactions have been executed around the core ring-system, leading to the controlled synthesis of a multitude of biologically active structures. Moreover, the reactivity of the ketone and enone functionalities is influenced by the 1,6-anhydro bridge, which strongly biases reaction to occur from the less hindered exo-face of the molecule. [1]
In this work, LGO was explored as the starting point for the green and scalable synthesis of a series of novel high boiling solvents having varying polarity called Cygnets. These solvents were then used for polymer chemistry applications such as the production of membranes [2] and the enzymatic synthesis of aliphatic and aromatic polyesters allowing both the synthesis and the work up of the obtained polymers to be performed without the use of halogenated and/or toxic solvents. [3, 4]

Acknowledgements
Funded by the European Union (ERC, CIRCULARIZE, 101114664). Views and opinions expressed are, however, those of the author(s) only and do not necessarily reflect those of the European Union or the European Research Council. Neither the European Union nor the granting authority can be held responsible for them.

References
1. Camp J. E., Greatrex B. W., Front. Chem. 2022, 10.
2. Milescu R. A. et al., ChemSusChem. 2021, 14:3367-3381.
3. Warne C. M. et al. Green Chem. Lett. Rev. 2023, 16:2154573.
4. Warne C. M. et al., ChemSusChem. 2024, 17:e202301841.

VANADIUM METALLODRUGS: THE ALTERNATIVE TO TRADITIONAL CANCER CHEMOTHERAPEUTICS

Athanasios SALIFOGLOU

School of Chemical Engineering, Faculty of Engineering, Aristotle University of Thessaloniki, Thessaloniki, 54124 Greece
salif@auth.gr

Cancer has been a disease plaguing the human population over ages. Its many types and forms is a direct consequence of the magnitude of human genetic base and the consequences on its evolution as a result of environmental pressure exerted over the duration of a person's life. The heterogeneous spectrum and often unpredictable influence of variably configured factors on a cell's life cycle over various tissues of the human body confer multilateral phenotypes exemplified as cancer forms with usually detrimental repercussions to the patients. Regardless of the phenotypic emergence of the various forms of cancer, the course of diagnosis and concomitant therapeutics remains a formidable challenge for researchers and clinicians alike. In the framework of developing therapeutics for specific types of cancer, metallodrugs emerged as viable options, due to their unique mode of action either as front line agents or supporting agents in cocktail therapeutic regimens. Prominent of such drugs have so far been molecular agents of Pt, Ru, Ti, among others. [1] Due to undesired, however, side effects and extensive non-specificity of such agents, new alternative metallodrugs have been sought after over the past years. One such metal ion that has been introduced in our research is vanadium [2]; an early transition metal of variable oxidation states and multifaceted chemistry that has shown merit in Diabetes mellitus II. [3] The distinct behavior of that metal ion in the case of cancer therapeutics comes from the notion that it could a) carry bound ligands (e.g. peroxido ions) capable of inducing the demise of cancer cells, and b) bear bound zwitterionic ligands promoting intramolecular polarity with immediate consequences on the uptake and subsequent biological chemistry with key targets in the cancer cell's life cycle machinery. In that respect, ternary V(V)-peroxido-betaine systems were synthesized and fully characterized in the solid state and in solution. The emerging properties were subsequently used to probe into the in vitro biological activity of well-defined materials, taking into consideration the a) tissue type associated with the cancerous phenotype (lung, hepatocellular carcinoma, etc.), b) structure of the vanadium complex species (nuclearity, composition, coordination number), c) culture dimensionality (2D, 3D), and d) potential mechanistic pathways, through which the cancer cell demise may be brought about upon exposure to the specific ternary vanadoforms. [4]

The collective results suggest that a) vanadium in the V(V) oxidation state exerts biochemical reactivity that leads cancer tissue cells to their apoptotic demise, b) the structure of vanadium complex should bear both peroxido and zwitterionic derivatives of amino acids in the coordination sphere, c) exert reactivity commensurate with apoptotic mechanistic pathways in cellular demise, and c) provide specificity in the involved interactions with cellular targets in the cytoplasmic and nuclear milieux, thereby denoting the extent of activity contributing to the importance of such molecular agents as potential anticancer drugs. The chemistry and biology of such agents formulate a globally distinct profile that merits their further perusal as metallodrugs in tissue-specific cancer therapeutics.

References

1. Chen T.W., Fan H.L., Liu S.T., Huang S.M. Int. J. Mol. Sci. 2025, 26:7137
2. Evangelou A.M. Crit. Rev. Oncol. Hematol. 2002, 42(3):249–265.
3. Domingo J. L., Gómez M. Food Chem. Toxicol. 2016, 95:137–141.
4. Kioseoglou E., Petanidis S., Gabriel C., Salifoglou A. Coord. Chem. Rev. 2015, 301-302:87–105.

TOWARD NOVEL LIGHT-RESPONSIVE HETEROARYL-AZO MOLECULES

Bogdan C. ENACHE[1,2], George COSTACHE[1,3], Adela DOBRE[1,2], Maria POPESCU[1], Anamaria HANGANU[1,3], Augustin M. MĂDĂLAN[1], Codruța C. POPESCU[1], Mihaela MATACHE[1,4]

[1]University of Bucharest, Faculty of Chemistry, Department of Inorganic, Organic Chemistry, Biochemistry and Catalysis, Research Centre of Applied Organic Chemistry, 90 Panduri Street, 050663, Bucharest, Romania;
[2]SC Microsin SRL, Department of Research and Development, 51-63 Pericle Papahagi Street, 032364 Bucharest, Romania;
[3]Institute of Organic and Supramolecular Chemistry "C.D. Nenițescu" of the Romanian Academy, 202B Spl. Independenței, 060023, Bucharest, Romania.
[4]University of Bucharest, Faculty of Interdisciplinary Studies, Interdisciplinary School of Doctoral Studies (ISDS-UB), 6 Transilvaniei Street, Bucharest, Romania;
mihaela.matache@g.unibuc.ro

Molecular photoswitches are defined as compounds able to exist in two different states when light is used as trigger. [1] *E-Z* geometrical isomers are common examples of such light-responsive molecules. In the case of azo photoswitches, reversible photochemical conversion occurs between the thermally stable *E* isomer and metastable *Z* isomer, which reverts thermally to *E* isomer in the dark; the timescale of this conversion is highly tunable by molecular design. [2] By replacing a phenyl with a heterocycle residue, the heteroarylazo photoswitches [3] were born and this has opened new avenues in the molecular switches field. Facile access to novel heteroaryl azo molecules provides very large number of possibilities to explore their structures, properties and mechanisms of actions. This talk refers to design and synthesis of novel (hetero)arylazo molecules and their switching ability under light irradiation. We present our progress and work from the well-known pyrazole derivatives to new classes of heteroaryl azo molecules based on 1,3,4-thiadiazoles and triazapentalenes that we have recently developed.

Aknowledgments
This research was partially carried out and financed through ANC-UEFISCDI, within the framework of the second Swiss contribution MAPS project code F-RO-CH-2024-0178, contract no. 8ROCH/01/07/2025 as well as ANC-UEFISCDI, PN-IV-P6-6.1-CoEx-2024-0088, TheraFast 9CoEx/2026. Romanian Ministry of Education and Research, PNRR/2022/C9/MCID/I8, project number CF 760056/23.05.2023, code 235/29.11.2022 is also aknowledged for partial funding.

References

1. Lerch M. M., Szymański W., Feringa B. L., Chem. Soc. Rev. **2018**, 47, 1911–1937.
2. Bandara H. M. D. Burdette S. C., Chem. Soc. Rev. **2012**, 41, 1809–1825.
3. Crespi S., Simeth N. A., König B., Nat. Rev. Chem. 2019, 3:133–146.
4. a) Enache B.C., Simene A.F., Hanganu A., Tablet C., Mădălan A.M., Popescu C.C., Matache M. Synthesis-Stuttgart, 2025, 57(23): 3587-3598.
   b) Dobre A.F., Hanganu A., Nicolau I., Popescu C.C., Paun A., Madalan A.M., Tablet C., Mirea A.G., Matache M. ChemPlusChem. 2024, 89: e202300504.
   c) Enache B.C., Hanganu A., Tablet C., Anghel C.C., Popescu C.C., Paun A., Hădade N.D., Mădălan A.M., Matache M., ACS Omega. 2022, 7:39122−39135.

FROM FERROFLUIDS TO FERROFLUID DRIVEN MANUFACTURING OF NEW MATERIALS-THE ROLE OF CHEMISTRY

Ladislau VÉKÁS

Romanian Academy – Timișoara Branch, Center for Fundamental and Advanced Technical Research, Laboratory of Magnetic Fluids, Timișoara, Romania

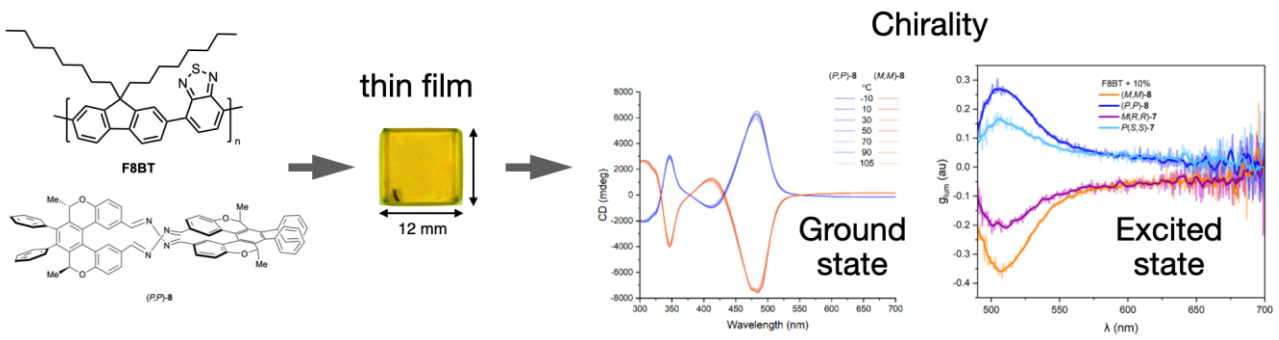
Following a short introduction the talk offers an overview of the most recent achievements on ferrofluid synthesis, advanced characterization, as well as on the governing equations of ferrohydrodynamics, the most important interfacial phenomena and the flow properties. Their magnetically controllable and tunable feature proved to be from the beginning an extremely fertile ground for a wide range of engineering applications. More recently, biocompatible ferrofluids attracted a huge interest and produced a considerable increase in the applicative potential in nanomedicine, biotechnology and environmental protection. Finally, the talk gives some details of recent advances in tunable and adaptive multifunctional materials derived from ferrofluids and a brief presentation of the recent progress of applications in the field, among them magnetoresponsive adsorbents, nano-micro composite magnetorheological fluids, new types of leakage-free rotating seals, as well as magnetorheological brakes and clutches.

CHIRAL EMISSIVE THIN FILMS

G. Dan PANTOȘ

University of Bath, Department of Chemistry, United Kingdom

We will discuss two strategies of producing chiral thin films on fused silica plates, firstly by spincoating/dropcasting chiral phthalocyanines and secondly by spincoating achiral polymer/chiral dopant blends. The film chirality has been investigated using benchtop spectrophotometers, CDi mapping and Mueller matrix polarimetry in order assess their homogeneity and chiroptical properties. We will also discuss the design and synthesis of enantiomers of a [5]helicenoid derived molecular lemniscate (figure-of-eight shaped molecule), in which two homochiral helicenes are linked via the formation of two azine motifs. We demonstrate that these molecules, and their helicenoid constituents, are also excellent chiral dopants that induce dissymmetry in the ground and excited states of the achiral emissive polymer F8BT, leading to high CPL activity. The ability to control the handedness of the helicenoid dopants via enantiopure synthesis affords control of the sign of circularly polarised emission. This method of inducing large dissymmetry factors in achiral emissive polymers allow us to produce new materials of great interest for next-generation optoelectronic technologies.



INNOVATIVE MATERIALS FOR ENVIRONMENTAL APPLICATIONS, RESOURCES RECOVERY AND REUSE

Marcela MIHAI

Petru Poni Institute of Macromolecular Chemistry, Grigore Ghica Voda Alley No 41A, Iasi – 700487, Romania
marcela.mihai@icmpp.ro

Currently there is a strong need for polymeric materials from more sustainable sources and polysaccharides, as an important and abundant class of biomacromolecules, can be the answer to human needs now and in the future. Natural biopolymers can be chemically modified owing to the presence of numerous and free functional groups, such as amine, hydroxyl, carboxyl, and sulfate sites displayed along their backbones. Our group scientific interest is focused on finding integrated research solution (Figure 1) both by capitalizing on the knowledge and skills in the field of ionic polymer synthesis and functionalization of synthetic/natural polymers, obtaining complex multi-component systems with applications in different fields.

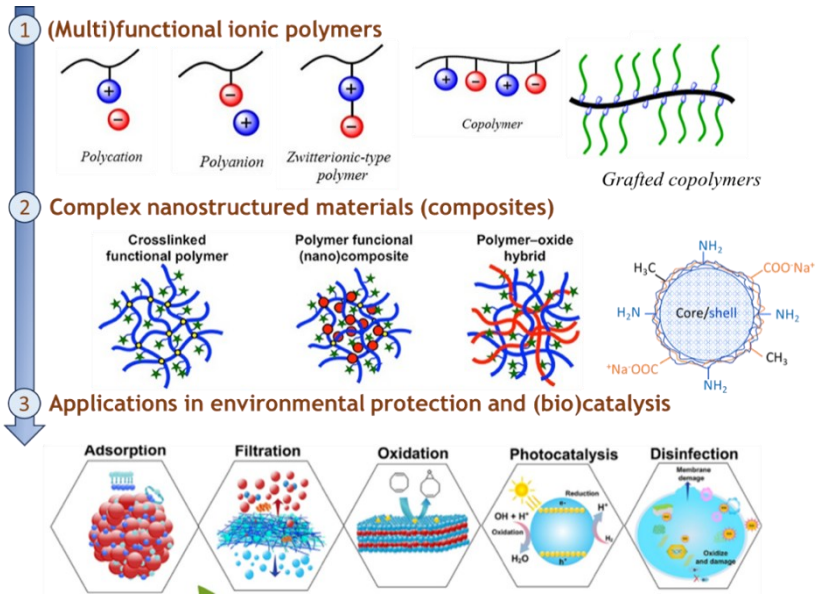


Figure 1. Integrated research solution on (1) synthesis of (multi)functional polymers, (2) fabrication of complex nanostructured materials and (3) testing in specific applications

Finding efficient and economical methods for removing metal ions and organic pollutants from surface water or wastewater is a priority worldwide. Therefore, the obtained materials, which combine rapid sorption with the possibility of immobilizing large amounts of pollutants, are of extraordinary practical interest, especially in water treatment. Controlling the chemical composition of nanoscale surfaces and creating specific functional groups for subsequent molecular interactions is essential not only in water purification but also in sensor design, controlled drug release, photocatalysis, chromatography, etc.

Acknowledgements
This work was supported by a grant of the Ministry of Education and Research, CCCDI - UEFISCDI, through the project *Center of Excellence in water management, materials, by-products and waste valorisation for circular bioeconomy implementation*, project code PN-IV-P6-6.1-CoEx-2024-0056, contract 6CoEx/02.06.2026 and through the project *Multifunctional hybrid nanostructures of natural macromolecules and metals,* PN-IV-P1-PCE-2023-0738, contract 71PCE/01.07.2025, within PNCDI IV.

SNAIL-BASED PRODUCTS AS SUSTAINABLE RESOURCES FOR CIRCULAR BIOECONOMY APPLICATIONS

Dana-Maria COPOLOVICI [1,2], Cristian MOISA [2], Andreea LUPITU [2], Flavia BORTES [1,3], Elena Rusandra ILLYES [4], Luminița ANDRONIC [4], Lucian COPOLOVICI [1,2,3]

[1] "Aurel Vlaicu" University of Arad, Faculty of Food Engineering, Tourism, and Environmental Protection; Elena Dragoi St., Nr. 2, Arad, 310330, Romania,
[2] "Aurel Vlaicu" University of Arad, Institute for Interdisciplinary Research, Romania, Elena Dragoi St., Nr. 2, Arad, 310330, Romania,
[3] "Aurel Vlaicu" University of Arad, Interdisciplinary School of Doctoral Studies, Elena Dragoi St., Nr. 2, Arad, 310330, Romania, Romania
[4] Transilvania University of Brasov, Faculty of Product Design and Environment, B-dul Eroilor nr. 29, 500036, Brașov,
dana.copolovici@uav.ro

The transition toward a circular bioeconomy increasingly relies on the sustainable valorization of biological by-products, and snail-derived materials-including meat, shells, mucus, and internal organs-represent promising renewable resources for food production, agriculture, environmental remediation, and biomaterial development. This study evaluates the potential integration of these snail-derived fractions into circular bioeconomy models by considering their chemical and biological characteristics and their possible use as nutritional resources, environmentally friendly fertilizers, adsorbents, composite fillers, and sources of biologically active compounds, with particular attention to nutrient recovery and hydroponic cultivation. Snail by-products are rich in high-quality proteins and peptides, essential amino acids, minerals, and other bioactive constituents, while shells, composed predominantly of $CaCO_3$, can be processed into soil amendments, fertilizer components, adsorbent materials, or fillers for composite biomaterials. Furthermore, other snail-derived fractions may provide nutrients and biologically active compounds capable of supporting plant development and improving nutrient-use efficiency. Their integration into sustainable agricultural systems, including combinations with photocatalytic processes, could contribute to contaminant removal, water reuse, and reduced dependence on conventional synthetic inputs, thereby supporting more resource-efficient production systems. Overall, snail-derived products and processing residues show substantial potential for circular bioeconomy applications, although their broader implementation requires standardized processing protocols, comprehensive physicochemical characterization, safety and toxicity assessment, agronomic validation, life-cycle evaluation, and economic feasibility analysis.

Acknowledgements
This work was supported by a grant of the Ministry of Education and Research, CNCS - UEFISCDI, project number PN-IV-P7-7.1-PTE-2024-0387, within PNCDI IV.

References
1. Surowka K., Ligaszewski M., Szymczyk B., Anthony B., J. Food Compost. Anal. 2025, 140:107221.
2. Adepitan O.L., Alabi O.O., Gbadeyan O.J., Deenadayalu N., Jayeola A.T., Discover Material 2025, 5:25.
3. Anand M.A.V., Wang W.L., Yang C.J., Lai J.Y., Yao C.H., Food. Res. Int. 2006, 223:117872.

CAN METALS BIND TO BILIPROTEINS?

Alexandru SONICA, Radu SILAGHI-DUMITRESCU

Babeș-Bolyai University, Faculty of Chemistry and Chemical Engineering, 11 Arany János Street, 400028 Cluj-Napoca, Romania
alexandru.sonica@ubbcluj.ro

The chemistry of metal complexes binding to proteins through residues or cofactors [1, 2] lies at the heart of many essential biological processes. The so-called pigments of life are almost entirely cyclic tetrapyrroles acting as the first coordination sphere to metals, as in heme, chlorophyll or cobalamin, and are the driving force in giving very specific reactivities. Bilins instead arise from oxidative heme opening followed by reductive conversion to linear tetrapyrroles; such catabolites were evolutionarily recruited by oxygenic phototrophs for light harvesting and photoreception. In this context, it remains unclear whether bilins can also support biologically relevant chemistry as a first coordination sphere to metals. We therefore explore whether biliproteins can support metal coordination under two distinct scenarios: (1) an ideal scenario representing de novo protein scaffolds designed for this purpose, and (2) in existing biliproteins, by outlining the different protonation states of the cofactor and its metal-binding capabilities, employing spectroscopic methods. [3, 4]

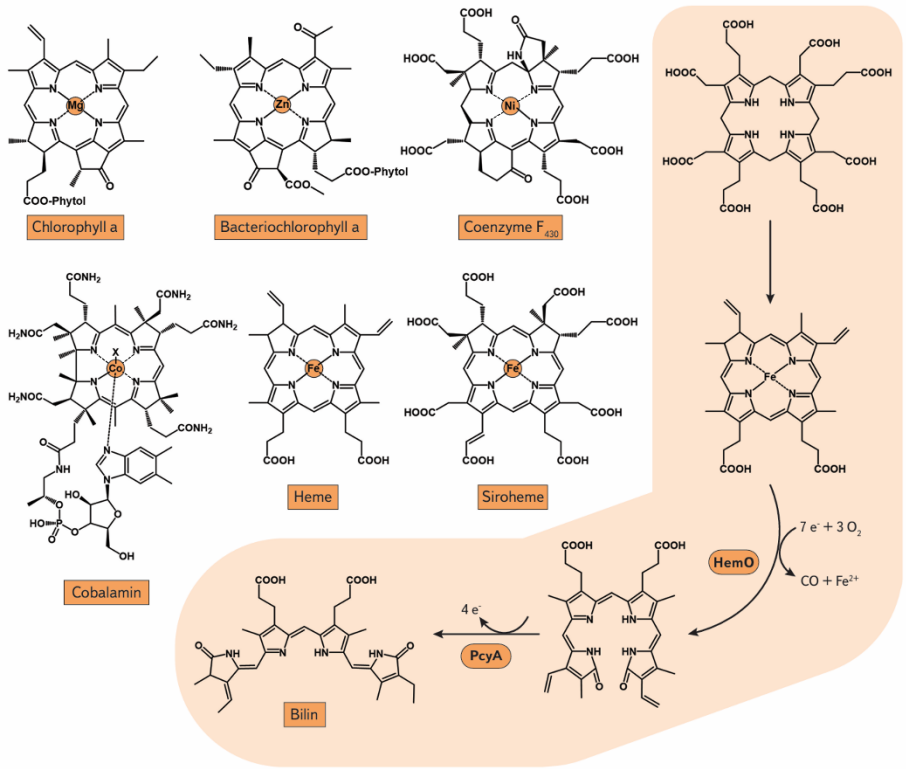


Figure 1. An overview of the tetrapyrrolic pigments of life.

Acknowledgements
I gratefully acknowledge Dr. Alida Timar-Gabor (Babeș-Bolyai University) for her assistance with the low-temperature EPR measurements, Dr. Bogdan Drugă and Dr. Adriana Hegedus (Institute for Biological Research) for kindly providing the *Spirulina platensis* sample used in this study.

References
1. Valentová J., Humboldt A., Korcová J., Svitková B., Silaghi-Dumitrescu R., Sonica A., et al., Chem. Eur. J. 2025, e01578.
2. Lehene, M.; Simon, J.; Zagrean-Tuza, C.; Aghion, A.; Vasile, B.; Sonica, A., et al., Biochim. Biophys. Acta, Proteins Proteomics. 2025, 1873:141086.
3. Wegner H., Roitman S., Kupczok A., Braun V., Woodhouse J. N., Grossart H.-P., et al., Nat. Commun. 2024, 15:8783.
4. Krishna R., Wang J., Ahern W., Sturmfels P., Venkatesh P., Kalvet I., et al., Science. 2024, 384:6693.

NEW REACTIVITY PATTERNS IN THE DOEBNER REACTION OF CYCLIC SECONDARY AMINE-SUBSTITUTED BENZALDEHYDES WITH ELECTRON-WITHDRAWING ANILINES

Maria Cristina AL-MATARNEH[1], Alina NICOLESCU [2], Mihaela SILION[3], Kulcitki VEACESLAV[4]

[1]Research Institute of the University of Bucharest-ICUB, 91-95 Spl. Independentei, 050095 Bucharest, Romania
[2]NMR Laboratory "Petru Poni" Institute of Macromolecular Chemistry of Romanian Academy, 41A Grigore Ghica Voda Alley, Iasi 700487, Romania
[3]Physics of Polymers and Polymeric Materials Department, "Petru Poni" Institute of Macromolecular Chemistry, 41A Grigore Ghica Voda Alley, 700487, Iasi, Romania
[4]Moldova State University, Institute of Chemistry, 3, Academiei str., Chişinău MD-2028, Republic of Moldova
almatarneh.cristina@icmpp.ro

The Doebner reaction is a well-established synthetic method for the preparation of α,β-unsaturated carboxylic acids. However, when electron-withdrawing anilines are employed instead of electron-donating analogues, the reaction follows a distinct pathway, predominantly leading to the formation of pyrrol-2-one derivatives rather than the expected cinnamic acid products. This altered reactivity highlights the complexity of the reaction mechanism and the influence of substrate electronic properties. [1]

Our research group has previously demonstrated that, besides the electronic nature of the aniline, the aldehyde component can also play a decisive role in determining the reaction outcome. In particular cases, the aldehyde directs the reaction toward the formation of complex product mixtures or promotes the selective formation of unique heterocyclic scaffolds, including furan-based derivatives and other unexpected structural motifs. [2, 3]

Motivated by these findings, the present study investigates the influence of aromatic aldehydes substituted with cyclic secondary amines, namely morpholine, piperidine, and pyrrolidine, on the Doebner reaction with electron-withdrawing anilines. The objective is to elucidate how these N-heterocyclic substituents affect the reaction pathway and product selectivity while providing access to novel heterocyclic compounds with potential applications in medicinal chemistry and organic synthesis.

Acknowledgements
This work was supported by a bilateral grant of the Romanian National Authority for Scientific Research (CNCS – UEFISCDI) project PN-IV-PCB-RO-MD-2024-0018. (43PCBROMD/01.09.2025) and National Agency for Research and Development (ANCD) of the Republic of Moldova, program PN-IV-PCB-RO-MD-2024-0018 (25.80013.8007.05ROMD).

References
1. Omidkhah N, Ghodsi R. Synth Commun. 2021, 51(13):1947–1955.
2. Al-Matarneh C.M., Nicolescu A., Marinaş I.C., Găboreanu M.D., Shova S., Dascălu A., Silion M., Pinteală M. Molecules. 2024, 29(4):772.
3. Nicolescu A., Pinteală M., Al-Matarneh C.M.. Rev Roum Chim. 2025, 70(7–8):475–482.

NON-CONJUGATED POLYAMIDE FOR FLEXIBLE SUPERCAPACITORS WITH ELECTROCHROMIC STATE-OF-CHARGE VISUALIZATION

Andra-Elena BEJAN, Catalin-Paul CONSTANTIN, Mariana-Dana DAMACEANU

Petru Poni Institute of Macromolecular Chemistry, Romanian Academy, Electroactive Polymers and Plasmochemistry Department, Grigore Ghica Voda Alley, 41A, 700487, Iasi, Romania
bejan.andra@icmpp.ro

Flexible electrochromic energy storage devices have emerged as promising candidates for next-generation wearable and smart optoelectronic technologies by integrating reversible optical modulation with electrical energy storage into a single multifunctional platform. Although indium tin oxide deposited on polyethylene terephthalate (ITO-PET) is widely employed as a transparent flexible electrode, the influence of substrate flexibility on device performance remains insufficiently explored. [1–3] Herein, a non-conjugated aromatic polyamide was investigated as a multifunctional electrode material for flexible electrochromic supercapacitors. [4] Uniform thin films were deposited onto ITO-PET substrates and evaluated by electrochemical, spectroelectrochemical and chronoamperometric techniques in both three-electrode cells and flexible prototype devices under planar and bent conditions.

The polymer-modified electrode exhibited hybrid battery-type charge storage with an areal capacitance of **3.95 mF cm^{-2}**, while the flexible devices retained comparable electrochemical performance in both configurations. The bent device maintained Coulombic efficiencies above **96%** after **500** charge-discharge cycles, demonstrating excellent mechanical stability. The polyamide also displayed a reversible **yellow-to-green** electrochromic transition with **67.12%** optical contrast at **880 nm**, switching times of **3.3/2.3 s** (coloration/bleaching), and improved coloration efficiency upon cycling. The flexible prototypes combined stable optical modulation with charge-storage capability (Figure 1), demonstrating the potential of non-conjugated polyamides for durable flexible electrochromic energy-storage devices, smart windows and wearable optoelectronics. [5–7]

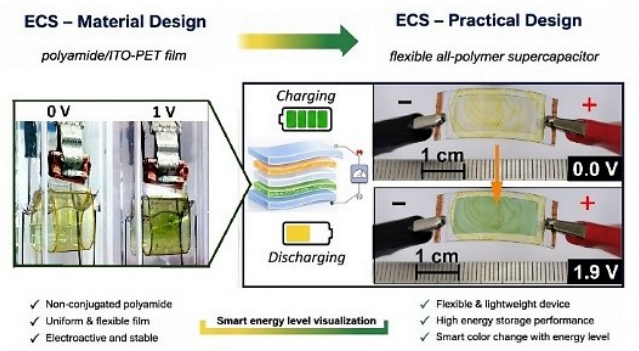


Figure 1. Flexible polyamide-coated ITO-PET electrode and supercapacitor device.

Acknowledgements
This work was financially supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS – UEFISCDI, project number PN-IV-P2-2.1-TE-2023-0213, contract no. 36TE/08.01.2025, within PNCDI IV.

References
1. Zardetto V., Brown T.M., Reale A., Di Carlo A., J. Polym. Sci. B Polym. Phys. 2011, 49:638-648.
2. Nuroldayeva G., Balanay M.P., Polymers 2023, 15:2924.
3. Xie Y., Li M., Chen J., Cao N., Gu G., Liu X., Chao D., J. Colloid Interface Sci. 2025, 693:137592.
4. Bejan A.E., Constantin C.P., Damaceanu M.D., J. Power Sources 2024, 613:234829.
5. Bejan A.E., Constantin C.P., Stoica I., Damaceanu M.D., ACS Appl. Polym. Mater. 2026, 8(12):6c01056.
6. Constantin C.P., Trofin I.A., Damaceanu M.D., Rusu R.D., J. Power Sources 2025, 644:237098.
7. Bejan A.E., Constantin C.P., Nicolescu A., Damaceanu M.D., Chem. Eng. J. 2026, 532:174223.

RATIONAL DESIGN AND STRUCTURAL INVESTIGATION OF LANTHANIDE AND TRANSITION METAL COMPLEXES WITH EXTENDED π-CONJUGATED LIGANDS

Robert I. BOTEA, Augustin MĂDĂLAN

University of Bucharest, Faculty of Chemistry, Regina Elisabeta Blvd. 4-12, Bucharest – 030018, Bucharest, Romania
ioan.botea@s.unibuc.ro

Polydentate Schiff base ligands derived from N-(1-naphthyl)ethylenediamine and substituted salicylaldehydes were employed for the synthesis of mono- and heteronuclear complexes containing 3d, 4d, and 4f metal ions. Owing to their extended π-conjugated systems and multiple coordination sites, these ligands promote the formation of structurally diverse metal complexes with a broad range of functional properties. [1]
Mononuclear complexes of Zn(II), Cu(II), Pd(II), Eu(III), and Tb(III) were synthesized and extensively characterized using spectroscopic techniques and single-crystal X-ray diffraction. The crystallographic analyses confirmed coordination geometries ranging from tetrahedral and square-planar to square-antiprismatic. A schematic representation of the synthetic route for the 3d metal complexes is presented in Figure 1.

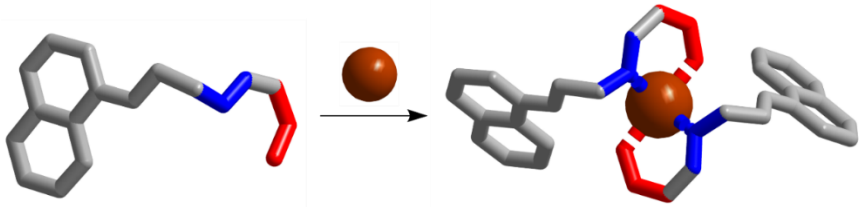


Figure 1. Schematic synthesis of 3d complexes using Schiff base ligands.

Luminescence studies demonstrated emission from Eu(III) and Tb(III) complexes, generated from efficient ligand-to-metal energy transfer. Furthermore, stepwise synthetic approaches enabled the synthesis of heterometallic Zn-Ln complexes, which showed enhanced luminescent properties.
Special attention was given to Pd(II) complexes due to their potential interactions with biomolecules. Their square-planar geometry, together with previous DNA-binding studies, suggests a possible intercalative mode of interaction, making these compounds promising candidates for further investigation as potential intercalators. [2] Figure 2 shows the X-ray crystal structures of two Pd(II) complexes with differing metal-to-ligand stoichiometries.

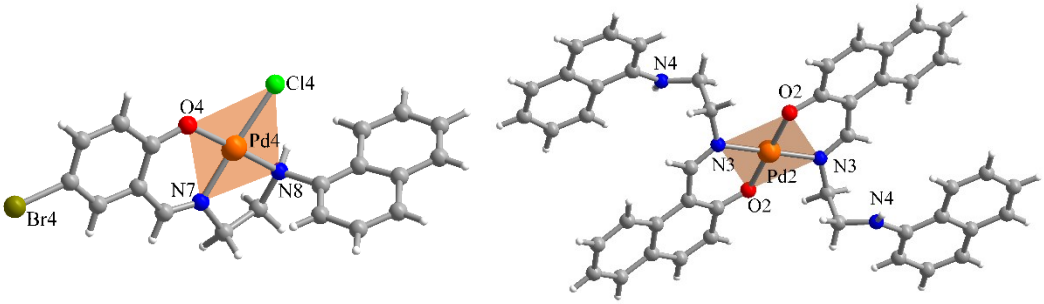


Figure 2. X-ray crystal structures of two Pd(II) complexes featuring 1:1 and 1:2 metal-to-ligand ratios.

References
1. Andruh M., Dalton Trans. 2015, 44:16633-16653.
2. Mbugua S.N., Sibuyi N.R.S., Njenga L.W., ACS Omega. 2020, 5:14942–14954.

SYNTHESIS AND CHARACTERISATION OF FLEXIBLE POLYIMIDE BLENDS INCORPORATING BULKY AND FLUORINATED UNITS

Adriana-Petronela CHIRIAC, Dan-Radu RUSU, Mariana-Dana DAMACEANU

Petru Poni Institute of Macromolecular Chemistry, Electroactive Polymers & Plasmochemistry Laboratory, 41A Grigore Ghica Voda Alley, Iasi, Romania
chiriac.adriana@icmpp.ro

Polyimides are a class of high-performance polymeric materials widely used in various applications due to their high glass transition temperatures, high thermal and chemical stability, and good mechanical and optical properties. Their applications include engineering plastics, insulating coatings for aerospace applications, separation membranes, sensors, and various optical and electronic devices. [1, 2]
However, aromatic polyimides generally show poor solubility and processability due to the rigid polymer chains and strong intermolecular interactions, which significantly limit their applicability. To improve their properties, various monomers with different structures, such as spiro, cardo, aliphatic, bulky, and fluorinated units, have been incorporated into polyimides, making materials with improved solubility, low dielectric constant, high optical transparency, and other properties. [3]. Among the most efficient strategies, the introduction of semi-aromatic or fluorine-containing groups into polymer backbones to prepare fluorinated aromatic polyimides has proven to enhance optical transparency and lower dielectric constants. [4, 5] In addition, fluorinated groups also enhance the hydrophobicity of polyimide films. [6]
A versatile, cost-effective pathway to bypass most drawbacks of aromatic polyimides is blending neat polymers with already certified performance. It enables the development of tailored polymer materials that synergistically combine the specific thermal, mechanical, and transport characteristics of multiple individual polymers into a single, high-performance material. [7]
In this context, we report the synthesis of a series of polymeric blends based on polyimides with bulky groups combined with a fluorinated counterpart, which were further employed to obtain flexible free-standing films by the drop-casting method. Besides detailed structural and physico-chemical characterization of the polyimides, the resulting polymer blends were investigated concerning the components' miscibility, by using scanning electron microscopy, FTIR spectroscopy, and differential scanning calorimetry, as well as from the perspective of their thermal, mechanical, hydrophobic, and dielectric behavior.
The obtained materials represent promising candidates for the development of dielectric components in electronic and optical applications.

Acknowledgements
This work was financially supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS – UEFISCDI, project number PN-IV-P2-2.1-TE-2023-1896, contract no. 143TE/05.01.2026, within PNCDI IV.

References
1. Ma J., Liu X., Wang R., Lu C., Wen X., Tu G., Nanomaterials. 2023, 13:656.
2. Nagella S.R., Ha C.S., Nanomaterials. 2023, 13, 2090.
3. Liaw D.J., Wang K.L., Huang Y.C., Lee K.R., Lai J.Y., Ha, C.S., Prog. Polym. Sci. 2012, 37:907−974.
4. He J.J., Yang H.X., Zheng F., Yang S.Y., Polymers. 2022, 14:649.
5. Peng W.F., Lei H.Y., Zhang X.X., Qiu L.H., Huang, M.J., Chinese J. Polym. Sci. 2022, 40:781–788.
6. Shi Y., Hu J., Li X., Jian J., Jiang L., Yin C., Xi Y., Huang K., Su L., Zhou L., RSC Adv. 2024, 14:32613.
7. Yong W.F., Zhang H., Prog. Mater. Sci. 2021, 116:100713.

BIOINSPIRED ARSENIC-SEQUESTERING MEMBRANES FOR SUSTAINABLE WATER DECONTAMINATION

Francesco GALIANO[1], Raffaella MANCUSO[2], Lorenzo GUAZZELLI[3], Christian Silvio POMELLI[3], Jochen BUNDSCHUCH[4], Jörg RINKLEBE[5], Shan-Li WANG[6], Carmine APOLLARO[7], Fabio PALUMBO[8], Cinzia CHIAPPE[3], Bartolo GABRIELE[2], Alberto FIGOLI[1]

[1]Institute on Membrane Technology "Enrico Drioli", National Research Council of Italy (CNR-ITM), Italy
[2] Dep. Chemistry and Chem. Technol., University of Calabria, Italy
[3]University of Pisa, Italy
[4]University of Southern Queensland, Australia
[5]University of Wuppertal, Germany
[6]National Taiwan University, Taiwan
[7]Dep. Biology, Ecology and Earth Sci., University of Calabria, Italy
[8]Institute of Nanotechnology, National Research Council, 70125 Bari, Italy
f.galiano@itm.cnr.it

Arsenic contamination of groundwater represents a major global challenge, affecting millions of people and posing serious risks to human health. [1] Conventional arsenic removal technologies often suffer from high energy consumption, limited selectivity, generation of secondary waste, and poor efficiency towards arsenite (As(III)), the most toxic and difficult-to-remove arsenic species. [2] In this work, a novel bioinspired porous membrane was developed for the selective sequestration of both arsenate (As(V)) and arsenite (As(III)) from contaminated water. The membrane was prepared through the polymerization of a tailored sulfur-containing polymerizable ionic liquid (PIL-S) within a porous polymer matrix, mimicking the arsenic-binding mechanisms found in biological systems. [3] The resulting membrane exhibited high water permeability and outstanding arsenic removal performance, achieving extraction efficiencies up to 99.6% in model solutions and reducing arsenic concentrations below the World Health Organization guideline value of 10 μg L^{-1}. Synchrotron-based EXAFS analyses confirmed the formation of strong As–S covalent interactions responsible for the selective capture mechanism. The membrane was successfully tested on naturally arsenic-contaminated groundwater, reducing arsenic concentrations from 65 μg L^{-1} to below the drinking water limit in a single filtration step while preserving the mineral composition of the water. Furthermore, the membrane could be easily regenerated through a simple acidic treatment without loss of performance over multiple cycles.

These results demonstrate the potential of bioinspired selective membranes as an effective, low-energy and sustainable solution for arsenic remediation, offering a promising alternative to conventional treatment technologies for the production of safe drinking water.

References

1. Bhattacharya P., Bundschuh J., CRC Press. 2010.
2. Figoli A., Criscuoli A., J. Hazardous Material. 2019, 370:147-155.
3. Galiano F., Mancuso R., Guazzelli L., Pomelli C. S., Bundschuch J., Rinklebe J., Wang S.-L., Apollaro C., Palumbo F., Chiappe C., Gabriele B., Figoli A., Nature Water. 2023, 2:350-359.

SUSTAINABLE-SOLVENT-PROCESSED PVDF/CARBON NANOHORN MEMBRANES FOR ENHANCED SEPARATION PERFORMANCE

Giuseppe DI LUCA, Francesco GALIANO, Alberto FIGOLI

Istituto per la tecnologia a membrana "E. Drioli" (CNR-ITM), Via P. Bucci 17/c, 87036 Rende (CS), Italy
g.diluca@itm.cnr.it

Polyvinylidene fluoride (PVDF) membranes are widely used in water treatment for their excellent chemical stability and mechanical robustness. [1] However, their intrinsic hydrophobicity and the use of toxic aprotic solvents during fabrication remain critical challenges for sustainable membrane engineering. [2]

This work presents a green strategy for preparing high-performance PVDF membranes by combining sustainable solvent processing with advanced surface functionalisation. Membranes were fabricated via phase inversion using triethyl phosphate (TEP) as an environmentally friendly solvent, followed by cross-linking ammonia-plasma-treated carbon nanohorns (CNHs) with sulphonic and zwitterionic functionalities to tailor surface chemistry and antifouling properties.

A comprehensive physicochemical analysis-including ATR-FTIR, XPS, Raman spectroscopy, TEM, water contact angle, and zeta potential measurements, confirmed successful covalent immobilisation of functional groups and the development of charge-adjustable membrane interfaces. The synergistic effect of plasma-functionalised CNHs and ionic surface groups markedly improved membrane wettability, surface hydration, and electrostatic repulsion against organic foulants.

Filtration tests using humic acid solutions under cross-flow conditions showed significant enhancements in permeability and fouling resistance. The modified membranes achieved water permeabilities of up to 2268 L m^{-2} h^{-1} bar^{-1}, about 94% higher than pristine PVDF membranes, while still providing excellent rejection and stable long-term performance.

The proposed approach offers a viable pathway to developing sustainable, high-flux, and antifouling PVDF membranes for advanced water treatment applications, combining green fabrication processes with durable, nanostructured surface engineering.

Acknowledgements
The authors acknowledge the financial support of the project "FUTURAW" FOE 2024, "The raw materials of the future from non-critical, residual and renewable sources", financed by MUR (Riparto Fondo Ordinario Enti di Ricerca), CUP: B53C24011380001, DCM.AD004.304.001.

References
1. Pendergast M.M., Hoek E.M.V., Energy Environ Sci. 2011, 4:1946–1971.
2. Figoli A., Marino T., Simone S., Di Nicolò E., Li X.M., He T., Tornaghi S., Green Chem. 2014, 16(9):4034– 4059.

EMERGING TRENDS IN ENANTIOSELECTIVE LIQUID CHROMATOGRAPHIC SEPARATIONS: FOCUS ON ION-EXCHANGE-BASED CHIRAL STATIONARY PHASES

István ILISZ, Gábor NÉMETI, Róbert BERKECZ

Institute of Pharmaceutical Analysis, Faculty of Pharmacy, University of Szeged, H-6720 Szeged, Somogyi u. 4., Hungary
ilisz.istvan@szte.hu

Chirality is a fundamental property of molecular structure that plays a crucial role in biological systems, since living organisms are inherently stereoselective. Enantiomers of the same compound may exhibit markedly different pharmacological, toxicological, or metabolic behavior. Therefore, the separation and analysis of enantiomers remain essential in pharmaceutical, biomedical, and agrochemical research. Among the available analytical techniques, high-performance liquid chromatography (HPLC) has become the most powerful and versatile method for enantioselective analysis due to its high efficiency, robustness, and broad applicability. The success of enantioselective HPLC is closely linked to the continuous development of chiral stationary phases (CSPs), which provide the basis for selective enantiomer recognition. Recent developments in CSPs include improved selector design, advanced immobilization and coating strategies, as well as the application of modern particle technologies such as superficially porous and sub-2 μm materials. These innovations have significantly enhanced separation efficiency, selectivity, and robustness while enabling faster analyses. In addition, they have expanded the applicability of CSPs to a broader range of enantioselective separations under diverse chromatographic conditions.

Among the numerous CSP families, ion-exchange-based CSPs have gained considerable attention because of their outstanding performance in the separation of ionizable compounds, including pharmaceutically relevant analytes. Particular attention has been devoted to *Cinchona* alkaloid-based CSPs, which represent one of the most versatile and successful ion-exchange selector classes. Derived from quinine and quinidine, these selectors possess a rigid chiral scaffold and ionizable functional groups, enabling efficient and complementary enantiomer recognition. Their chiral recognition mechanism is based on the synergistic contribution of ionic interactions, hydrogen bonding, π–π interactions, and steric effects, allowing highly selective and tunable enantioseparations.

This presentation summarizes emerging trends in enantioselective liquid chromatography, with special focus on ion-exchange-based CSPs and *Cinchona* alkaloid-derived selectors. In addition to mechanistic aspects, recent methodological developments, and representative pharmaceutical applications, particular attention will be given to the green chemical aspects of enantioselective separations.

SUSTAINABLE BAMBOO-DERIVED BIOCHAR AS A FUNCTIONAL ENZYME SUPPORT: EFFECT OF PYROLYSIS CONDITIONS

Lizeth Marlen MORENO PASCUAL[1] , Natalia Nicotra[1], Francesco Papatola[1], Omar Ginoble PANDOLI[2], Alessandro PELLIS[1]

[1]*University of Genova, Department of Chemistry and Chemistry of Materials, Via Dodecaneso 31, 16146, Genova, Italy.* S4646706@edu.unige.it, alessandro.pellis@unige.it
[2]*University of Genova, Department of Pharmacy, Viale Cembrano 4, 16148, Genova, Italy*
omar.ginoblepandoli@unige.it

Bamboo is a renewable lignocellulosic biomass with significant potential as a sustainable precursor for functional carbon materials. In this work, untreated *Dendrocalamus giganteus* was converted into bamboo-derived activated carbons (BACs) through fast pyrolysis (300–600 °C) under nitrogen followed by in situ CO_2 activation. This approach enabled precise tuning of the structural, surface, and paramagnetic properties of the resulting carbon like material, including permanent free radical formation. The materials were characterized by DRIFT, BET surface area analysis, and nitrogen adsorption–desorption measurements. Pyrolysis temperature strongly influenced pore architecture, with B600 being predominantly microporous, B500 exhibiting a mesoporous structure, and B400 displaying a macroporous network, making these materials attractive candidates for enzyme immobilization. [1]
The biochars were evaluated as support for *Candida antarctica lipase* B (*CaL*B). The catalytic performance of immobilized *CaL*B was assessed using a model polycondensation reaction of 1,8-octanediol and dimethyl adipate, producing an aliphatic polyester. The monomer conversion and the polymer properties were analyzed by NMR and GPC. High monomer conversions were achieved across all materials (97% B300, 97% for B400, 94% for B500, and 75% for B600), with substantial differences in the obtained polymer molecular weight. B300 enabled the formation of polyesters with a number-average molecular weight of approximately 4 kDa while B400 yielded the highest molecular weight of 11 kDa, compared to 7.5 kDa for B500 and only 1.5 kDa for B600. These results indicate that macroporous biochars promote more favorable enzyme orientation and accessibility, whereas microporous structures impose steric constraints that limit polymer chain growth.

Acknowledgements
Project Funded by the European Union ERC Starting Grant CIRCULARIZE 101114664

References
1. Franchi P., Turchetti A., Lucarini M., et al., Catal. Sci. Technol. 2025, 15:6161–6178.

SWEET SUGAR-BASED PLASTICIZERS FOR POLYMERS

Andrea PASQUALE[1], Martina GALATINI[1], Giacomo DAMONTE[1], Anamaria TODEA[2], Laura CIPOLLA[3], Dario CAVALLO [1]*, Alessandro PELLIS[1]*

[1]Department of Chemistry and Industrial Chemistry, University of Genova, via Dodecaneso 31, 16146, Genova (GE), Italy
[2]Faculty of Industrial Chemistry and Environmental Engineering, Polytechnic University of Timisoara, Carol Telbisz 6, 300001 Timisoara, Romania
[3]Department of Biotechnology and Biosciences, University of Milano-Bicocca, Piazza della Scienza 2, Milano I-20126, Italy
dario.cavallo@unige.it and alessandro.pellis@unige.it

Carbohydrates are among the most abundant polymers in the world and offer a promising alternative for valorization and synthesis of value-added chemicals. Galactaric acid is an attractive bio-based building block; however, it has not yet been fully exploited. [1, 2] Currently, regulatory, sustainability, safety-by-design and performance requirements for additives are becoming increasingly strict. As a result, innovation in this field must be accelerated to develop new materials with enhanced properties. With this objective, new sugar-based plasticizers: GalO-2EH, GalA-2EH and GalX-2EH, have been synthesized (*Figure 1.*). In this framework, PLA was selected as a model bio-based polymer due to its inherent brittleness, in order to evaluate the ability of these innovative additives to improve its properties. [3] GalA-2EH showed the best performance in terms of reducing the glass transition temperature (*Tg*) and increasing the elongation at break up to 260% of PLA thin films. Experimental results have been supported by computational results to highlight how small modifications in the molecular structure can influence both the synthesis and the performance of these additives. These new plasticizers could be used in a wide range of applications across different types of polymers.

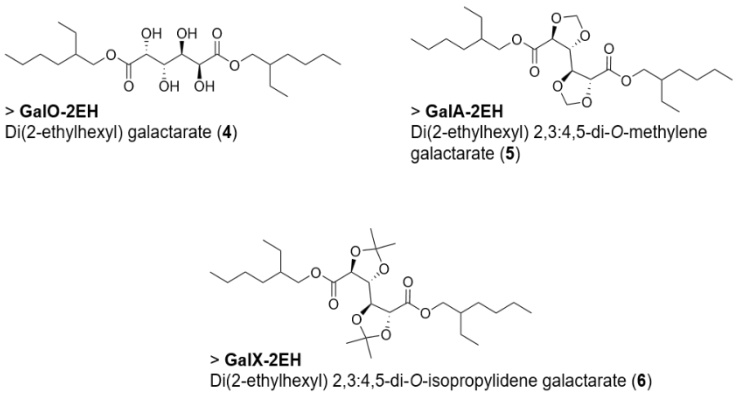


Figure 1. Novel galactarate-based plasticizers GalO-2EH, GalA-2EH and GalX-2EH synthesized.

Acknowledgements
Funded by the European Union (ERC, CIRCULARIZE, 101114664). Views and opinions expressed are, however, those of the author(s) only and do not necessarily reflect those of the European Union or the European Research Council. Neither the European Union nor the granting authority can be held responsible for them.

References
1. Muñoz-Guerra S., Lavilla C., Japu C. and Martínez De Ilarduya A., Green Chem. 2014, 16:1716–1739.
2. Trapasso G., Annatelli M., Dalla Torre D. and Aricò F., Green Chem. 2022, 24:2766–2771.
3. Ramezani Dana H. and Ebrahimi F., Polym. Eng. Sci. 2023, 63:22–43.

TRENDS TO DYE FOR: FLAVONOIDS AS ECO-COLORANTS OF TEXTILE FIBERS WITH 2-IN-1 RESULTING PROPERTIES

Leposava PAVUN

University of Belgrade - Faculty of Pharmacy, Vojvode Stepe 450, 11221 Belgrade, Serbia
leposava.pavun@pharmacy.bg.ac.rs

Flavonoids are a large group of polyphenolic compounds widely found in the plant kingdom. These plant pigments give rise to the bright and attractive colors of flowers, fruits and leaves (from yellow and orange to red, blue and purple). These bioactive compounds attract attention due to their numerous bioactive properties. Fresh fruits and vegetables and their products, along with traditional and herbal teas, are prominent sources of dietary polyphenols, a class of bioactive molecules closely linked to various health benefits.

Beyond the undeniable benefits of consuming foods rich in bioactive molecules, their beneficial effects are also observed when used as natural dyes for textiles. From the literature review, it is evident that the extracts of various parts of plants and product of plants, such as roots, bark, peels, leaves, berries, and pomaces, are used as sources of natural ecological dyes. [1-3] These dyes are skin-friendly, biodegradable, and do not cause environmental pollution. Apart from color, the great majority of them can impart functional properties to textile materials, such as UV protection, antioxidant and antimicrobial activity attributed to polyphenolic compounds, primarily flavonoids, present in the extract. Fabrics with such improved characteristics may be suitable for medical use because, thanks to their antioxidant properties, they can capture free radicals and reactive oxygen species and prevent cell decay.

For an extract obtained from natural sources, it is necessary to determine the total polyphenol content (TPC) and evaluate its antioxidant (DPPH and ABTS test) and antimicrobial activity. The antioxidant activity of the dyed and functionalized fabrics were evaluated using the DPPH and ABTS methods, while their antimicrobial activity was tested against the same bacterial and yeast strains. [4,5]

On the other hand, this method of dyeing and functionalization with dyes from natural sources is significant from an environmental perspective. The use of industrial waste, such as cask industry waste [6] or food industry waste [3] as a natural source of dye for textiles, on the one hand, reduces water and atmospheric pollution caused by the use of synthetic dyes and pigments, while on the other hand, it reduces the amount of waste, resulting in fabrics dyed with/or functionalized with natural dyes.

Acknowledgements
This research was funded by the Ministry of Science, Technological Development and Innovation, Republic of Serbia through two Grant Agreements with University of Belgrade-Faculty of Pharmacy No 451-03-136/2025-03/ 200161 and No 451-03-137/2025-03/ 200161.

References
1. Mansour R., Dhouib S., Sakli F., J. Nat. Fibers. 2020, 19:610–620.
2. Ivanovska A., Gajić I.S., Lađarević J., Milošević M., Savić I., Mihajlovski K., Kostić M., Antioxidants. 2022, 11:2059.
3. Ugrinović V., Simović A., Ćorović M., Mihajlovski K., Lađarević J., Bajat J., Ivanovska, A., Sustain. Chem. 2025, 6:46.
4. Pavun L., Đurđević P., Jelikić-Stankov M., Đikanović D., Uskoković-Marković, S., Czech. J. Food Sci. 2018, 36:233–238
5. Pavun L., Spasojević D., Ivanovska A., Milenković M., Uskoković-Marković S., Mac. J. Chem. Chem. Eng. 2023, 42: 263–273.
6. Ivanovska A., Veljović S., Reljić M., Lađarević J., Pavun L., Natić M., Kostić M., J. Nat. Fibers. 2022, 19:11050-11063.

LEVOGLUCOSENONE-DERIVED DIOLS FOR BIOCATALYTIC POLYESTER SYNTHESIS

Francesco RABONI[1], Atsushi TAHARA[2], Lisa MONI[1], Alessandro PELLIS[1]

[1]*Università degli Studi di Genova, Dipartimento di Chimica e Chimica Industriale, Via Dodecaneso 31, 16146, Genova, Italy*
[2]*Tohoku University, Graduate School of Pharmaceutical Sciences, and FRIS, 6-3 Aoba, Aramaki, Aoba-ku, 980-8578, Sendai, Japan*
Francesco.raboni@edu.unige.it

Levoglucosenone (LGO; 1,6-Anhydro-3,4-dideoxy-β-D-glycero-hex-3-enoyranos-2-ulose) is a versatile platform molecule derived from cellulose waste such as sawdust through a simple process of acidification and pyrolysis [1]. The interest towards this structure arises from the two stereocenters, the enone functional group and the cyclic acetal bridge that can be easily exploited through many different reactions [2]. Recently the synthesis of polyhydrazones containing two LGO units linked through a double Thia-Michael rection was reported [3]. However, while aromatic dithiols readily afford the product, they are petrol-derived, possess a foul smell and give excessive rigidity to the final product. In this work, two LGO units were linked using flexible biobased aliphatic diols such as 1,4-butanediol, 1,6-hexanediol and 1,8-octanediol. The diketone structure was obtained through an acid-catalyzed Oxa-Michael reaction using LGO itself as the solvent. Following this, a Baeyer-Villiger oxidation was performed, using hydrogen peroxide in neat conditions to obtain a molecule bearing two primary alcohols, as well as two lactone functions, Figure 1. The newly synthesized diols monomers were then used in an enzymatic polymerization reaction with dimethyl esters using *Candida antarctica* Lipase B (CaLB) as a selective biocatalyst in order to leave the lactone structures unaffected. Moreover, the mild conditions used during the synthesis allow for the preservation of stereochemical information, possibly making these molecules interesting also for their chiroptical properties.

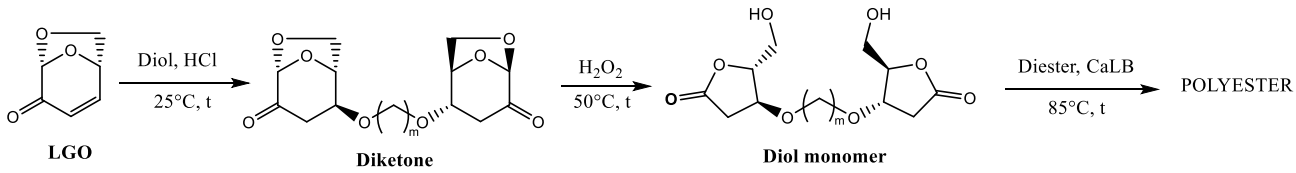


Figure 1. Synthetic procedure for the obtainment of the LGO-derived monomers

References
1. Klepp J., Dillon W., Lin Y., Feng P., Greatrex B.W., Org. Synth. 2020, 97:38.
2. Camp J., Greatrex B. W, Front. Chem. 2022, 10:902239.
3. Tahara A., Yashiro S., Hokajo T., Kudo S., Yoshizaki Y., Konno T., Doi T., Polym. Chem., 2024, 16:800.

NANO-ONCOLOGY: CHALLENGES, HOPES, AND SUCCESSES

Radostina ALEXANDROVA[1], Orlin ALEXANDROV[2], Eliya STOILOVA[1], Silvia MANCHEVA[1,3], Tanya ZHIVKOVA[1], Lora DYAKOVA[4], Abedulkadir ABUDALLEH[1], Hristo HRISTOV[1], Ildiko BUTA[5], Teodora MOCANU[6], Daniela-Cristina CULITA[6], Gabriela MARINESCU[6]

[1] *Institute of Experimental Morphology, Pathology and Anthropology with Museum, Bulgarian Academy of Sciences, Sofia, Bulgaria*
[2] *Faculty of Medicine, Medical University - Sofia, Bulgaria*
[3] *New Bulgarian University, Sofia, Bulgaria*
[4] *Institute of Neurobiology, Bulgarian Academy of Sciences, Sofia, Bulgaria*
[5] *"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd. 300223, Timişoara, Romania*
[6] *"Ilie Murgulescu" Institute of Physical Chemistry, Romanian Academy, Bucharest, Romania*
rialexandrova@hotmail.com

Despite advances in prevention, early diagnosis and treatment, cancer remains one of the leading medical and societal challenges of our time. According to World Health Organization (WHO) projections, the number of people diagnosed with cancer is expected to double by 2050.
Among the major challenges limiting the effectiveness of cancer treatment are the high plasticity and adaptability of cancer cells, the multidrug resistance of tumor cells, their ability to escape the immune response, and the toxicity of currently used antineoplastic agents.
Nano-oncology, the application of nanotechnology to cancer diagnosis and treatment, is revolutionizing the way tumors are diagnosed and treated. Its main advantages include unprecedented precision in targeted drug delivery, significantly reduced systemic side effects, the ability to cross biological barriers (such as the blood-brain barrier), and the integration of diagnostics with therapy (theranostics).
Nanotherapeutic agents can circumvent key obstacles to conventional cancer therapies by improving drug solubility and overcoming limitations associated with multidrug resistance.
At least 15 nanomedicines have been approved worldwide for cancer treatment by regulatory agencies such as the US Food and Drug Administration (FDA) and the European Medicines Agency (EMA). These include liposomes, polymeric micelles, and albumin-bound nanoparticles, such as Doxil (liposomal doxorubicin) and Abraxane (albumin-bound paclitaxel).
However, the clinical application of nanomedicines still faces several challenges, including the interaction of nanoparticles with biological systems, efficient accumulation within tumor tissues, and precise production of therapeutic agents.
This review summarizes the major challenges facing preclinical and clinical nano-oncology, and discusses potential strategies to overcome them from the perspectives of cell biology and experimental oncopharmacology.

Acknowledgements
Supported by Grant КП-06-Н91-15 from 11.12.2025, National Science Fund, Bulgaria, and Bulgarian Academy of Sciences (Bilateral project between the Bulgarian Academy of Sciences and the Romanian Academy, project IC-RO/04/2026-2028);

BIOAVAILABILITY OF POTENTIALLY TOXIC ELEMENTS: IMPLICATIONS FOR SUSTAINABLE ENVIRONMENTAL AND HUMAN HEALTH RISK ASSESSMENT

Svetlana ĐOGO MRAČEVIĆ[1], Almasa LEKPEK[2], Zoran DINIĆ[3], Aleksandra ŠAJNOVIĆ[4], Slavica RAŽIĆ[1], Milan STANKOVIĆ[1], Branimir JOVANČIĆEVIĆ[2]

[1] University of Belgrade - Faculty of Pharmacy, Vojvode Stepe 450, 11221 Belgrade, Serbia
[2]University of Belgrade - Faculty of Chemistry, Studentski trg 12-16, 11000 Belgrade, Serbia
[3]Institute of Soil Science, Teodora Drajzera 7, 11000 Belgrade, Serbia
[4]University of Belgrade, Institute of Chemistry, Technology and Metallurgy, Njegoševa 12, 11000 Belgrade, Serbia
svetlana.djogo@pharmacy.bg.ac.rs

Soil contamination by potentially toxic elements (PTEs) poses a persistent environmental challenge due to their long-term stability and bioaccumulation in the food chain. Effective assessment of environmental and human health risks associated with PTEs requires a thorough understanding of the processes governing their transformation and immobilization in soil.

In this study the long-term behavior of Pb, As, Cd, and Cr in soils from a historically contaminated mining area was analyzed using both individual and integrated soil pollution indices, including the enrichment factor (EF), geoaccumulation index (Igeo), Nemerow index (NI), Pollution Load Index (PLI), Environmental Risk Index (ERI), and Potential Ecological Risk Index (PERI). A sequential extraction procedure was performed to assess the geochemical partitioning and potential mobility of these elements. In addition, a plant growth experiment was conducted under controlled conditions to evaluate the transfer of PTEs from soil to plants, their accumulation in plant tissues, and their effects on plant development. Furthermore, potential impacts on human health were evaluated through carcinogenic and non-carcinogenic risk assessments that considered multiple exposure pathways. In addition, chromium speciation was analyzed, taking into account the distinct behavior and impacts of chromium (III) and chromium (IV).

The results demonstrate that the speciation and transformation of PTEs are critical determinants of their environmental behavior, bioavailability, and potential ecological and health risks. Moreover, integrating experimental and field-based studies provides new insights into the mechanisms that control the environmental fate of PTEs and their interactions within the soil-plant system.

Acknowledgements
This research was funded by the Ministry of Science, Technological Development and Innovation, Republic of Serbia through two Grant Agreements with University of Belgrade-Faculty of Pharmacy No. 451-03-33/2026-03/200161 and No. 451-03-34/2026-03/200161, University of Belgrade - Faculty of Chemistry No. 451-03-33/2026-03/200168, Institute of Soil Science No. 451-03-33/2026-03/ 200011, and University of Belgrade - Institute of Chemistry, Technology and Metallurgy No .451-03-33/2026-03/200026

References
1. Guillevic F., Rossi M., Develle A.-L., Spadini L., Martins J.M.F., Arnaud F., Poulenard J., Appl. Geochem. 2023, 150:105556.
2.Đogo Mračević S., Stanković M., Đurđević M., Vizi A., Ražić S., Environ. Geochem. Health. 2025, 47:401.

HIGHLY THERMALLY CONDUCTIVE EPOXY-BASED PHASE-CHANGE COMPOSITE MATERIALS FOR EFFICIENT CHIP THERMAL MANAGEMENT

Yanhui CHEN, Bingying HUANG

Chang'an Campus of Northwestern Polytechnical University, Chang'an District, Xi'an City, 710029, Shaanxi Province, China
yanhuichen@nwpu.edu.cn

To address the challenge of balancing high thermal conductivity and high phase transition enthalpy in thermal phase-change composite materials, this research work designed and synthesized an epoxy resin (*TEMP*$_0$) containing a large number of ether bonds. When combined with polyethylene glycol (PEG-6000), a stable phase-change composite material (*TEMP*$_x$) was obtained, which exhibited excellent heat storage performance and effectively encapsulation ability. The phase transition latent heat reached up to 148.0 J/g, and the energy storage efficiency was as high as 94% (Figure 1). After 100 heating-cooling cycles, the enthalpy remained basically unchanged, demonstrating the excellent thermal cycling stability. Further introducing copper foam (CuF) into *TEMP*$_x$ fabricated the epoxy phase-change thermal composite material (*TEMP*$_x$-Cuy). As the thermally conductive framework, the CuF significantly increased the thermal conductivity of *TEMP*$_x$-Cuy. The thermal conductivity of *TEMP*$_{80}$-Cu60 reached as high as 8.26 W/(m·K), representing an approximately 33-fold increase compared to *TEMP*$_0$. This material effectively promotes heat dissipation in electronic devices and suppresses temperature rise. In the simulated chip thermal management tests, the time required for the chip surface temperature to rise from 30°C to 90°C is approximately 14 times longer than that of the blank control group. The epoxy phase-change thermal composite material prepared in this work has the potential for application in the thermal management of electronic devices.

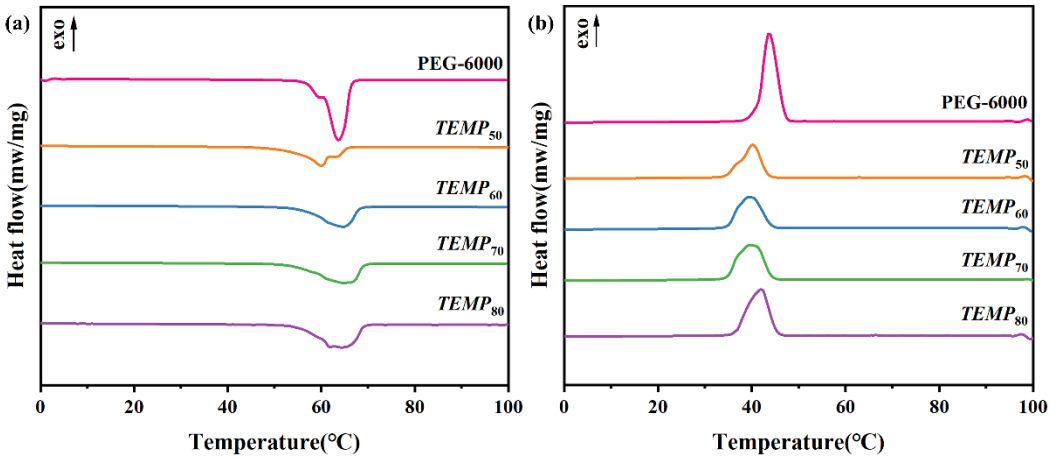


Figure 1. (a) DSC heating and (b) cooling curves of PEG-6000 and *TEMP*$_x$ samples.

Acknowledgements
The authors gratefully acknowledge the financial support of this work by the National Natural Science Foundation of China (Nos. 22378332).

References
1. Guo X., Wei K., Ni T., et al. J. Energy Storage. 2024, 88:111525.
2. Li Y., Wang T., Zhang J., et al. Compos. Part A Appl. Sci. Manuf. 2025, 193:108849.
3. W. Lee, J. Kim. J. Energy Storage. 2025, 110:115283.
4. Huang B., Hu G., Wang H., Liang H., Zhang Q., Chen Y., Composites Part A. 2026, 208:109873.

GREEN APPROACH IN MEMBRANE FABRICATION

Alberto FIGOLI, Francesca RUSSO, Giuseppe DI LUCA, Francesco GALIANO

Institute on Membrane Technology "Enrico Drioli", National Research Council of Italy (CNR-ITM), via P. Bucci 17c, Rende (CS) Italy
a.figoli@itm.cnr.it

The use of more and more green solvents in membrane fabrication is increasingly recognized as a priority, with growing efforts focused on replacing toxic solvents with environmentally benign alternatives. Conventional membrane preparations are still largely dependent on hazardous organic solvents such as N,N-dimethylformamide (DMF), N,N-dimethylacetamide (DMAc), and N-methyl-2-pyrrolidone (NMP), widely adopted for their polymer dissolution efficiency but classified as substances of very high concern due to their reprotoxic and environmentally harmful profiles. Recent research has focused on the replacement of traditional solvents with green alternatives in accordance with the 12 Principles of Green Chemistry, particularly the number 5 principle, which encourages the use of safer solvents and auxiliaries. Current research is therefore moving beyond solvent substitution toward the design of customized green solvent systems capable of controlling polymer dissolution, membrane morphology and processability. [1-2] Recent advances in sustainable membrane fabrication are presented through two complementary case studies. The first focuses on the preparation of flat-sheet membranes by phase inversion using bio-based and low-toxicity solvents, including dimethyl isosorbide (DMI) [3] and other emerging sustainable solvent platforms. The influence of these solvents on phase inversion, membrane morphology, pore-size, and separation performance is highlighted, demonstrating how solvent can be exploited to fabricate high-performance membranes while reducing environmental impact. The second case study concerns the potentiality of tailored made blends of solvents for specific polymer membrane fabrication. [4-5] Finally, future perspectives on the development of fully bio-based membrane systems are outlined.

Acknowledgements
NextGeneration EU from the Italian Ministry of Environment and Energy Security POR H2 AdP MMES/ENEA with involvement of CNR and RSE, PNRR - Mission 2, Component 2, Investment 3.5 "Ricerca e sviluppo sull'idrogeno", CUP: B93C22000630006.

References
1. Figoli A., Marino T., Simone S., Di Nicolò E., Li X.M., He T., Tornaghi S., Drioli E., Green Chemistry. 2014, 14: 4034-4059.
2. Zou D., Nunes S.P., F.J. Vankelecom, Figoli A., Y.M. Lee, Green Chemistry. 2021, 23:9815–9843.
3. Russo R., Galiano F., Pedace F., Aricò F., Figoli A., ACS Sustain. Chem. Eng. 2020, 8:659–668.
4. Figoli A., Galiano F., Russo F., Zago M., Manetti A., 2023, Patent No. IT2023000003420
5. Fontananova E., Figoli A., Galiano F., Russo F., Di Profio G., Zago M., (2025) Patent No. IT2025000028249

SELF-ASSEMBLED LACCASE-BASED BIOHYBRIDS: A ROBUST BIOCATALYTIC PLATFORM FOR EFFICIENT DYE DEGRADATION

Larisa-Maria PETRILA, Cristina BOSTACĂ, Marius-Mihai ZAHARIA, Ana-Lavinia VASILIU, Marcela MIHAI

Petru Poni Institute of Macromolecular Chemistry,
Grigore Ghica Voda Alley No 41A, Iasi – 700487, Romania
larisa.petrila@icmpp.ro

Enzymes are protein structures which possess catalytic activity, finding applications in a wide range of domains, including organic synthesis, pharmaceuticals or environmental protection. Despite their high specificity and catalytic efficiency, the use of enzymes is hindered by their susceptibility to denaturation under non-native conditions and difficulties in their recovery and reuse. [1] As a potential solution, the immobilization of enzymes has imposed as an effective method to increase their stability and facilitate their reusability. The immobilization of enzymes by organic-inorganic biomineralization, with the formation of enzymatic biohybrids, has emerged as an efficient method to increase the stability of enzymes while preserving their catalytic activity. The obtained biohybrids are particularly attractive due to their large surface-to-volume ratio, high loading capacity and increased catalytic efficiency. [2]

Herein, we report an easy and environmentally friendly method for the preparation of *Trametes versicolor* laccase-based biohybrids. The biohybrids were prepared using a one-step self-assembly biomineralization process using laccase and various metal precursors. The presence of the enzyme in the crystallization media offered an organic template for the nucleation of the metal phosphate crystals, which further underwent anisotropic growth and maturation, leading to the formation of enzyme-based hierarchical biohybrids.

Morphological characterization by scanning electron microscopy revealed a distinctive flower-like morphology of the obtained biohybrids, with the overall aspect and structural features depending on the metal precursor used and self-assembly conditions. Moreover, structural characterization by energy-dispersive X-ray analysis, X-ray diffraction and Fourier-transform infrared spectroscopy confirmed the successful encapsulation of the enzyme and the crystalline structure of the materials. Additionally, the enzymatic activity of the obtained biohybrids was tested, observing satisfactory enzymatic activity as well as increased stability under various experimental conditions, compared to the native enzyme.

To test the potential applicability of the obtained biohybrids, the degradation of the organic dye Indigo Carmine was investigated. The complete enzymatic degradation of the dye was achieved in the presence of the laccase-based biohybrids, with degradation times varying between 30 minutes and a few hours, depending on the metal precursor and preparation conditions.

In summary, this study provides important insights into the enzyme biomineralization, confirming the efficacy of the proposed method for the preparation of stable and reusable biocatalysts with potential environmental applications following the implementation of circular bioeconomy concept.

Acknowledgements
This work was supported by a grant of the Ministry of Education and Research, CCCDI - UEFISCDI, through the project *Center of Excellence in water management, materials, by-products and waste valorisation for circular bioeconomy implementation*, project number PN-IV-P6-6.1-CoEx-2024-0056, contract 6CoEx/02.06.2026, within PNCDI IV.

References
1. Petrila L.M., Bucatariu, F., Stoica I., Mihai M., Froidevaux R., J. Environ. Chem. Eng. 2025, 13: 115631.
2. Han Z., Wang H., Zheng J., Wang S., Yu S., Lu L., Environ. Res. 2023, 216: 114690.

Special session for Project 6CoEx/2026

CENTER OF EXCELLENCE IN WATER MANAGEMENT, MATERIALS, BY-PRODUCTS AND WASTE VALORISATION FOR CIRCULAR BIOECONOMY IMPLEMENTATION – CERSUS

Elisabeta I. SZERB[1], **Florica MANEA**[2]

[1] *"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223, Timisoara, Romania*
eszerb@acad-icht.tm.edu.ro
[2]*Politehnica University of Timisoara, Bvd. Vasile Parvan No. 6, 300223 Timisoara, Romania*
florica.manea@upt.ro

Project **CERSUS** is one of the 4 centers of excellence covering circular bioeconomy, biodiversity, resilient agriculture and food security financed by UEFISCDI in the framework of strengthening Romanian scientific research by establishing partnerships in areas of demonstrated scientific excellence of research organizations, aiming to form the critical mass of researchers and the interdisciplinarity necessary to address main challenges of the European Strategic Research Agenda. The CERSUS project, coordinated by Prof. Carmen TEODOSIU from Gheorghe Asachi Technical University of Iași and developed by 7 partners - Politechnica University Timişoara (UPT), Petru Poni Institute of Macromolecular Chemistry Iaşi, Transilvania University of Braşov, Alexandru Ioan Cuza University of Iași, University of Agronomic Sciences and Veterinary Medicine Bucharest, "Coriolan Dragulescu" Institute of Chemistry, Timişoara - Romanian Academy (ICCD) and National Institute for R&D for Industrial Ecology Bucharest aims to contribute to sustainable social and economic development by bringing excellence in research at international level, paving the way for ground breaking research results, technology transfer to industrial partner and providing opportunities for young researchers training.
The presentation will include research methodologies applied by the research team of ICCD for the synthesis and characterization of innovative materials and detection of priority/emerging pollutants and integrating advanced wastewater treatment and by-products/waste characterization/valorization by UPT team.

Acknowledgements
This work was supported by a grant of the Ministry of Education and Research, CCCDI - UEFISCDI, through the project Center of Excellence in water management, materials, by-products and waste valorisation for circular bioeconomy implementation, proposal number PN-IV-P6-6.1-CoEx-2024-0056, contract 6 CoEx/02.06.2026, within PNCDI IV.

SYNTHESIS AND ANTIBACTERIAL POTENTIAL OF QUATERNARY PHOSPHONIUM SALTS

Alexandru BUHAI[1], Andrei IVAN[2], Aurelia VIŞA[1]

[1] "Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223, Timişoara, Romania
[2]Faculty of Veterinary Medicine, University of Life Science "King Mihai I", 119 Calea Aradului, 300465, Timisoara, Romania
buhaialex9@gmail.com

Growing interest in quaternary phosphonium salts is driven by the development of antimicrobial resistance (AMR), which threatens the effectiveness of antimicrobial therapies. Owing to their unique physicochemical properties, structural versatility, and straightforward synthesis, these compounds are promising candidates for medicinal chemistry and are consistent with the principles of green chemistry.

A series of quaternary phosphonium salts was synthesized and structurally characterized using one- and two-dimensional nuclear magnetic resonance (NMR) spectroscopy, FTIR spectroscopy, and elemental analysis. The compounds were systematically modified by varying the alkyl chain length (C2–C5), halide counterions, and aryl substituents attached to the phosphorus atom to investigate their influence on physicochemical properties and biological activity. These structural modifications provide valuable insights into structure–activity relationships and support the development of more effective antimicrobial agents. [1–3] Progressive substitution of phenyl groups with 3-furyl moieties induced an upfield shift in the ^{31}P NMR resonances, reflected by decreasing chemical shift (δ, ppm) values with increasing 3-furyl content. Conversely, changes in alkyl chain length (C2–C5) did not significantly affect the ^{31}P NMR chemical shifts. [4] The antimicrobial activity of the synthesized compounds was evaluated against the Gram-positive bacteria *Staphylococcus aureus* and *Bacillus cereus*, Gram-negative bacteria *Escherichia coli* and *Pseudomonas aeruginosa*, and the yeast *Candida albicans* using the Kirby–Bauer disk diffusion method. Fresh 24-hour bacterial cultures and 48-hour yeast cultures were used for testing. The synthesized salts demonstrated antimicrobial activity against both Gram-positive and Gram-negative bacteria, as well as *Candida albicans* [1,5], highlighting their potential as broad-spectrum antimicrobial agents. Antibacterial activity was determined by measuring the diameters of the inhibition zones around each disc. The antimicrobial performance of the synthesized compounds was evaluated relative to the control (ethanol solutions, coded as 1). Figure 1 summarizes the antimicrobial susceptibility results against *Pseudomonas aeruginosa*.

The synthesized compounds exhibited significant antibacterial activity, producing inhibition zones comparable in size to those observed for the reference antibiotic, gentamicin.

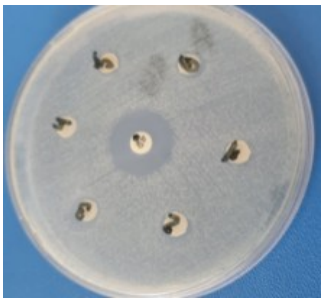


Figure 1. Antibacterial studies on *Pseudomonas aeruginosa*.

Acknowledgements
This work is supported by Research Program No. 2 of the „Coriolan Dragulescu" Institute of Chemistry, Timisoara, Romania.

References
1. Ibrahim M.K., Haria A., Mehta N.V., Degani M.S., Future Med. Chem. 2023, 15:2113.
2. McDonough D., Sanchez C.A., Wuest W.M., Minbiole K.P.C., RSC Medicinal Chemistry. 2025, 16:1000.
3. Nichita I., Lupa L., Visa A., Dragan E.-S., Dinu M.V., Popa A., Molecules. 2024, 29:6054.
4. Ackermann M., Pascariu A., Höcher T., Siehl H.-U., Berger S., J. Am. Chem. Soc. 2006, 128:8434.
5. Wang L., Xu G., Tang M., Liang Y., Prog. Org. Coat. 2023, 175:107337.

SYNTHESIS AND CHARACTERIZATION OF α-AMINOPHOSPHONATE LIGANDS AS PRECURSORS FOR METAL-ORGANIC FRAMEWORKS

Iosif-Cristian MOCAN[1], Bianca MARANESCU[1], Aurelia VIŞA[2]

[1]West University of Timişoara, Faculty of Chemistry, Biology, Geography, 16A Pestalozzi Street, Timişoara, Timiş, 300115, Romania
[2]"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223, Timişoara, Romania
iosif.mocan04@e-uvt.ro

Metal-organic frameworks (MOFs) represent an important class of porous crystalline materials, formed through the coordination of metal ions or clusters with organic ligands. Their structural diversity, high surface area and tunable functionality make them promising candidates for applications such as gas storage, catalysis, drug delivery, sensing and biomedical materials. [1] Since the properties of MOFs are strongly influenced by the nature of the organic linker, the design and synthesis of new ligands remain an essential step in the development of advanced metal–organic materials. [1, 3]

Among the different classes of ligands used in MOF chemistry, phosphonic ligands are particularly attractive due to their ability to form strong metal–oxygen–phosphorus bonds. Compared with conventional carboxylate linkers, phosphonate-based systems can offer improved chemical, thermal and hydrothermal stability. [3] However, their multiple coordination modes may also lead to dense or poorly crystalline structures, which makes the rational design of suitable organic precursors more important. [3]

In this study, a series of α-aminophosphonate derivatives was synthesized via the Kabachnik–Fields (Phospha–Mannich) reaction using aromatic aldehydes, aniline, and dialkyl phosphites as starting materials. [2]

Two synthetic approaches were investigated: an alternative one-pot method performed under ultrasound irradiation, in solvent-free and catalyst-free conditions, and a classical reflux method using oxalic acid as catalyst. The comparison between these approaches allows an evaluation of their efficiency, accessibility and compatibility with greener synthetic principles.

The synthesized compounds were purified by column chromatography and recrystallization and characterized by elemental analysis, TLC, FT-IR, Raman, and ^{1}H NMR spectroscopy. Spectroscopic data confirmed the formation of the targeted α-aminophosphonates through characteristic amino, aromatic, and phosphonate signals. Hydrolysis of the phosphonate ester groups provides the corresponding α-aminophosphonic acids with free –$PO(OH)_2$ functionalities, enabling coordination with metal ions such as Zr(IV), Al(III), Fe(III), and lanthanides for potential application as ligands in metal–organic frameworks (MOFs) [3]. The amino group may further contribute to framework assembly through secondary interactions.Therefore, the synthesized α-aminophosphonates represent valuable organic precursors for the development of phosphonate-based MOF ligands. Their conversion into aminophosphonic acids may provide access to robust metal–organic materials with enhanced stability and functional potential. [1, 3]

Acknowledgements
This work was partially supported by West University of Timisoara, Faculty of Chemistry, Biology, Geography, and by Research Program No. 2 of the „Coriolan Dragulescu" Institute of Chemistry, Timisoara, Romania

References
1. Furukawa H., Cordova K.E., O'Keeffe M., Yaghi O.M., Science. 2013, 341:1230444.
2. Cherkasov R.A., Galkin V.I., Russ. Chem. Rev. 1998, 67:857-882.
3. Clearfield A., Prog. Inorg. Chem. 1998, 47:371-510.

[*3+2*] DIPOLAR CYCLOADDITION-BASED FUNCTIONALIZATION OF PHENANTHRIDINE AND THE SYNTHESIS OF LOW-MOLECULAR-WEIGHT QUATERNARY SALTS USING SHORT ALIPHATIC CHAINS

Ashraf AL-MATARNEH[1], Florentina Gabriela LAZĂR[2], Mariana PINTEALĂ[2], Ionel MANGALAGIU[1], Maria Cristina AL-MATARNEH[2]

[1]Faculty of Chemistry, Alexandru Ioan Cuza University of Iasi, Iasi, Romania
[2]Centre of Advanced Research in Bionanoconjugates and Biopolymers, "Petru Poni" Institute of Macromolecular Chemistry of Romanian Academy, Iasi, Romania
dr.ashraf.matarneh@gmail.com

Phenanthridine is a privileged heteroaromatic scaffold with significant potential for the development of functional molecules owing to its structural versatility and valuable physicochemical properties. [1] In the present work, [*3+2*] dipolar cycloaddition reactions were employed as an efficient synthetic strategy for the functionalization of the phenanthridine core, enabling the preparation of a series of novel derivatives. [2]

A key aspect of this study is the conversion of these derivatives into quaternary salts using short aliphatic substituents. The use of short alkyl chains was intentionally chosen to maintain a low molecular weight while minimizing steric effects and avoiding unnecessary increases in molecular size. This approach also provides an effective means of tuning the physicochemical properties of the resulting compounds, including their solubility, without significantly altering the aromatic framework. The combination of [*3+2*] dipolar cycloaddition chemistry with the rational design of low-molecular-weight quaternary salts highlights an efficient route toward structurally diverse phenanthridine-based compounds. This strategy provides a versatile platform for the synthesis of functional heterocyclic molecules with optimized structural and physicochemical characteristics, offering promising opportunities for further investigation in medicinal, supramolecular, and materials chemistry.

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).

References
1. Zhang S., Zhang S., Wang Y., Zhang Y., Liang S., Fan S., Chen D., Liu G. Arch Microbiol. 2023, 205(12):371.
2. Al-Matarneh A., Simionescu N., Nicolescu A., Cibotariu N., Danac R., Al-Matarneh M.C., Mangalagiu II. J. Biochem. Mol. Toxicol. 2025, 39(9):e70443.

THEORETICAL INSIGHTS INTO THE INTERACTIONS OF DACARBAZINE TAUTOMERS WITH FULLERENE NANOCARRIERS

Raluca POP[1], Adina Căta[2], Daniela Velciov[1], Alexandra Masuti[1], Ioana M. C. Ienaşcu[2,3]

[1]Victor Babeş University of Medicine and Pharmacy, Faculty of Pharmacy, Eftimie Murgu Square No.2, RO-300041 Timişoara, România
[2]National Institute of Research and Development for Electrochemistry and Condensed Matter, 144 Dr. A. P. Podeanu Str., 300569, Timisoara, Romania
[3]Vasile Goldis Western University of Arad, Faculty of Pharmacy, 86 Liviu Rebreanu, 310045, Arad, Romania
pop.raluca@umft.ro

Dacarbazine is an alkylating anticancer agent whose biological behavior may be influenced by its tautomeric equilibrium and interactions with nanostructures carriers. [1-3]
In this work, an *in silico* investigation was performed to evaluate the interactions between dacarbazine and its tautomeric forms and a series of fullerene nanostructures. Geometry optimizations and interaction energy calculations were carried out to assess the stability and binding characteristics of the resulting complexes. The influence of the different tautomers on the affinity toward fullerenes was analyzed by comparing the structural and energetic properties of the complexes.
The study aims to offer a theoretical basis for the rational design of nanomaterial-assisted anticancer drug delivery systems and to contribute to the understanding of fullerene-based nanocarriers as potential drug delivery systems.
The investigated structures of dacarbazine and its two tautomeric forms are depicted in scheme below:

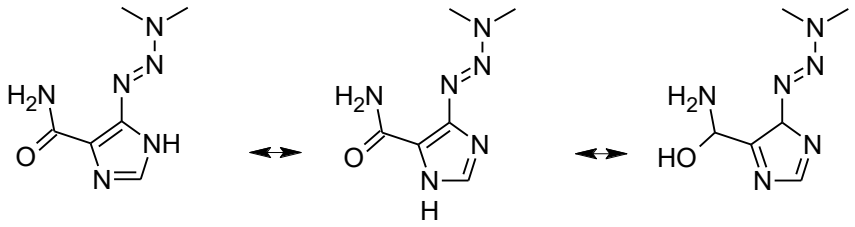


Figure 1. The structures of Dacarbazine and its two tautomers. T1 and T2

References
1. Al-Otaibi J.S., Mary Y.S., Mary Y.S., Ullah Z., Yadav R., Gupta N., Churchill D.G. Spectrochim Acta A Mol Biomol Spectrosc. 2022, 268:120677.
2. Hoelm M., Kinart Z, Porwański S. Molecules. 2025, 30(24):4819.
3. Larina L.I. Crystals. 2019, 9:366.

THE BIO-TEXTILE-SSBD PROJECT: DEVELOPING SAFE AND SUSTAINABLE BY DESIGN BIO-BASED LIQUID REPELLENT TEXTILE COATINGS

Cicely M. WARNE[1], Lucia GARDOSSI[2], Anamaria TODEA[3], Alessandra OPERAMOLLA[1]

[1]University of Pisa, Department of Chemistry and Industrial Chemistry, Via Giuseppe Moruzzi 13, 56124, Pisa, Italy.
[2]Universita' degli Studi di Trieste, Dipartimento di Scienze Chimiche e Farmaceutiche, Via Licio Giorgieri,1 34127, Trieste, Italy.
[3]University Politehnica Timisoara, Biocatalysis and Green Chemistry Group, Faculty Chemical Engineering, Biotechnologies and Environmental Protection, Bulevardul Vasile Pârvan 6, 300322, Timisoara, Romania.
cicely.warne@unipi.it

Omniphobic materials, defined by their hydrophobic and oleophobic traits, have a wide array of commercial uses, including in the textile industry. Traditionally, per- and poly-fluoroalkyl substances (PFAS) are used to confer omniphobicity, but these substances are set to become even more tightly restricted [1] due to their high persistency in the environment, tendency to bioaccumulate, and documented negative effects on human health. [2] PFAS alternatives such as polysiloxanes exist, but synthesis is extremely energy intensive, and recycling of these materials is not commercially mature. [3] Further research into coatings that are safe and sustainable by design (SSbD) is therefore needed. To address this need, the BIO-TEXTILE-SSbD project aims at designing and synthesizing a fully bio-based omniphobic coating for textile applications, keeping SSbD principles in mind and using sustainable methodologies at every stage of the process. Firstly, BIO-TEXTILE-SSbD will utilize computational techniques for design of molecules from bio-based feedstocks suitable for omniphobic coatings, reducing energy usage and waste. Sustainable synthesis routes to these compounds will be investigated, prioritizing those which utilize enzymes as a catalyst. Before application to textiles, the ecotoxicity and biodegradability of these new coatings will be assessed. Finally, infrared thermal activation (IRTA), as an efficient surface functionalization technique that offers great potential for scale up [4], will be applied in the final textile coating step.

Acknowledgements
This project has received funding from the European Union's Horizon Europe research and innovation programme under the Marie Skłodowska-Curie grant agreement No 101277185.

References
1. Yu R.S., Yu H.C., Yang Y.F., Singh S. Toxics. 2025, 13(4):251
2. Fenton S.E., Ducatman A., Boobis A., DeWitt J.C., Lau C., Ng C., et al. Environ Toxicol Chem. 2021, 40(3):606–30.
3. Brook M.A., Chen Y. Macromolecules. 2025, 58(8):3742–63.
4. D'Orsi R., Danielli C., Spennato M., Guazzelli E., Martinelli E., Asaro F., et al. ChemSusChem. 2025, 18(11):e202500164.

HUMAN SKIN CELL CULTURE MODELS FOR COMPARATIVE EVALUATION OF NOVEL METAL-BASED ANTITUMOR COMPOUNDS

Abedulkadir ABUDALLEH[1], Tanya ZHIVKOVA[1], Hristo HRISTOV[1], Lora DYAKOVA[2], Peter DORKOV[3], Juliana IVANOVA[4], Teodora MOCANU[5], Daniela-Cristina CULITA[5], Gabriela MARINESCU[5], Radostina ALEXANDROVA[1]

[1] *Institute of Experimental Morphology, Pathology and Anthropology with Museum, Bulgarian Academy of Sciences, Sofia, Bulgaria*
[2] *Institute of Neurobiology, Bulgarian Academy of Sciences, Sofia, Bulgaria*
[3]*Chemistry Department, R&D, BIOVET JSC, Peshtera, Bulgaria*
[4]*Faculty of Medicine, Sofia University "St. Kliment Ohridski", Sofia, Bulgaria*
[5] *Institute of Physical Chemistry "Ilie Murgulescu", Romanian Academy, Bucharest, Romania*
alkader78mah@yahoo.com

Human skin cell culture models represent valuable in vitro platforms for the identification of novel anticancer agents and comparative evaluation of their biological activity and selectivity. In the present study, human melanoma cell lines (A375 and SH-4), together with non-tumor cell lines (HaCaT keratinocytes and Lep-3 embryonic fibroblastoid cells), were used to investigate the cytotoxic activity of two classes of newly synthesized metal-based compounds: mixed-ligand Cu(II) Schiff base complexes derived from o-vanillin and amino acids, and salinomycin-derived metal complexes containing Zn(II), Cu(II), Co(II), Mn(II), and Gd(III).

Cell viability was evaluated using MTT, Neutral Red and Crystal Violet assays. Cytopathological alterations and cell migration were investigated by acridine orange/propidium iodide (AO/PI) fluorescence staining and the scratch test, whereas long-term antitumor activity was determined using the three-dimensional (3D) cell colony formation method.

Both classes of compounds exhibited concentration- and time-dependent cytotoxic effects against melanoma cells - reduced cell viability and/or proliferation, inhibition of cell migration, suppression of long-term 3D cell colony formation, and characteristic morphological changes associated with apoptotic cell death were observed. Comparative analysis of tumor and non-tumor cell models demonstrated distinct sensitivity and selectivity profiles, enabling identification of the most promising metal-based compounds for further investigation.

Overall, these findings demonstrate that human skin cell culture models provide robust and informative experimental systems for comparative screening of novel metal-based compounds and support their application in the early identification and preclinical evaluation of potential antitumor agents.

Acknowledgements
The study was supported by Bulgarian National Science Fund (Grant N КП-06-КОСТ/18 from 12.08.2024), Bulgarian Academy of Sciences (Bilateral project between the Bulgarian Academy of Sciences and the Romanian Academy, project IC-RO/04/2026-2028); European Union Next Generation EU through the National Recovery and Resilience Plan of the Republic of Bulgaria (project no. BG-RRP-2.004-0008).

MECHANOCHEMICAL FUNCTIONALIZATION OF CHITOSAN WITH METAL IONS USING PLANETARY BALL MILLING

Adriana POPA[1], Aurelia VISA[1], Lavinia LUPA[2], Ionela FRINGU[1], Bianca MARANESCU[3], Anca FILIMON[4]

[1] "Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223, Timisoara, Romania
[2] Politehnica University Timişoara, Faculty of Chemical Engineering, Biotechnology and Environmental Protection, 6 Vasile Parvan Blvd., 300223, Timisoara
[3] Faculty of Chemistry, Biology, Geography, West University of Timisoara, 16 Pestalozzi Street, Timisoara 300115, Romania
[4] "Petru Poni" Institute of Macromolecular Chemistry, 41A Aleea Grigore G. Voda, 700487, Iasi
[*]coresponding e-mail: capataanca@yahoo.com; apopa@acad-icht.tm.edu.ro

In recent years, mechanochemical reactions have gained increasing attention as a highly efficient and environmentally friendly approach for the synthesis of novel functional materials. [1, 2] The mechanochemical modification of biopolymers, such as chitosan, presents significant opportunities for the development of novel functional composites. [2] Chitosan, a naturally abundant polysaccharide [3], exhibits intrinsic biocompatibility [4], chemical versatility, and metal binding capacity, making it an excellent candidate for functionalization with metal ions.

In this study, we used a planetary ball mill type MN200 to perform the mechanical activation of chitosan under solvent-free conditions and at ambient temperature. Potassium dichromate ($K_2Cr_2O_7$) was introduced as an oxidizing agent in varying concentrations, and its influence on the structural, chemical and physicochemical properties of chitosan was investigated. UV-Vis spectroscopy (Figure 1) indicates the formation of new absorption bands upon treatment. After heat treatment, $K_2Cr_2O_7$ decomposes, releasing oxygen that contribute to chitosan oxidation, accompanied by the reduction of Cr(VI) to Cr(III), as suggested by the appearance of an absorption band around ~560 nm.

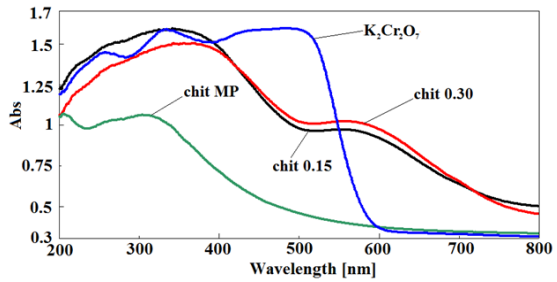


Figure 1. UV-Vis spectra for chitMP, $K_2Cr_2O_7$, and final samples (chit0.15 and chit0.30).

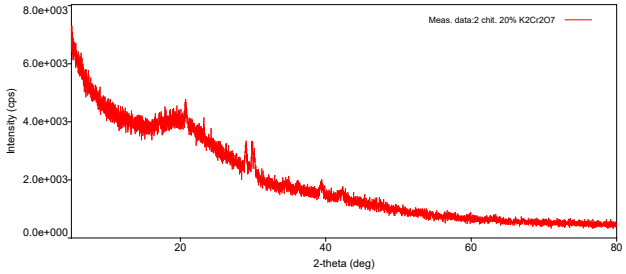


Figure 2. XRD pattern of chit0.30.

X-ray diffraction analysis (Figure 2) of the modified samples shows weak and shifted diffraction peaks in the 10–30° range, indicating a predominantly amorphous structure and possible interactions between chitosan and chromium species. These results highlight the potential of mechanochemical approaches for the synthesis of chitosan-metal composites with tailored functional properties, in agreement with the principles of green chemistry.

Acknowledgments
This work was partially supported by Research Program No. 2 of the "Coriolan Dragulescu" Institute of Chemistry, Timisoara, Romania.

References
1. Wang G.-W., Chem. Soc. Rev., 2013, 42:7668-7700.
2. Vakili M., Qiu W., Cagnetta G., Huang J., Yu G., J. Environ. Chem. Eng. 2021, 9:105454
3. Bhatnagar A., Sillanpää M., Adv. Colloid Interface Sci. 2009, 152:26–38.
4. Singh J., Dutta P. K., Int. J. Polym. Mater. 2010, 59:793–807.

EVALUATION OF THE CHEMICAL COMPOSITION AND BIOLOGICAL ACTIVITIES OF DIFFERENT PLANT EXTRACTS - GREEN SYNTHESIS OF NANOPARTICLES

Alexandra-Mariana IONESCU[1], Andreea Veronica BOTEZATU[1], Ana-Maria MOCANU[1], Bianca FURDUI[1], Alina Viorica IANCU[2], Luminita MARIN[3], Mihaela SILION[3], Maria Paula Cabral CAMPELLO[5], Fernanda Marujo MARQUES[5], Costel VINATORU[4], Rodica Mihaela DINICA[1*]

[1] "Dunarea de Jos" University, Faculty of Sciences and Environment, Galati, Romania
[2] "Dunarea de Jos" University, Faculty of Medicine and Pharmacy, Galati, Romania
[3] "Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania
[4] Genetic and Vegetal Resources Bank (GVRB), Buzau, Romania
[5] Instituto Superior Técnico, Universidade de Lisboa, Campus Tecnológico e Nuclear, Bobadela, Lisbon, Portugal
alexandra.ionescu@ugal.ro, rodica.dinica@ugal.ro

The genus *Sideritis* (Lamiaceae) comprises over 150 species distributed across the Mediterranean basin, the Canary Islands, and Madeira. Traditionally prepared as an infusion or decoction, these beverages are widely used for alleviating common colds, respiratory discomfort, and mild gastrointestinal ailments. Mountain tea (*Sideritis spp*.), locally known as "tsai tou vounou," is among the most popular traditional herbal infusions in the Mediterranean region. Throughout Greece, it is consumed under various vernacular names—such as "Olympus tea," "Taygetus tea," "Malotira," and "Vlach tea"—each referring to distinct species or subspecies within the genus *Sideritis L*. Although several *Sideritis* species have been extensively studied for their phytochemical composition and pharmacological properties, research efforts have concentrated primarily on *S. scardica*, *S. raeseri*, and *S. syriaca.* [1]

Various extraction techniques and HPLC were used to highlight specific chemical compounds. The biological activities evaluated in this study included antioxidant, antitumor, and antimicrobial activities. The study was also based on green synthesis of nanoparticles using the extract and characterizing them through different methods, such as UV-VIS, FTIR, DLS, and zeta potential.

Thus, based on chromatographic analyses and chemical and biological tests, *Sideritis spp.* can be considered a promising representative of its family, with significant medicinal properties for the prevention and treatment of infections, but also with potential for oncological diseases.

Acknowledgements
This work was partially supported by ADER grant 5.2.1. "Conservation and valorization of the genetic heritage of aromatic and medicinal species that can be cultivated on the territory of Romania" and UDJG internal Grant "Targeted therapeutic molecules, anti-inflammatory and antitumor, isolated from exotic plants acclimatized in Romania", funding contract no. 7956/31.03.2025.

References
1. Eleftheria H. Kaparakou, Charalabos D. Kanakis, Dimitra Daferera, Petros A. Tarantilis, Phytochemical composition, antioxidant potential, and toxicity of infusions and decoctions of Greek mountain tea (*Sideritis clandestina* subsp. *clandestina*) from the Peloponnese, Elsevier, Amsterdam, 2025.

CONSERVATION IMPLICATIONS DUE TO CHEMICAL CHARACTERIZATION OF 20TH-CENTURY CELLULOSIC PAPER SUPPORTS IN THE STEFAN JÄGER COLLECTION AT THE MNART

Andreea PETCU FOANENE[1], Filip Adrian PETCU[1], Daniela MĂNESCU[1], Mariana SUBA[2]

[1]National Museum of Art Timişoara, Uniri Square No.1, 300085, Timişoara, România

[2]"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223, Timişoara, România

Andreea.foanene@mnart.museum

The National Museum's collection of more than 500 watercolours created by the renowned painter Stefan Jäger represents an important cultural heritage resource whose long-term preservation depends on understanding the chemical nature and degradation behaviour of its constituent materials. This study focuses on the characterization of the paper supports used in Jäger's watercolours, with particular emphasis on their relevance within the field of organic polymer sciences. Stefan Jäger (1877–1962) was one of the most important painters of the Banat region and is often called "the painter of the Banat Swabians." Today, many of his paintings are held in museums, private collections, and cultural institutions in Romania, Germany and other European countries. Depending on size, condition, and subject, works attributed to Stefan Jäger have appeared at European art auctions with estimates ranging from several hundred euros to over €5,000–€8,000 for significant oil paintings, while exceptional historical works are considered culturally invaluable. The analyzed artworks consist of drawing and watercolour paper support, typical of the first half of the twentieth century, manufactured predominantly from cellulose fibers derived from mechanical and semi-chemical wood pulp, potentially blended with recycled textile fibers such as cotton or flax. Chemically, the primary component is cellulose, a natural polysaccharide polymer composed of β-D-glucose repeating units. Variable amounts of hemicelluloses, residual lignin, and papermaking additives - including rosin sizing, alum (potassium aluminium sulfate), and other sizing agents - are also present and significantly influence the material's long-term stability. He has used a large selection of paper, dating from the end of XIX century the beginning-middle of XX century. Visual and physical examination in our graphic storage revealed a cream-yellow coloration, moderate embrittlement, folds, and dimensional deformations, all characteristic of naturally aged cellulosic materials. These alterations are associated with oxidative and hydrolytic degradation processes affecting the cellulose macromolecular network. Residual lignin further contributes to progressive yellowing through photochemical reactions induced by ultraviolet radiation and atmospheric oxygen. Moreover, the acidic sizing systems commonly employed during the period promote a decrease in paper pH, accelerating cellulose depolymerization and leading to reduced flexibility and increased brittleness. From a polymer science perspective, the deterioration mechanisms observed illustrate the complex interaction between cellulose structure, residual lignocellulosic components, environmental factors, and manufacturing additives. Through comparative analyses of paper samples from different centuries, using FTIR spectra with the contribution of *the Coriolan Drăgulescu Institute of Chemistry*, we observed differences in the degradation/oxidation peak at approximately 1720 cm^{-1}, characteristic of carbonyl (C=O) groups, as well as information regarding moisture retention and a structure less affected by acidity. These data are important for understanding the support material and for adapting appropriate conservation conditions to ensure the preservation and exhibition of these works of art.
The findings highlight the importance of preventive conservation strategies, including. environmental control, appropriate storage conditions, and handling protocols specifically adapted to the chemical properties of historic cellulosic polymers, ensuring the sustainable preservation of this significant artistic collection.

SYNERGISTIC MODULATION OF AROMATIC POLYAMIDE BLENDS PROPERTIES FOR FLEXIBLE SUBSTRATE APPLICATIONS

Andra-Elena BEJAN, Catalin-Paul CONSTANTIN, Irina BUTNARU, Mariana-Dana DAMACEANU, Radu-Dan RUSU

Petru Poni Institute of Macromolecular Chemistry, Romanian Academy, Electroactive Polymers and Plasmochemistry Department, Grigore Ghica Voda Alley, 41A, 700487, Iasi, Romania
bejan.andra@icmpp.ro

Modern technological advancements constantly push the functional limits of engineering materials performance. High-performance polymers are one of the most effective solutions provided by macromolecular materials science, yielding the resilience to withstand arduous mechanical, thermal, and chemical environments and thus representing the long-term driving force behind the evolution of electronics, automotive, aerospace, and energy-related industrial areas. [1] As always, with every structural-derived advantage comes an inherent drawback: such polymers frequently face a dense matrix of challenges, covering development timeframe and effort, diversity, processability, property modulation and high cost, intensive synthesis. [2, 3] One feasible mitigation strategy to tackle most liabilities is polymer blending: a straightforward and cost-effective pathway which combines the synergistic properties of already validated materials and increases the options of performance fine-tuning. [1–3] The impact of blending on material properties is deeply complex and multidimensional. It improves film-forming properties, enabling the fabrication of thin, defect-free materials from otherwise intractable resins and boosting the application options. It allows the optimization and incremental adjustment of the dielectric constant and the reduction and control of dielectric loss. Optical transparency is also achievable, either through miscible systems with uniform refractive indices or by matching indices in immiscible pairs where domain sizes are smaller than the wavelength of light. Furthermore, this approach provides the means to master and expand the spectrum of attainable morphologies, a critical determinant of the final physical features. [1–4]

We deployed this versatile strategy to overcome the traditional trade-offs in materials science and developed new aromatic polyamide blends starting from the already acquired, comprehensive structure-property relationships of the precursor polymers. [5–8]

The primary research trajectory was to evaluate the multi-scale structural and dynamic interplay governing polymer morphology, multi-scale relaxation modes, and macroscopic phase compatibility and the performance control possibilities derived from changing the nature or the ration of the repeating units. The investigation was focused on miscibility confirmation, film-forming properties and processability improvement, mechanical performance, dielectric features, optical behavior (with a focal point on transparency) and morphological outcome.

The study confirms the viability of this macromolecular blending approach for robust flexible dielectric substrates applications.

Acknowledgements
This work was financially supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS – UEFISCDI, project number PN-IV-P2-2.1-TE-2023-1896, contract no. 143TE/05.01.2026, within PNCDI IV.

1. Goh S.H., in: L.A. Utracki. C.A. Wilkie (Eds.), Polymer blends handbook, Springer, New York, 2014. pp. 1915-2151.
2. Xavier S.F. in: L.A. Utracki. C.A. Wilkie (Eds.), Polymer blends handbook, Springer, New York, 2014. pp. 1031-1201.
3. Yong W.F., Zhang H., Prog. Mater. Sci. 2021, 116:100713.
4. Park H.B., Kamcev J., Robeson L.M., Elimelech M., Freeman B.D., Science. 2017, 357(6352):eaab0530.
5. Iosip M.D., Bruma M., Ronova I., Szesztay M., Müller P., Eur. Polym. J. 2003, 39(10):2011-2021.
6. Damaceanu M., Rusu R.D., Nicolescu A., Bruma M., Rusanov A.L., Polym. Int. 2011, 60:1248-1258.
7. Damaceanu M., Rusu R.D., Nicolescu A., Bruma M., J. Polym. Sci. A Polym. Chem. 2011, 49:893-906.
8. Damaceanu M.D., Rusu R.D., Cristea M., Musteata V.E., Bruma M., Wolinska-Grabczyk A., Macromol. Chem. Phys. 2014, 215:1573-1587.

SYNTHESIS AND CHARACTERIZATION OF MCM-48 AND MCM-41 MESOPOROUS MATERIALS

Silvana BORCĂNESCU, Orsina VERDES, Mariana SUBA

"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223, Timisoara, Romania
silvana.borcanescu@gmail.com

In this paper are summarized results about synthesis and characterization of functionalization of MCM-48 and MCM-41 mesoporous materials by grafting techique. For the synthesis, tetraethylorthosilicate (TEOS) was used as pure silica source, cetyltrimethylammonium bromide (CTAB) as surfactant and 3-aminopropyltrimethoxysilane (APTES) as the modifying agent. MCM-48 was synthesized by the method developed by Ortiz et al. [1], while MCM-41 was prepared after the method developed by Beck et al. [2]
The mesoporous materials were investigated by IR spectroscopy, XRD spectra, nitrogen adsorption/desorption measurements and thermogravimetric analysis investigations. From FT-IR spectra, it can be observed that the succsessful grafting of MCM-48 material with APTES, reflected by newly introduced organic aminopropyl bands as described in Fig 1.

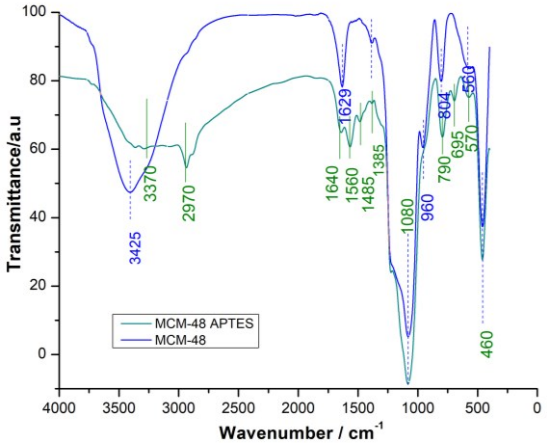


Figure 1. FT-IR spectra of the MCM-48 and MCM-48 APTES materials.

Investigated materials present high surface areas and uniform pores. Results obtained from N_2 adsorption-desorption isotherms, show that MCM-41 and MCM-48 presents type IV isotherm assigned to mesoporous materials with large surface areas (1460 m^2/g for MCM-48 and 1300 m^2/g for MCM-41).Due to high surface area and large pore size distribution, MCM-48 and MCM-41 functionalized mesoporous materials represent promising structures for CO_2 adsorbents and catalyst support. [3, 4]

Acknowledgments
This work was supported by Research Program No. 4 of the "Coriolan Dragulescu" Institute of Chemistry, Timisoara, Romania.

References
1. Meléndez-Ortiz H. I., Perera-Mercado Y., Mercado-Silva J. A., Olivares-Maldonado Y., Castruita G., García-Cerda L. A., Ceram. Inter. 2014, 40:9701-9707.
2. Beck J.S., Vartuli J.C., Roth W.J., Leonowic M.E., Kresge C.T., Schmitt K.D., Chu C.T.W., Olson D.H., Sheppard E.W., J. Am. Chem. Soc. 1992, 114:10834–10843.
3. Borcănescu S., Popa A., Verdeş O., Suba M., Int. J. Mol. Sci. 2023, 24(12):10345.
4. Debatrayee D., Anjali P., RSC Adv. 2025, 15(40):33657–33666.

PRELIMINARY STUDIES ON WATER BASED FERROFLUID WITH APPLICATION IN WASTEWATER TREATMENT

Ildiko BUTA[1], Vlad Mircea SOCOLIUC[2], Mariana SUBA[1], Catalin IANASI[1], Liliana CSEH[1], Ladislau VÉKÁS[2]

[1] "Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223, Timisoara, Romania
[2]Romanian Academy – Timisoara Branch, Center for Fundamental and Advanced Technical Research, Laboratory of Magnetic Fluids, Timisoara, Romania

Water-stable ferrofluids are of considerable interest due to their compatibility with aqueous and physiological environments, making them suitable for a wide range of biomedical applications [1] as well as environmentally sustainable processes, including wastewater remediation. [2] Consequently, achieving long-term colloidal stability in aqueous media is a key prerequisite for their practical implementation. [3]

Here, we report the preparation of a colloidally stable aqueous ferrofluid based on hydrophilic azelaic acid-coated Fe_3O_4 nanoparticles (FeAA). Hydrophobic oleic acid-coated Fe_3O_4 nanoparticles were first synthesized by chemical coprecipitation and dispersed in hexane. The FeAA nanoparticles were subsequently obtained through the oxidative cleavage of the oleic acid coating using a green oxidation process. This transformation converts the hydrophobic oleic acid shell into a hydrophilic, carboxyl-functionalized surface, providing excellent colloidal stability in aqueous media.

The FeAA nanoparticles were characterized using Fourier-transform infrared spectroscopy (FTIR), thermogravimetric analysis (TG), small-angle X-ray scattering (SAXS), and wide-angle X-ray scattering (WAXS). The magnetic properties of the aqueous ferrofluid were investigated by vibrating sample magnetometry (VSM), while its colloidal stability was assessed using dynamic light scattering (DLS) and static light scattering (SLS).

Aknowledgements
The work of I.B. was supported by Research Program No. 4, Subprogramme 4.1, Theme 4.1.2 of the "Coriolan Dragulescu" Institute of Chemistry, Timisoara, Romania, and the work of V.M.S. and L.V. by the RA-TB/CFATR/LMF Multiannual Research Program 2026–2030.

References
1. Socoliuc V., Peddis D., Petrenko V.I., Avdeev M.V., Susan-Resiga D., Szabó T., Turcu R., Tombácz E., Vékás L., Magnetochemistry 2020, 6:2.
2. Yaqoob S., Hanif M.A., Environ. Monit. Assess. 2025, 197: 917.
3. Vasilescu C., Latikka M., Knudsen K.D., Garamus V.M., Socoliuc V., Turcu R., Tombácz E., Susan-Resiga D., Ras R.H.A., Vékás L., Soft Matter. 2018, 14:6648-6666.

POLYMERS OBTAINED BY ELECTROPOLYMERIZATION AS ELECTRODE MATERIALS FOR NIR ELECTROCHROMIC AND ENERGY STORAGE APPLICATIONS

Adriana-Petronela CHIRIAC, Catalin-Paul CONSTANTIN, Mariana-Dana DAMACEANU

Petru Poni Institute of Macromolecular Chemistry, Electroactive Polymers & Plasmochemistry Laboratory, 41A Grigore Ghica Voda Alley, Iasi, Romania
chiriac.adriana@icmpp.ro

Conducting polymers are recognized for their remarkable electrical and optical properties, including low density, high flexibility and electrical conductivity, low band gap energy, and facile synthesis and processing. For these reasons, they have been extensively studied in electrical, electronic, and optoelectronic fields, as well as in energy storage applications such as supercapacitors, fuel cells, and batteries, and also in photocatalysis, anticorrosion coatings, biomedical, and sensing applications. [1, 2] They also exhibit high coloration efficiency, color versatility, high color contrast, and rapid response times, making them attractive for electrochromic devices and smart windows. [3] Among the most well-known classes of conducting polymers, polythiophenes (PTh) and their derivatives have been extensively studied for their thermal stability, high optical properties, and excellent electrical conductivity, and are widely used in the fabrication of optical, energy storage, and electrochromic devices. [1, 3]

Several methods are available for the synthesis of conducting polymers, such as chemical oxidative polymerization, electrochemical synthesis, and photochemical synthesis, and among these, the electropolymerization has attracted significant attention due to many advantages, such as short reaction time, cost-effectiveness, the possibility to obtain thin and uniform polymer films on conducting surfaces with controlled thickness and surface morphology. [4]

Therefore, the present work is focused on developing two conjugated 3,4-propylenedioxythiophene (ProDOT)-based polymers functionalized with two different polar groups, hydroxymethyl and oligooxyethylene-benzoester unit, deposited by electropolymerization on both rigid (ITO-coated glass) and flexible (ITO-coated PET) substrates, and evaluated for their dual functionality in electrochromic and energy storage applications. [5] A detailed study of their electrochromic performance and energy storage capability was carried out using spectroelectrochemistry, chronoamperometry, cyclic voltammetry (CV), and galvanostatic charge-discharge (GCD) measurements to demonstrate their potential as active materials in energy storage smart windows. In a three-electrode cell configuration, the polymer substituted with an ester group exhibited a specific areal capacitance of 7.063 mF/cm^2 at a scan rate of 20 mV/s and 9.96 mF/cm^2 at 0.01 mA/cm^2, as determined by CV and GCD measurements, respectively, and a high optical contrast of 83% and a coloration efficiency of 1036 cm^2/C. Therefore, both polymers were evaluated as active electrode materials in an electrochromic energy storage device prototype configuration, displayed comparable capacitive performance, and confirmed their use as active materials for energy storage smart windows applications.

Acknowledgements
This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-IV-P2-2.1-TE-2023-0213, within PNCDI IV (contract no. 36TE/08.01.2025).

References
1. Namsheer K., Rout C.S., RSC Adv. 2021, 11:5659–5697.
2. Hasan M.B., Parvez M.M., Abir A.Y., Ahmad, M.F., Heliyon. 2025, 11:e42375.
3. Kim J., Rémond M., Kim D., Jang H., Kim, E., Adv. Mater. Technol. 2020, 5:1900890.
4. Khatak M., Balkhandia M., Kedia R., Patra A., ACS Appl. Polym. Mater. 2025, 7:0016−10025.
5. Chiriac A.P., Constantin C.P., Damaceanu M.D., J. Energy Storage. 2026, 175:123190.

PHYSIOLOGICAL AND METABOLIC RESPONSES OF *GALIUM VERUM* AND *HELICHRYSUM ITALICUM* TO OZONE EXPOSURE

Lucian COPOLOVICI[1,2], Andreea LUPITU[3], Flavia BORTES[2,3], Maria COJOCARU-TOMA[4], Angelica OHINDOVSCHI[4], Mihaela NARTEA[4], Cristian MOISA[3], Dana COPOLOVICI[1]

[1]Faculty of Food Engineering, Tourism and Environmental Protection, Aurel Vlaicu University, Elena Dragoi St. 2, Arad, 310330, Romania
[2]Interdisciplinary Doctoral School of Aurel Vlaicu University, Elena Dragoi St. 2, Arad, 310330, Romania
[3]Institute for Interdisciplinary Research, Aurel Vlaicu University, Elena Dragoi St. 2, Arad, 310330, Romania
[4]State University of Medicine and Pharmacy "Nicolae Testemițanu" of the Republic of Moldova, Stefan cel Mare si Sfant Boulevard 165, MD-2004, Chișinău, Moldova
lucian.copolovici@uav.ro

Tropospheric ozone is one of the most damaging phytotoxic air pollutants, as it promotes oxidative stress and interferes with several physiological and metabolic processes in plants. Its effects may include reduced carbon assimilation, changes in stomatal regulation and chlorophyll fluorescence, pigment degradation, activation of antioxidant defenses, stimulation of secondary metabolite synthesis, and modification of volatile organic compound emissions. Medicinal and aromatic species may respond differently to ozone exposure, with possible consequences for both stress tolerance and phytochemical quality. This study investigated the physiological, biochemical, and metabolic responses of *Galium verum* and *Helichrysum italicum* cultivated under controlled environmental conditions and exposed to ozone treatments. Net photosynthetic rate, stomatal conductance, and chlorophyll fluorescence were monitored weekly, while HPLC analyzed individual phenolic compounds. Total polyphenol and flavonoid contents were determined spectrophotometrically, and volatile organic compounds released by the plants were characterized using PTR–TOF–MS. Ozone exposure significantly reduced photosynthetic performance in both species, indicating limitations in carbon assimilation and gas exchange. At the same time, the accumulation of secondary metabolites increased, suggesting the activation of biochemical defense mechanisms against ozone-induced oxidative damage. Changes in volatile emission profiles also differed between the two species, highlighting distinct metabolic adjustment strategies. Overall, *G. verum* and *H. italicum* exhibited coordinated yet species-specific responses, including photosynthetic downregulation, enhanced secondary metabolism, and altered VOC emissions, which may contribute to their tolerance and influence their phytochemical value under increasing atmospheric pollution.

Acknowledgements
This work was supported by a grant from the Romanian National Authority for Scientific Research, CNCS – UEFISCDI, project number PN-IV-P8-8.3-ROMD-2023-0022.

CHITOSAN-DERIVED INHIBITORS AS SUSTAINABLE AGENTS FOR METAL CORROSION PROTECTION

Anemona CORNEA, Milica ŢARĂ-LUNGĂ-MIHALI, Adriana POPA, Nicoleta PLEŞU

"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223, Timişoara, Romania
plesu_nicole@yahoo.com

The present study investigates the electrochemical behavior of iron in a 2 wt.% citric acid solution containing chitosan-based corrosion inhibitors. Chitosan is a naturally occurring cationic biopolymer produced by the alkaline deacetylation of chitin, the second most abundant natural polymer after cellulose. Structurally, it is a linear polysaccharide composed of D-glucosamine and N-acetyl-D-glucosamineunits. Owing to its remarkable properties, including biocompatibility, biodegradability, low toxicity, and intrinsic antimicrobial activity, chitosan has attracted considerable interest in biomedical, cosmetic, food, and environmental applications. [1–6] From the perspective of corrosion protection, chitosan and its derivatives are considered promising environmentally friendly inhibitors because their molecular structure contains numerous oxygen- and nitrogen-containing functional groups. The amino ($-NH_2$) and hydroxyl ($-OH$) groups can adsorb onto their surface, promoting the formation of a protective film that reduces the corrosion rate in acidic media. The effectiveness of chitosan as a corrosion inhibitor depends on several factors, including the solution pH, citric acid concentration, temperature, molecular weight, and degree of deacetylation. This work also evaluates whether the inhibitor performance can be enhanced through mechanical treatment or chemical modification of chitosan. Two types of inhibitors were investigated: untreated chitosan supplied by Sigma-Aldrich and ball-milled chitosan. Electrochemical polarization and electrochemical impedance spectroscopy (EIS) measurements were carried out while maintaining constant experimental conditions, including citric acid concentration, pH, temperature, and inhibitor concentration. Analysis of the polarization curves and impedance spectra demonstrated that iron immersed in the citric acid solution containing ball-milled chitosan exhibited the highest corrosion resistance. Under these conditions, the corrosion current decreased to approximately $4.67 \cdot 10^{-6}$ A, representing an approximately 11.3% reduction compared with iron exposed to the solution containing untreated chitosan and nearly a 39.6% reduction relative to iron immersed in the citric acid solution without inhibitor. These findings demonstrate the significant potential of mechanically processed chitosan as an eco-friendly corrosion inhibitor for iron in acidic environments and provide a solid basis for further investigations aimed at optimizing its performance and understanding its inhibition mechanism.

Acknowledgments
This work was supported by Research Programs No. 2 and 3 of the "Coriolan Dragulescu" Institute of Chemistry, Timisoara, Romania.

References
1. Marin L., Stoica I., Mihai M.[b], Dinu V., C. Simionescu B.C. and Barboiu M., J. Mater. Chem. B. 2013, 1:3353.
2. Marguerite R., Elsevier, Prog. Polym. Sci. 2006, 31:603-632.
3. Li M.,Li F., Hu J., Cui N., Su H, Li.L., Wang. Z.,Sun S., and Hu S., Royal Society of Chemistry, New J. Chem., 2024, 48:3064.
4. Zhang W., Zhang J., XiaW., Int. J. Food Prop. 2014,17:26-37.
5. Riham. R.M., Fekry A.M., Int. J. Electrochem. Sci. 2011, 6:2488 – 2508.
6. Karaer H., Kaya İ., Iran Polym J. 2015, (24) 6.

FROM TRIETHANOLAMMONIUM 4-NITROBENZOATE TO Ni(II) COORDINATION COMPOUNDS: SUPRAMOLECULAR ARCHITECTURES AND SOLID-STATE PHOTOLUMINESCENCE

Manuela CRISAN[1], Anastasia GOROBET[2], Paulina BOUROSH[2], Anatolii SIMINEL[2], Lilia CROITOR[2], Marina FONARI[2], Victor KRAVTSOV[2]

[1] *"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223, Timisoara, Romania*
mdorosencu@yahoo.com
[2] *Institute of Applied Physics, Academy Str., 5 MD2028, Chisinau, Republic of Moldova*
nasteagorobet@gmail.com

Systems based on alkanolamines and aromatic carboxylic acids provide versatile platforms for the construction of organic salts and metal coordination compounds in which proton transfer, hydrogen bonding, metal coordination and π–π interactions can be used to direct supramolecular organization. [1-3] In this study, triethanolammonium 4-nitrobenzoate, (HTEA)(4NB), and four Ni(II) complexes were obtained from the same $NiCl_2$-(HTEA)(4NB) chemical system under different reaction conditions, demonstrating structural diversity. [4]

The compounds form supramolecular systems stabilized by hydrogen bonds, π–π interactions and metal coordination in the case of Ni(II) complexes. In the ionic Ni(II) complexes, O–H···O hydrogen bonds generate well-defined 2D layers that are further consolidated into 3D supramolecular networks through π–π stacking interactions. By contrast, the neutral Ni(II) complex forms a 3D supramolecular network governed predominantly by hydrogen bonding.

Solid-state photoluminescence measurements show that the emission response is influenced not only by the molecular components, but also by the crystal structure, packing arrangement, and intermolecular interactions. In this context, two Ni(II) complexes exhibit room-temperature solid-state emission under UV excitation, with distinct red and blue photoluminescent responses.

Acknowledgements
This work was partially supported by Research Program No. 2
of the "Coriolan Drăgulescu" Institute of Chemistry, Timișoara, Romania, and by Project ANCD 20.80009.5007.15 and subprogram 011202 of Ministry of Education and Research of R. Moldova.

References

1. Crisan M, Petric M., Vlase G., Vlase T., Siminel A.V., Bourosh P., Croitor L., J. Therm. Anal. Calorim. 2022, 147(2):1203-1213.
2. Gorobet A., Crisan M., Petric M., Bourosh P., Croitor L., Rev. Roum. Chim. 2018, 63(12):1175-1179.
3. Crisan M., Bouros P., Chumakov Y., Petric M., Ilia G., Cryst. Growth Des. 2013, 13(1):143-154.
4. Gorobet A., Crisan M.E., Bourosh P., Siminel A.V., Croitor L., Polyhedron. 2021, 193:114893.

INTENTIONAL SOLVENT-DRIVEN STANDARDIZATION OF ROSEMARY EXTRACTS: DIRECTING HYDROPHILIC AND LIPOPHILIC PHYTOCHEMICALS TOWARD FUNCTIONAL COSMETIC INGREDIENTS

Daniela HAIDU[1], Manuela CRIȘAN[1], Mariana SUBA[1], Luminița CRIȘAN[1], Ildiko BUTĂ[1], Camelia OPREAN[2,3]

[1]"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223 Timişoara, Romania
danielahaidu1@gmail.com
[2]Faculty of Pharmacy, "Victor Babeş" University of Medicine and Pharmacy, E. Murgu Sq., No. 2, 300041 Timişoara, Romania
[3]OncoGen Centre, County Hospital Pius Brînzeu, 156 Liviu Rebreanu Blvd., 300736, Timişoara, România;

There is a growing demand for natural cosmetic ingredients modulating the need for standardized extracts with reproducible botanic composition and functionality with industrial applicability. *Rosmarinus officinalis L.*, adaptogen increasingly cultivated in Romania, is a valuable source of phytochemicals with antioxidant, anti-inflammatory, antimicrobial, immunomodulatory skin effects and wound healing properties. [1, 2] Considering the natural variability of raw plant material and extraction procedures the reproducibility of rosemary derived cosmetic ingredients is limited. [3]
This study proposes a solvent-guided strategy for the standardization of rosemary extracts using cosmetic compatible solvents spanning a broad hydrophilic-lipophilic polarity range. By selectively extracting phytochemicals according to their polarity, the approach generates chemically distinct extracts with targeted cosmetic potential while supporting a sustainable value chain based on locally cultivated rosemary.
The extracts were characterized by FT-IR spectroscopy, GC-MS, total phenolic content, antioxidant activity, and stability studies under UV-visible irradiation, temperature, and pH variations. Representative lipophilic compounds were further evaluated *in silico* for physicochemical descriptors relevant to cosmetic performance.
Preliminary results consolidate solvent dependent extraction selectivity, yielding distinct chemical fingerprints, antioxidant capacities, and stability profiles. The proposed workflow provides a practical framework for developing standardized functional botanical ingredients and facilitates the sustainable transfer of Romanian plant resources into science-based cosmetic formulations.

Acknowledgements
This work was partially supported by Research Program No. 2 of the "Coriolan Dragulescu" Institute of Chemistry, Timisoara, and by a grant of the Ministry of Education and Research, CCCDI-UEFISCDI, project number PN-IV-P6-6.1-CoEx-2024-0196, within PNCDI IV.

References
1. Meziane H., Zraibi L., Albusayr R., Bitari A., Oussaid A., Hammouti B., Touzani R., J Umm Al-Qura Univ Appl Sci. 2025, 11(1):9-37.
2. González-Minero F.J., Bravo-Díaz L., Ayala-Gómez A., Cosmetics (Basel). 2020, 7(4):77.
3. Erdoğan Ü., Öztürk T., Önder S., Tonguç M., J Mol Liq. 2024, 407:125167.

NEW PYRIDINE HYDRAZIDE ISOMERS: SYNTHESIS, SUPRAMOLECULAR ARCHITECTURE, BIOLOGICAL AND PHOTOLUMINESCENT PROPERTIES

Olga DANILESCU[1], Maria COCU[1], Ion BULHAC[1], Alexandru CIOCARLAN[1], Paulina BOUROSH[2], Vlad GHENEA[2], Olga KULIKOVA[2], Nicoleta VORNICU[3], Yurii CHUMAKOV[2]

[1]Moldova State University, Institute of Chemistry, 3, Academiei str., MD2028, Chisinau, R. Moldova
[2]Moldova State University, Institute of Applied Physics, 5, Academiei str., MD2028, Chisinau, R. Moldova
[3]Metropolitan Centre of Research T.A.B.O.R, 700066 Iasi, Romania
olgadanilescu@gmail.com, maria.cocu@sti.usm.md

Hydrazone-based ligands and their derivatives continue to attract significant attention in coordination chemistry and materials science due to their versatile structural features, chelating abilities, tuneable electronic properties, and structural diversity.

The solvothermale reaction involving benzene-1,4-dicarboxaldehyde and picolinic/nicotinic/isonicotinic acid hydrazides in ethanol at 100ºC led to the formation of colourless elongated prismatic crystals of three positional isomers of *N′,N″*-(1,4-phenylenedimethanilidene)bis(pyridine-2,3,4-carboxaldehyde) H_2L^1 (**1**), H_2L^2 (**2**), and H_2L^3 (**3**).

The structural data reveal that the changing of nitrogen atom position within the aromatic ring resulted in different crystal packing arrangements of compounds **1**–**3**. This shift significantly alters the intermolecular interactions, such as hydrogen bonding and $\pi\cdots\pi$ stacking, which, in turn, affects the assembly of molecules in the crystal structures of the studied compounds.

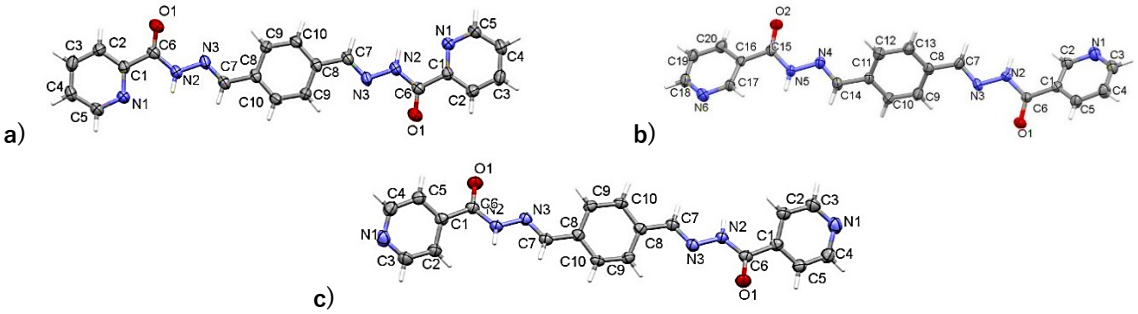


Figure. The molecular structures of the compounds **1**(a), **2**(b) and **3**(c). Displacement ellipsoids are drawn at the 30% probability level

The DFT calculations identified the potential reactive sites in compound **1**. This compound was shown to be the most reactive of the compounds studied. The molecular docking was subsequently performed to determine the binding conformation of compound **1** to 1,3-β-glucan synthase, and this compound may be considered as promising for further development.

The compounds **1**–**3** demonstrated significant antifungal and antibacterial activities, comparable to and in some cases surpassing the reference drugs Caspofungin and Kanamycin.

The photoluminescence measurements showed that the PL intensity of compound **2** was higher than that of compounds **1** and **3**. Shifting the substitution position in studied compounds alters the spatial arrangement of atoms, leading to changes in orbital overlap and electron delocalization. Isomer **2** is structurally favourable for concentrating electron states at the band edges, thereby maximizing emission efficiency compared to isomers **3** and **1**.

Acknowledgement
The authors are grateful for the subprograms financed by the Ministry of Education and Research of the Republic of Moldova 010602, 011202 and 011201.

ANTITUMOR ACTIVITY OF NOVEL COPPER(II) COMPLEXES IN A ROUS SARCOMA VIRUS - TRANSFORMED CELL CULTURE MODEL

Eliya STOILOVA[1], Ildiko BUTA[2], Silvia MANCHEVA[1,3], Mara BOGDAN[2], Tanya ZHIVKOVA[1], Lora DYAKOVA[4], Abedulkadir ABUDALLEH[1], Hristo HRISTOV[1], Radostina ALEXANDROVA[1], Liliana CSEH[2]

[1] *Institute of Experimental Morphology, Pathology and Anthropology with Museum, Bulgarian Academy of Sciences, Sofia, Bulgaria*
[2] *"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223, Timisoara, Romania*
[3] *New Bulgarian University, Sofia, Bulgaria*
[4] *Institute of Neurobiology, Bulgarian Academy of Sciences, Sofia, Bulgaria*
eliya_st@yahoo.com

Schiff base ligands containing thiophene and piperidine moieties represent promising scaffolds for the development of novel metal-based anticancer agents. In the present study, a thiophene-derived Schiff base ligand (HL) and its binuclear copper(II) complex, $[Cu_2LCl_4H_2O]\cdot 1.5H_2O$ (LCu2), were synthesised and structurally characterized by ^1H NMR, FT-IR, UV–Vis spectroscopy, single-crystal X-ray diffraction, and elemental analysis. Their antitumor activity was evaluated using Rous sarcoma virus (RSV)- transformed rat sarcoma cells expressing v-src (cell line LSR-SF-SR), a well-established experimental model of virus-induced oncogenic transformation.

The Cells were treated with the compounds under investigation at concentrations ranging from 0.5 to 200 µg/mL for 24–72 h. Cell viability and proliferative activity were examined using the MTT, Neutral Red and Crystal Violet assays. Cytopathological alterations were determined by acridine orange/propidium iodide (AO/PI) fluorescence staining, cell migration was evaluated using the scratch test, and long-term antiproliferative activity was assessed by the three-dimensional (3D) cell colony formation assay.

Both the Schiff base ligand and the binuclear Cu(II) complex exhibited concentration- and time-dependent cytotoxic effects against RSV-transformed cells. Treatment with both compounds resulted in reduced cell viability and proliferation, inhibition of cell migration, suppression of long-term 3D cell colony formation, and characteristic cytopathological changes associated with apoptotic cell death. The binuclear Cu(II) complex consistently demonstrated greater biological activity than the free Schiff base ligand, indicating that copper coordination enhanced the antitumor potential of the ligand.

Overall, these findings demonstrate that the LSR-SF-SR cell model provides a reliable in vitro platform for evaluating novel compounds with potential antitumor activity and supports their further biological investigation

Acknowledgements
This study was supported partially by the National Science Fund, Ministry of Education and Science of Bulgaria (Grant No. КП-06-КОСТ/18, 12.08.2024), by the bilateral project between the Bulgarian Academy of Sciences and the Romanian Academy (Project No. IC-RO/04/2026–2028) and by Research Program No. 4, Subprogramme 4.1 of the "Coriolan Dragulescu" Institute of Chemistry, Timisoara, Romania.

OPTICAL SENSOR FOR THE DETECTION/QUANTIFICATION OF COPPER

Ionela FRINGU, Anca LASCU, Nicoleta PLESU

"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223 Timisoara, Romania
ionelacreanga@yahoo.com

Porphyrins are well-known spectrophotometric sensors for a variety of metal ions. Copper ions can be quantified by many methods, among which the colorimetric [1] and potentiometric [2] are the most cost-effective.

The spectrophotometric detection of copper chloride was performed using 5,10,15,20-tetra-(4-carboxy-phenyl)-porphyrin (4-COOHPP) as sensitive compound, resulting in a detection of the copper ion of 10^{-8} M, in the limit that proves to be toxic for humans [3]. The linear dependence between the absorption intensity of 4-COOHPP measured at 420 nm and the $CuCl_2$ concentration (Figure 1) presents a confidence coefficient of 99.5% in the 1.22 x 10^{-8} to 2.45 x 10^{-7} M concentration domain.

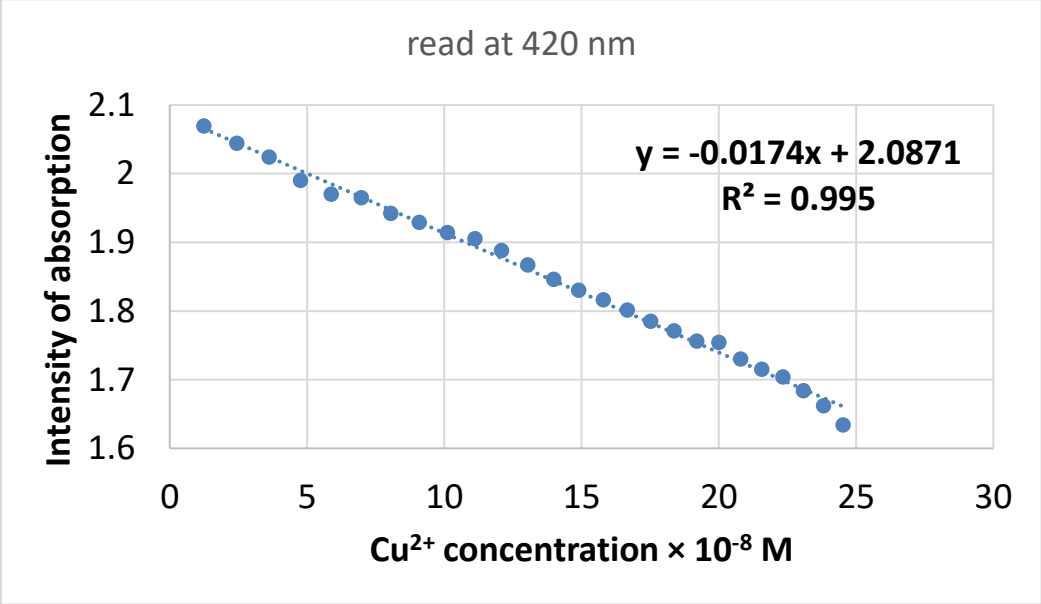


Figure 1. Linear dependence between the absorption intensity of 4-COOHPP measured at 420 nm and the $CuCl_2$ concentration

Acknowledgments
This work was supported by Research Program No. 3 of the "Coriolan Dragulescu" Institute of Chemistry, Timisoara, Romania.

References
1. Deng H.H., Li G.W., Liu A.L., Chen W., Lin X.H., Xia X.H., Microchim. Acta. 2014, 181:911–916.
2. Vlascici D., Popa I., Chiriac V.A., Fagadar-Cosma G., Popovici H., Fagadar-Cosma E., Chem. Cent. J. 2013, 7:111.
3. Anan J.K., Inchulkar S.R., Eur. J. Pharma. Med. Res. 2018, 5(11):232-237.

VIRTUAL SCREENING AND COMPUTATIONAL DESIGN OF POTENTIAL ANTI-INFLAMMATORY BILIRUBIN-LIKE ANALOGUES

Lucia GRADINARU, Alina BORA, Luminita CRISAN*

"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223, Timisoara, Romania
lumi_crisan@acad-icht.tm.edu.ro

Inflammation plays a central role in the pathogenesis of numerous chronic diseases, making the identification of safe and effective anti-inflammatory agents a major research priority. Bilirubin, once regarded solely as a toxic byproduct of heme catabolism, is now recognized as a biologically active endogenous molecule with potent antioxidant and anti-inflammatory properties, mediated in part through inhibition of the NF-κB signalling pathway and modulation of inflammasome activation. However, its therapeutic potential is limited by its poor aqueous solubility. [1, 2]
To address this limitation, the present study integrates molecular docking, quantum chemical calculations, and *in silico* pharmacological evaluation to identify bilirubin-like compounds with improved physicochemical and pharmacological properties.
Following an initial virtual screening and evaluation of drug-like characteristics, top ten promising candidates were selected for further computational investigation. Their structural, electronic, pharmacokinetic, and molecular docking profiles were comprehensively analysed, leading to the identification of one compound (Figure 1) as the most promising candidate based on its overall computational performance.

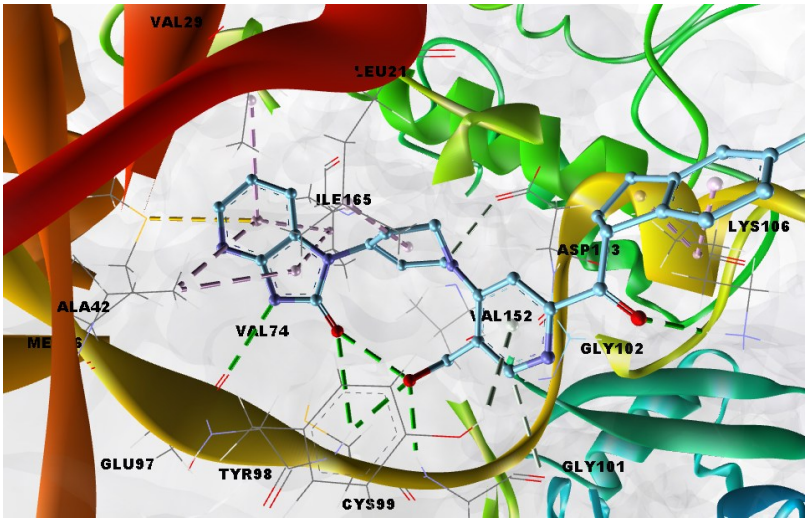


Figure 1. Molecular docking poses of the selected compound in IKKβ (3RZF).

Although promising, these findings should be further validated through *in vitro* and *in vivo* studies before their therapeutic potential can be confirmed.

Acknowledgements
This work was supported by Research Program No. 1 of the "Coriolan Dragulescu" Institute of Chemistry, Timisoara, Romania. The authors would like to thank BIOVIA Software Inc. for providing a free academic license for BIOVIA Discovery Studio Visualizer (v. 19.1.0).

References
1. Čepelak I, Dodig S, Pavić I. Biochem Med (Zagreb). 2025, 35(2):020501.
2. Li Y, Huang B, Ye T, Wang Y, Xia D, Qian J. Int Immunopharmacol. 2020, 84:106520.

IONIC LIQUIDS SYNTHESIS AND CHARACTERIZATION OF POROUS SILICA FOR ENHANCED HYDROGEN STORAGE

Ana-Maria LACRĂMĂ[1], Carlo Poselle BONAVENTURA[2,4], Raffaele G. AGOSTINO[2,3,4], Alfonso POLICICCHIO[2,4]

[1] *"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223, Timisoara, Romania.*
[2] *Department of Physics, Università della Calabria, Via P. Bucci, Cubo 31C, 87036 di Rende (CS), Italy.*
[3] *Laboratorio di Spettroscopia Avanzata Dei Materiali, STAR IR, Via Tito Flavio, Università Della Calabria, 87036, Rende, CS, Italy.*
[4] *CNR-Nanotec, c/o Università della Calabria, Via P. Bucci, Cubo 31C, 87036 Rende (CS), Italy.*
lacramaanamaria@yahoo.com

Different series of mesoporous silica particles were synthesized using the sol-gel method, varying synthesis methods (stirring, microwave, sonication) and employing the Ionic Liquid (IL) as a co-solvent and directing agent. [1] The IL (N-butyl-3-methylimidazolium Octylsulfat ([BMIM][OctS]) was added to the silica precursors in an aqueous solution.
Afterwards, an acidified ethanol washing treatment was performed to remove the IL. Structural and textural properties, such as specific surface area, pore distribution, and total pore volume, were calculated from nitrogen isotherms at 77K up to a relative pressure of p/p°=1 by using the Brunauer–Emmett–Teller (BET) and Barrett-Joyner-Halenda (NLDFT) models. [2]
Preliminary hydrogen (H_2) adsorption/desorption tests were performed to evaluate samples performances for possible storage applications acquiring H_2 isotherms at liquid nitrogen (LN_2) temperature and low pressure (up to 1 bar). The synthesized nanostructures that demonstrated promising performance in gas adsorption at low pressure were further tested to higher pressure, up to of 80 bar, and at different temperatures, starting from 77 K to 298 K. [3] The research aimed to understand how synthesis methods, concentrations, and the extraction of IL affect the properties of materials, with a special attention on the relation between surface characteristics and structure of the produced samples and gas adsorption.

Acknowledgements
This work was partially supported by Research Program No. 4 of the "Coriolan Dragulescu" Institute of Chemistry, Timisoara, Romania.

References
1. Putz A.-M., Len A., Trif L., Horváth Z.E., Almásy, L., Gels, 2022, 8: 388.
2. Putz A.-M., Len A., Ianăşi C., Savii C., Almásy L., Korean J. Chem. Eng. 2016, 33(3):749-754.
3. Policicchio A., Conte G., Stelitano S., Bonaventura C.P., Putz A.-M., Ianăşi C., Almásy L., Horváth Z.E., Agostino R. G., Colloid. Surface A. 2020, 601:125040.

ONE PORPHYRIN-MULTIPLE APPLICATIONS

Anca LASCU, Ionela FRINGU, Nicoleta PLESU

[1] *"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223, Timisoara, Romania*
ancalascu@yahoo.com

The versatility of porphyrins is due to their amazing optical properties and is here presented by the application of a single compound, Pt(II)-5,10,15,20-tetrakis-(4-allyloxyphenyl)-porphyrin (PtTAOPP)(Figure 1), in:

- the fluorescent detection of H_2O_2 in the 1.05–3.9 - 10^{-7} M concentration domain (that is highly relevant for biological testing) [1];
- the electrochemical detection of same H_2O_2 in the concentration domain 1×10^{-6} M to 5×10^{-5} M by means of a glassy carbon electrode covered with PtTAOPP [1];
- the absorption of 0.025 mole CO_2/g, when incorporated in a silica matrix although the PtTAOPP content is 25000 times lower than that of the silica [2];
- the same porphyrin-silica hybrid is able to remove 7.261± 0.2 mg/g methylene blue from wastewaters [2]; and also 190.46 mg/g fuchsine B [3] and also 0.0022g of colored hybrid can electrochemically degrade 0.000519 g of malachite green. [4]

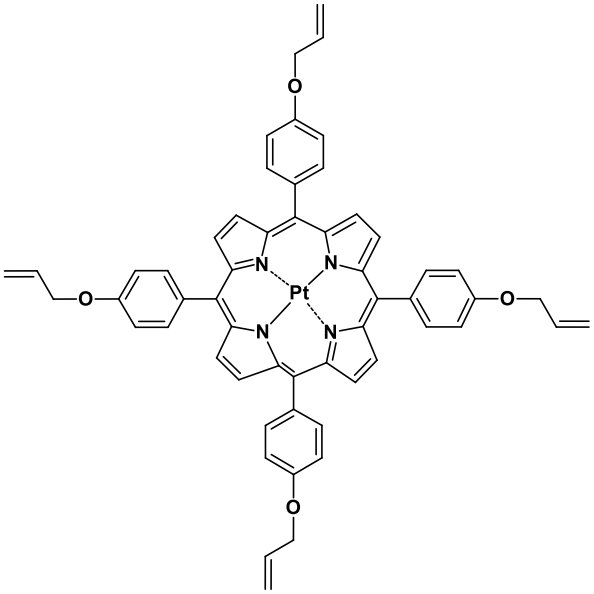


Figure 1. Structure of Pt(II)-5,10,15,20-tetrakis-(4-allyloxyphenyl)-porphyrin (PtTAOPP).

Acknowledgements
This work was supported by Research Program No. 3 of the "Coriolan Dragulescu" Institute of Chemistry, Timisoara, Romania.

References

1. Fagadar-Cosma E., Plesu N., Lascu A., Anghel D., Cazacu M., Ianasi C., Fagadar-Cosma G., Fratilescu I., Epuran C., Chemosensors, 2020, 8(2):29.
2. Anghel D., Lascu A., Epuran C., Fratilescu I., Ianasi C., Birdeanu M., Fagadar-Cosma E., Int J Mol Sci. 2020, 21(12):4262.
3. Fratilescu I., Dudas Z., Birdeanu M., Epuran C., Anghel D., Fringu I., Lascu A., Len A., Fagadar-Cosma E., Nanomaterials, 2021, 11(4):863.
4. Fringu I., Lascu A., Tara-Lunga-Mihali M., Plesu N., Fagadar-Cosma E., RSC Poster 3-4 March 2026.

NEWLY SYNTHESIZED SMALL MOLECULES: IN SILICO AND IN VITRO EVIDENCE OF ANTICANCER ACTIVITY AGAINST DIFFERENT CELL LINES

Bogdan-Ionuț MARA[1,2], Livia DEVESELEANU-CORICI[1], Alexandra MIOC[2], Ramona CURPĂN[1], Valentin BADEA[3], Alina NICOLESCU[4], Liliana CSEH[1]

[1]*Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223, Timişoara, Romania*
[2]*Victor Babeş University of Medicine and Pharmacy, Piata E. Murgu, 300041, Timişoara, Romania*
[3]*Politehnica University Timişoara, Vasile Pârvan 6 Boulevard, 300223, Timişoara, Romania*
[4]*Petru Poni Institute of Macromolecular Chemistry, 41 A, Gr. Ghica Voda Aley, 700487, Iaşi, Romania*
bmara@acad-icht.tm.edu.ro, alexandra.mioc@umft.ro, alina@icmpp.ro

Approved and emerging small-molecule-based therapies against various types of cancer are facing inevitable challenges due to low response rates and drug resistance. [1] Conventional chemotherapy, struggling with severe side effects and low efficacy, is considerably outperformed by the constant improvement in small molecule targeted therapy or therapeutic monoclonal antibodies which form the backbone of precision medicine for cancer treatment. [2]
In this context, we designed and synthesized six novel compounds bearing structural motifs commonly found in potent anticancer agents and marketed anticancer drugs. The compound's structures were confirmed by 1D, 2D NMR spectroscopy and HR-MS, with a purity of ≥95%.
In silico analysis compared the calculated physicochemical properties of the synthesized compounds with those of 242 kinase inhibitors and 3,892 approved drugs to assess similarity within this chemical space. The ADME profile was also evaluated, and molecular docking studies were performed against several kinases.
In vitro cytotoxicity assays in HaCat, HT-29, A375, MCF-7 and PANC-1 cell lines identified MB2-1 as the most active compound against PANC-1 cells, with an IC_{50} value of 26.12 μM.

Table 1. The calculated IC_{50} values (μM)

Compound	HaCat	A375	MCF-7	HT-29	PANC-1
MB2-1	63.34	55.84	>100	63.05	**26.12**
MB2-2	75.83	>100	>100	>100	>100
MB4-1	53.61	>100	86.65	76.93	66.72
MB4-2	72.93	55.71	>100	>100	75.08
MB4-3	>100	>100	>100	>100	>100
MB4-5	76.9	67.27	70.71	>100	>100

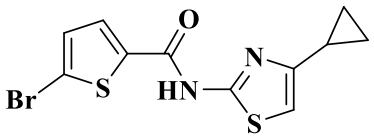


Figure 1. Structure of MB2-1

Acknowledgements
This work was supported by Research Program No. 4 of the "Coriolan Dragulescu" Institute of Chemistry, Timişoara, Romania, and by a grant from the Ministry of Education and Research, CCCDI–UEFISCDI, project no. PN-IV-P6-6.1-CoEx-2024-0196, within PNCDI IV. We acknowledge "Victor Babes" University of Medicine and Pharmacy Timisoara for the full support in providing us with in vitro assays. We are greatful to Alina Nicolescu from Petru Poni Institute of Macromolecular Chemistry, Iasi and Valentin Badea from Politehnica University Timisoara for recording NMR spectra.

References
1. Zhong L. et al., Signal Transduct. Target. Ther. 2021, 6:201.
2. Min H.-Y. & Lee H.-Y., Exp. Mol. Med. 2022, 54:1670–1694.

CONDUCTOMETRIC AND UV–VISIBLE STUDY OF METAL–ORGANIC FRAMEWORK DEGRADATION

Marcela IOSIVONI, Nicoleta PLESU, Aurelia VISA

"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223 Timisoara, Romania
miosivoni@gmail.com

Metal–organic frameworks (MOFs) have attracted considerable attention owing to their high surface area, tunable pore structure, and broad range of applications in catalysis, gas storage, drug delivery, and environmental remediation. However, their structural stability in aqueous and chemically aggressive environments remains a critical issue that can limit their practical use. In this study, the degradation behavior and stability of HEDP-based MOFs, derived from 1-hydroxyethylidene-1,1-diphosphonic acid (HEDP), were investigated using complementary analytical techniques under aqueous and UV–Vis irradiation conditions.

HEDP-based MOFs were synthesized using both conventional hydrothermal methods and alternative approaches, namely sonochemical and microwave-assisted synthesis, employing water as the reaction solvent in accordance with the 12 principles of green chemistry. [1, 2]

Two complementary analytical techniques were employed to investigate the degradation behavior of the HEDP-based metal–organic framework (MOF). Conductometric measurements were used to monitor the degradation process under acidic conditions, while X-ray diffraction (XRD) analysis was performed to evaluate the structural changes induced by ultraviolet (UV) irradiation. Conductometric analysis was employed to monitor changes in the ionic conductivity of the solution during degradation, providing information on the release of metal ions and linker-related species as the framework gradually decomposed. Complementary UV–Visible spectroscopy was used to detect changes in the concentration and electronic absorption characteristics of the dissolved organic components, allowing the degradation process to be followed over time. This methodology offers valuable insights into the degradation mechanism of MOFs and represents an effective tool for assessing their suitability for applications where long-term structural stability is essential. Zn HEDP show a good stability in acid solution; the release of parent acid is under 5%.

Additionally, X-ray Diffraction (XRD) was used to study the degradation process under UV-Vis radiation of MgHEDP. The diffraction patterns showed a nearly uniform decrease in peak intensities without abrupt disappearance or peak shifts, indicating a non-selective degradation mechanism and excluding violent photolysis or aggressive oxidation processes. The peak at ~5° does not shift significantly, indicating that there is no additional water intercalation but rather a stabilized structure that was likely initially hydrated and that UV exposure does not significantly eliminate it (in the range of 1–7h). The minor changes observed in the 30–35° range indicated limited amorphization, while the persistence of the Mg–O structure and lamellar organization demonstrated moderate stability under UV radiation. Analysis of the degradation constants suggested that structural and chemical degradation occurred simultaneously, with C–P bond cleavage representing the dominant degradation pathway.

Acknowledgements
This work is supported by Research Program No. 2 of the „Coriolan Dragulescu" Institute of Chemistry, Timișoara, Romania.

References
1. Anastas P.T., Warner J.C., Oxford University Press. 2000.
2. Zhao Y., Wang Z., Bao Z., Zing H., Zhang Z., Su B., Yang Q., Sep. Purif. Technol. 2018, 195:238-243.

SILICA DERIVED FROM RICE HUSK ASH: TAILORING PHASE STRUCTURE AND MORPHOLOGY BY CONTROLLING CALCINATION TEMPERATURE

Orsina VERDEŞ[1], Mariana SUBA[1], Silvana BORCĂNESCU[1], Cătălin IANAŞI[1], Paula SVERA[2] Livia DEVESELEANU-CORICI[1]

[1] *"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223, Timişoara, România*
[2]*National Institute for Research and Development in Electrochemistry and Condensed Matter-Timişoara - INCEMC, Dr. A. Păunescu Podeanu Street, No. 144, 300569 Timişoara, România*
orsinaverdes@acad-icht.tm.edu.ro

Rice husk, an abundant agricultural by-product, contains a high proportion of silica (SiO_2), making it a sustainable and low-cost precursor for silica synthesis. This study investigates the effect of calcination temperature on the phase structure and morphology of silica derived from rice husk ash (RHA), with the aim of identifying thermal treatment conditions suited to different target applications. Samples were calcined over a temperature range of 300–1200 °C, resulting in distinct structural characteristics depending on the applied conditions. At lower temperatures (300–600 °C), amorphous silica with a high surface area and a porous structure was obtained. At intermediate temperatures (600–800 °C), the amorphous character was largely preserved, although gradual changes in porosity and the onset of partial crystallization were observed. At higher temperatures (800–1200 °C), a progressive transformation toward crystalline silica phases, such as cristobalite and tridymite, occurred, significantly altering the thermal and mechanical properties of the resulting materials. The obtained samples were characterized by thermal analysis, Fourier-transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), and Brunauer–Emmett–Teller (BET) surface area analysis. These results show that controlled tailoring of phase composition and textural properties, through adjustment of the calcination temperature, is essential for optimizing RHA-derived silica for advanced applications, including lanthanide recovery from aqueous solutions and CO_2 capture. Given its silanol-rich, porous surface, RHA-derived silica obtained at lower calcination temperatures may also hold promise as a support for enzyme immobilization, potentially providing a favorable microenvironment for biocatalysts and enhancing enzyme loading and operational stability.

Acknowledgements
This work was supported by Research Program No. 4 of the "Coriolan Dragulescu" Institute of Chemistry, Timişoara, Romania, and by a grant from the Ministry of Research, Innovation and Digitization, CCCDI-UEFISCDI, project number PN-IV-P7-7.1-PED-2024-2513, within PNCDI IV. The authors also acknowledge the use of the RO-OPENSCREEN research infrastructure of the Institute (MySMIS code 127952, Contract No. 371/20.07.2020).

QUANTITATIVE ANALYSIS OF ARISTOLOCHIC ACID I IN AN ACTIVATED CHARCOAL SOLUTION BY ULTRA-HIGH PRESSURE LIQUID CHROMATOGRAPHY COUPLED WITH DIODE ARRAY DETECTION

Maria-Alexandra PRICOP[1,2], Camelia OPREAN[1,3,4] Alexandra T. LUKINICH-GRUIA[1], Alexandra IVAN[1,5], Virgil PĂUNESCU[1,5], Călin A. TATU[1,5]

[1] OncoGen Centre, Clinical County Hospital "Pius Branzeu", Blvd. Liviu Rebreanu 156, Timisoara, 300723, Romania
2 Department of Applied Chemistry and Environmental Engineering and Inorganic Compounds, Faculty of industrial Chemistry, Biotechnology and Environmental Engineering, Politehnica University Timisoara, Vasile Pârvan 6, 300223 Timişoara, Romania
3 Faculty of Pharmacy, Victor Babes, University of Medicine and Pharmacy Timişoara, E. Murgu Sq., no. 2, 300041 Timişoara, Romania
4 Center for Drug Data Analysis, Cheminformatics, and the Internet of Medical Things, Victor Babes, University of Medicine and Pharmacy, Timişoara, E. Murgu Sq., no. 2, 300041 Timişoara, Romania
5 Department of Functional Sciences, Center of Immuno-Physiology (CIFBIOTEH), Victor Babes, University of Medicine and Pharmacy, Timişoara, Eftimie Murgu Sq. 2, 300041 Timişoara, Romania

Aristolochia spp. are medicinal plants widely used in traditional medicine worldwide. However, their use is associated with significant health risks due to the presence of aristolochic acid I (AAI), the principal phytotoxin responsible for nephrotoxicity and carcinogenicity. Exposure to AAI may lead to acute and chronic kidney disease, as well as various types of cancer, depending on the dose and formulation. This study evaluated the ability of activated charcoal (AC) to adsorb and remove AAI as a simple and cost-effective detoxification strategy. AAI concentrations were determined qualitatively and quantitatively using ultra-high-performance liquid chromatography coupled with diode-array detection (UHPLC-DAD) at different contact times. The environmental sustainability of the analytical method was assessed using the AGREE greenness metric. Results: A single 250 mg dose of AC, corresponding to a standard medical tablet, removed 97.65% of AAI (125 µg/mL) from a methanolic solution within 30 minutes. The UHPLC-DAD method achieved an AGREE greenness score of 0.58, indicating a satisfactory level of environmental sustainability.
These findings demonstrate, for the first time, that AC provides an effective, affordable, and accessible approach for AAI removal, with potential applications in both the detoxification of Aristolochia-derived herbal preparations and the remediation of AAI-contaminated environments. Furthermore, the developed UHPLC–DAD method represents a reliable and environmentally responsible platform for the AAI-routine determination.

References

1. Pricop M.-A., Oprean C., Lukinich-Gruia A.T., Ivan A., Păunescu V., Tatu C.A., Processes. 2026, 14:1217.
2. Pricop M.-A., Negrea A., Ciopec M., Pascu I.B., Oprean C., Lukinich-Gruia A.T., Cristea I.-M., Ivan A., Păunescu V., Tatu C.A., Processes. 2025, 13:3397.
3. Pricop M.-A., Lukinich-Gruia A.T., Cristea I.-M., Păunescu V., Tatu C.A., Plants. 2024, 13:2987.

CELL CULTURE MODELS AND EXPERIMENTAL STRATEGIES FOR CYTOCOMPATIBILITY ASSESSMENT OF WOUND DRESSINGS AND SKIN CARE PRODUCTS

Radostina ALEXANDROVA[1], Orlin ALEXANDROV[2], Eliya STOILOVA[1], Silvia MANCHEVA[1],3, Tanya. ZHIVKOVA[1], Lora DYAKOVA[4], Abedulkadir ABUDALLEH[2], Hristo HRISTOV[2], Elena VASSILEVA[5], Erika ADOMAVIČIŪTĖ[6], Virginija JANKAUSKAITĖ[6], Ioana BALDEA[7], Monica NEAGU[8], Merve Erginer HASKOYLU[9]

[1] *Institute of Experimental Morphology, Pathology and Anthropology with Museum, Bulgarian Academy of Sciences, Sofia, Bulgaria*
[2] *Faculty of Medicine, Medical University - Sofia, Bulgaria*
[3] *New Bulgarian University, Sofia, Bulgaria*
[4] *Institute of Neurobiology, Bulgarian Academy of Sciences, Sofia, Bulgaria*
[5] *Faculty of Chemistry and Pharmacy, Sofia University "St. Kliment Ohridski",*
[6] *Kaunas University of Technology, Kaunas, Lithuania*
[7] *University of Medicine and Pharmacy, Cluj-Napoca, Romania*
[8] *"Victor Babes" National Institute of Pathology, Bucharest, Romania*
[9] *Istanbul University-Cerrahpaşa, Istanbul, Türkiye*
rialexandrova@hotmail.com

The aim of this study was to summarize the role, advantages, and limitations of different cell culture models (human keratinocytes, human and murine fibroblasts, and stem cells) in the cytocompatibility assessment of novel wound healing and skin care materials under laboratory conditions.
Our experience in evaluating wound dressings (polyzwitterionic hydrogels and cellulose-based materials) and skin care products (collagen-based formulations) with different structures and chemical/physicochemical properties is summarized.
Approaches for conducting both direct experiments, in which cells are cultured directly in or on the tested materials, and indirect experiments, in which cells are seeded into culture medium previously incubated with the tested materials, are also presented. These approaches are based on methods targeting different cellular components (molecules and organelles) and different mechanisms of action, including the MTT/MTS assay, neutral red uptake assay, crystal violet staining, trypan blue exclusion assay, acridine orange/propidium iodide double staining, and the scratch assay. The main challenges associated with these studies and possible strategies to overcome them are also discussed.

Acknowledgements
The study was supported by Bulgarian National Science Fund (Grant N КП-06-КОСТ/18 from 12.08.2024), Bilateral project between the Bulgarian Academy of Sciences and the Lithuanian Academy of Sciences and COST Action CA21108 „NETSKINMODELS".

References
1. Richter S., Lonnecke P., Bovan D., Andrian N., Stoean B., Lehene M., Silaghi-Dumitrescu R., Gaina L., Mijatovic S., Maksimovic-Ivanic D., Kaluderovic G.N., Hey-Hawkins E., Dalton Trans., 2025, 54:3597.
2. Zagrean-Turza C., Igescu I., Lupan A., Silaghi-Dumitrescu R., Inorg. Chim. Acta. 2024, 567:122053.

COMPARATIVE INVESTIGATION OF SOLVOTHERMAL AND MECHANOCHEMICAL SYNTHESIS OF Co-BTC METAL ORGANIC FRAMEWORKS

Ramona FARKAS (UNGUREAN)[1], Bianca MARANESCU[2], Aurelia VISA[3]

[1] *West University of Timisoara, Doctoral Sch Exact & Nat Sci, Bv Vasile Parvan 4, Timisoara 300223, Romania*

[2] *Faculty of Chemistry, Biology, Geography, West University of Timisoara, 16 Pestalozzi Street, 300115 Timisoara, Romania*

[3] *"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223, Timisoara, Romania*

ramona.farkas01@e-uvt.ro

Metal-organic frameworks (MOFs) are a rapidly expanding class of porous crystalline materials distinguished by their exceptionally high surface areas, tunable architectures, and broad potential in catalysis, gas storage, separation, and sensing. This work investigates the structural design and synthesis optimization of cobalt-based MOFs (Co-BTC), while emphasizing sustainable synthetic strategies aligned with green chemistry principles. [1] The experimental study focused on the synthesis and characterization of Co-BTC using trimesic acid and cobalt acetate as precursors.

Two preparation routes were comparatively evaluated: a conventional solvothermal method employing ethanol or dimethylformamide (DMF) as solvents, and a solvent-free mechanochemical approach based on ball milling. Structural and physicochemical properties were investigated by Fourier-transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), and X-ray diffraction (XRD).

The results demonstrate a clear trade-off between sustainability and structural quality. The mechanochemical route reduced the overall synthesis time by approximately 55% and lowered energy consumption by nearly 60%, while completely eliminating solvent waste, highlighting its significant environmental advantages. [2, 3] In contrast, solvothermal synthesis in DMF produced materials with superior crystallinity and enhanced thermal stability. Furthermore, precise pH control proved essential for directing framework formation, with optimal values of pH 4.6 for ethanol-based synthesis and pH 6.3 for DMF-based synthesis. These findings show that mechanochemical synthesis represents a promising low-energy alternative for MOF production, whereas solvothermal conditions remain preferable when maximum structural order and stability are required.

Acknowledgements

This work was partially supported by West University of Timisoara, Doctoral Sch Exact & Nat Sci, and by Research Program No. 2 of the „Coriolan Dragulescu" Institute of Chemistry, Timișoara, Romania.

References

1. Anastas P.T., Warner J.C., Oxford University Press, 2000.
2. Gines-Palestino R.S., Chiñas-Rojas L.E., Arenzano-Altaif J. A., Sánchez-Bazan I., Bello-Bello J., Rivera-Villanueva J. M., J. Solid State Chem. 2026, 360:126031.
3. Rajendran N., Karthikeyan S., ACS Omega. 2025, 10:43327–43362.

REPURPOSING OF AHAS-INHIBITING HERBICIDES AS ANTIFUNGAL AGENTS: STRATEGIES FOR OPTIMIZING ORAL BIOAVAILABILITY

Radu Daniel SĂVULESCU, Ana BOROTA, Sorin AVRAM, Sorin Alin MARINESCU

"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223, Timisoara, Romania

The increasing incidence of resistant fungal infections requires innovative drug development strategies. A rapid and efficient approach is the repurposing of acetohydroxyacid synthase (AHAS) inhibiting herbicides. Because AHAS is a vital enzyme for fungi such as Candida albicans, but completely absent in mammals, these compounds offer excellent selectivity. Although in silico studies have demonstrated their promising potential, a major barrier in the transition of these pesticides to human clinical use is oral bioavailability. Being initially optimized to penetrate plant structures, these compounds are often extremely lipophilic (high LogP values), which severely limits their aqueous solubility and absorption. The present work aims to experimentally evaluate these repurposed candidates and apply structural optimization strategies to improve their pharmacokinetic profile.

Acknowledgments
This work was supported by Research Program No. 1 of the "Coriolan Dragulescu" Institute of Chemistry, Timişoara, Romania.

ETHINYLESTRADIOL IN THE PREFORMULATION SPOTLIGHT: PRELIMINARY DATA

Sebastian SIMU[1], Yasmine BOUDALI[1], May ZIDI[1], Amalia RIDICHIE[1], Adriana LEDEŢI[1], Laura SBÂRCEA[1], Alina MOACĂ[2], Crinela-Mihaela ŞERBAN[3], Ionuţ LEDEŢI[1]

[1]University of Medicine and Pharmacy Victor Babeş Timişoara, Faculty of Pharmacy, Advanced Instrumental Screening Center, 2 Eftimie Murgu Square, Timişoara, Romania
[2]University of Medicine and Pharmacy Victor Babeş Timişoara, Faculty of Pharmacy, Research Center for Pharmacotoxicological Evaluations, 2 Eftimie Murgu Square, Timişoara, Romania
[3]Titu Maiorescu University, Faculty of Nursing, Târgu Jiu Branch, Department of General Nursing, 100 Ecaterina Teodoroiu Boulevard, Târgu Jiu, Romania
simu.sebastian@umft.ro

Ethinylestradiol (EE) is a synthetic estrogen widely used in oral contraceptive formulations and hormone replacement therapy, whose physicochemical profile - characterized by poor aqueous solubility, high lipophilicity and pH-dependent behavior - poses significant challenges to the development of stable and bioavailable pharmaceutical dosage forms. [1, 2] The present study follows the kinetic analysis of EE [3] and addresses the challenges through a two-pronged preformulation investigation encompassing solid-state compatibility screening with commonly used pharmaceutical excipients and the characterization of the interaction between EE and sulfobutylether-β-cyclodextrin (SBEBCD) in solution. Compatibility studies were performed on binary mixtures of EE with a selection of excipients representative of the main functional categories employed in solid dosage form development, using a complementary set of instrumental techniques including attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR), powder X-ray diffraction (PXRD) and thermal analysis (TG/DTG/DSC). The presence or absence of physicochemical interactions was assessed by comparing the spectral, diffractometric and thermoanalytical profiles of the pure components and their binary mixtures, both immediately after preparation and following a defined storage period.

The interaction between EE and SBEBCD in solution was investigated by the method of continuous variations, employing UV spectrophotometry to determine the stoichiometry of the inclusion complex formed. The complexation was further characterized by the determination of the binding constant, providing quantitative insight into the affinity of EE for SBEBCD and the potential of this cyclodextrin to enhance the apparent aqueous solubility and dissolution rate of the active ingredient. Collectively, the results of this study provide a rational preformulation framework for the development of EE-based pharmaceutical formulations with improved physicochemical performance, supporting the selection of compatible excipients and the use of SBEBCD as a solubility-enhancing agent.

References

1. Bitzer J., Minerva Ginecol. 2011, 63:299–304.
2. Simu S., Marcovici I., Dobrescu A., Malita D., Dehelean C.A., Coricovac D., et al., Molecules 2021, 26:2776.
3. Simu S., Ledeți A., Moacă E.-A., Păcurariu C., Dehelean C., Navolan D., Ledeți I., Processes 2022, 10:1518.

MAPPING OF PHARMACOLOGICAL SPACE BY STRUCTURE-TARGET RELATIONSHIPS THROUGH LAYERED SOM FRAMEWORK

Nicoleta STOIAN[1], Liliana HALIP[1]

"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223, Timişoara, Romania
nstoian@acad-icht.tm.edu.ro

Conventional methods in pharmacological analysis often fail to fully capture the relationships between ligand structures and biological response due to complexity of biological systems. Thus, there is interest in creating novel workflows which integrate both chemical and biological information to get a global overview of drug-target pairings.
We developed a machine learning framework with intuitive and interpretable output based on the classic Kohonen [1] sorting algorithm with two input matrices. Data consisted of 1600 approved drugs described further through a chemical layer (MACCS fingerprints) [2] and biological layer (ProtBERT embedding derived from protein sequences). [3] Model selection and validation were performed using established quality metrics, like Quantization Error (QE) and Topographic Error (TE). Clustering revealed aggregation based on both chemical similarities and biological criteria within the same cluster, thus proving the relevance of the biological information included. Mapping of new data post-training, revealed a coherent placement of drugs outside our data set in absence of an associated target. Mapping revealed chemical similarity between the novel structure and the previously mapped compounds' scaffolds, and hinted towards biological reasoning regarding the general use of the neighboring molecules and the new drug.
Overall, a SOM-based framework offers an intuitive approach to Structure-Target analysis and could be used in computational experiments as an early target assessment tool and polypharmacological tests.

Acknowledgements
This work was supported by Research Program No. 1 of the "Coriolan Dragulescu" Institute of Chemistry, Timisoara, Romania.

References
1. Kohonen T. Biol Cybern. 1982, 43(1):59-69.
2. Durant J.L., Leland B.A., Henry D.R., Nourse J.G., J Chem Inf Comput Sci. 2002, 42(6):1273-80.
3. Brandes N, Ofer D, Peleg Y, Rappoport N, Linial M., Bioinformatics. 2022, 38(8):2102-2110.

SYNTHESIS AND CHARACTERIZATION OF PRIMARY-, SECONDARY-, AND TERTIARY-AMINE-FUNCTIONALIZED KIT-6 MESOPOROUS SILICA

Mariana SUBA, Orsina VERDEȘ, Silvana BORCĂNESCU, Livia DEVESELEANU-CORICI, Cătălin IANAȘI

"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223 Timişoara, România
mariana_suba@acad-icht.tm.edu.ro

Amine-functionalized mesoporous silica materials have attracted considerable attention due to their enhanced adsorption performance and versatile surface chemistry, making them promising candidates for applications such as carbon dioxide capture, catalysis, and pollutant removal. Among mesoporous silicas, KIT-6 is particularly attractive because of its highly ordered three-dimensional bicontinuous pore structure, large specific surface area, and high pore volume, which facilitate the incorporation of functional groups while maintaining efficient mass transfer. These characteristics also make KIT-6 an excellent support for enzyme immobilization, providing a favorable microenvironment for biocatalysts, enhancing enzyme loading, improving operational stability, and reducing mass transfer limitations during catalytic processes. Surface functionalization through grafting enables the introduction of nitrogen-containing groups onto the silica framework, thereby tailoring the physicochemical properties of the material for specific applications.
In this study, amino-functionalized KIT-6 molecular sieves were prepared by post-synthetic grafting using different amine-containing silane and polymeric modifiers, namely 3-aminopropyltriethoxysilane (APTES), diethylamine (DEA), N,N-diethylethanolamine (DEEA), and polyethyleneimine (PEI). The influence of the grafting agents on the structural and surface characteristics of the resulting materials was investigated in order to evaluate their effectiveness in introducing accessible amino functionalities while preserving the mesoporous architecture of KIT-6. The materials obtained were characterized by IR spectroscopy and X-ray diffraction at low angles. Thermal stability was investigated by TGA-DTG, and the specific surface area and the mean pore diameter of the KIT-6 were determined by nitrogen adsorption in accordance with the BET method.

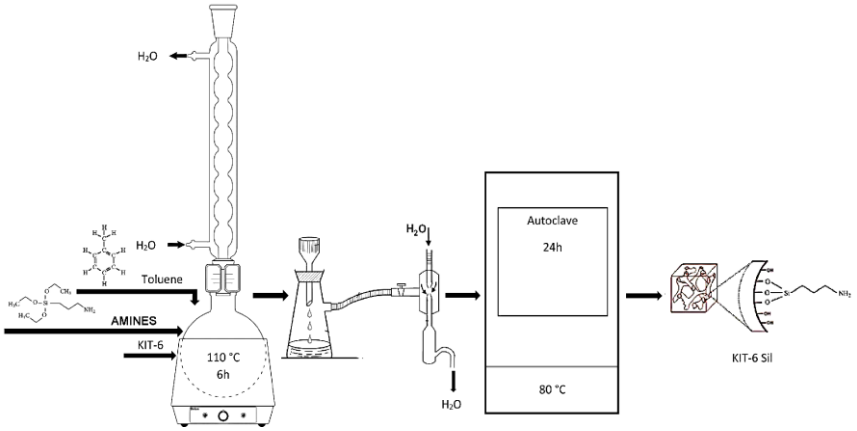


Figure 1. Schematic illustration of the synthesis of functionalized KIT-6

Acknowledgements
This work was supported by Research Program No. 4 of the "Coriolan Dragulescu" Institute of Chemistry, Timișoara, Romania, and by a grant from the Ministry of Research, Innovation and Digitization, CCCDI-UEFISCDI, project number PN-IV-P7-7.1-PED-2024-2513, within PNCDI IV. The authors also acknowledge the use of the RO-OPENSCREEN research infrastructure of the Institute ((MySMIS code 127952, Contract No. 371/20.07.2020).

ELECTROCHEMICAL INVESTIGATION OF CHITOSAN AS A CORROSION INHIBITOR FOR IRON IN LACTIC ACID

Milica ŢARĂ-LUNGĂ-MIHALI, Anemona Mariana CORNEA, Adriana POPA, Aurelia VIŞA, Nicoleta PLEŞU

"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223 Timişoara, Romania
milicamihali22@gmail.com

The development of environmentally friendly corrosion inhibitors has become an important research direction in the field of sustainable materials protection. In this study, the corrosion behavior of iron in a lactic acid solution containing chitosan was investigated using electrochemical techniques. Chitosan, a naturally derived biopolymer obtained by the deacetylation of chitin, possesses excellent biocompatibility, biodegradability, and a high density of amino and hydroxyl functional groups capable of interacting with metallic surfaces. These characteristics make it a promising green corrosion inhibitor for acidic environments. [1, 2]

The electrochemical performance of iron was evaluated in lactic acid solutions in the absence and presence of chitosan (non-ball-milled and ball-milled) under controlled experimental conditions. Potentiodynamic polarization (CP) and electrochemical impedance spectroscopy (EIS) were employed to assess the inhibition efficiency and to elucidate the corrosion mechanism. A corrosion rate of 0.744 mm/year was measured for iron without the inhibitor, 0.154 mm/year and 0.091 mm/year for iron with the non-ball-milled and ball-milled chitosan. The results indicate that the addition of chitosan significantly reduces the corrosion rate of iron by promoting the adsorption of inhibitor molecules onto the metal surface and the formation of a protective barrier that limits charge transfer and metal dissolution. The increase in polarization resistance (1127.7 Ω, 2109.3 Ω and 5358.3 Ω) and the corresponding decrease in corrosion current density (6.400×10^{-5} A/cm^2, 1.328×10^{-5} A/cm^2 and 7.815×10^{-6} A/cm^2) confirm the beneficial effect of chitosan on corrosion protection.

The inhibition performance is attributed to the adsorption of chitosan through its nitrogen- and oxygen-containing functional groups, leading to the formation of a compact and stable protective layer. These findings demonstrate that chitosan is an effective, biodegradable, and environmentally benign corrosion inhibitor for iron exposed to lactic acid solutions. The study provides a basis for the future development of sustainable corrosion protection systems for applications requiring non-toxic and biodegradable materials.

Acknowledgements
This work was supported by Research Programs no. 3, from the "Coriolan Dragulescu" Institute of Chemistry Timisoara, Romania.

References
1. Miretzky P., Cirelli A. F., J. Hazard. Mater. 2009, 167:10–23.
2. Verma C., Quraishi M.A., Alfantazi A., Rhee K. Y., Int. J. Biol. Macromol. 2021, 184:135–143.

SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF A NOVEL THIAZOLE-CONTAINING SULFONAMIDE DERIVATIVE AS A POTENTIAL BACTERIAL CARBONIC ANHYDRASE INHIBITOR

Ioana Andreea ANDREI, Bogdan MARA, Liliana CSEH

"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223, Timisoara, Romania
ioana13012000@gmail.com

Over the past decade, antimicrobial resistance has emerged as one of the greatest global threats to human health, according to the World Health Organization. [1] Consequently, the efficacy of conventional antibiotics has been severely limited, demanding the urgent identification of novel therapeutic targets.

Bacterial carbonic anhydrases play an essential role in the survival and virulence of pathogens. The selective inhibition of these enzymes offers a promising strategy for the development of novel antimicrobial agents. [2, 3]

This work encompasses the synthesis, physicochemical analysis, and structural characterization of a novel thiazole-containing sulfonamide derivative, designed as a potential bacterial carbonic anhydrase inhibitor.

The target compound was obtained in high purity, and spectroscopic characterization by 1H and 13C NMR and FT-IR supported the proposed molecular structure and the presence of the sulfonamide functional group.

Acknowledgements
This work was partially supported by Research Program No. 4 of the "Coriolan Drăgulescu" Institute of Chemistry, Timișoara, Romania, and by a grant from the Ministry of Education and Research, CCCDI–UEFISCDI, project number PN-IV-P6-6.1-CoEx-2024-0196, within PNCDI IV.

References
1. Ho C.S., Wong C.T.H., Aung T.T., Lakshminarayanan R., Mehta J.S., Rauz S, McNally A., Kintses B., Peacock S.J., de la Fuente-Nunez C., Hancock R.E.W., Ting D.S.J., Lancet Microbe. 2025, 6(1):100947.
2. Rowlett R.S., Biochim Biophys Acta. 2010, 1804(2):362-373.
3. Capasso C., Supuran C.T. J Enzyme Inhib Med Chem. 2015, 30(2):325-332.

SYNTHESIS OF pH-RESPONSIVE AMP-*g*-PAA COPOLYMER AND ITS APPLICATION IN THE GREEN FORMATION OF AuNPs

Melinda-Maria BAZARGHIDEANU[1], Larisa-Maria PETRILA[1], Marius-Mihai ZAHARIA[1], Ana-Lavinia VASILIU[1], Stergios PISPAS[1,2], Marcela MIHAI[1]

[1]*Petru Poni Institute of Macromolecular Chemistry, Iasi, Romania.*
[2]*Theoretical and Physical Chemistry Institute, Athens, Greece*
larisa.petrila@icmpp.ro

Over the past few years, gold nanoparticles (AuNPs), particularly recognized for their distinctive optical and catalytic characteristics, have attracted increasing attention due to their chemical stability and localized surface plasmon resonance properties, making them ideal candidates for a broad spectrum of applications, including biosensing, drug delivery, photomedicine and vaccine development [1]. Due to the increasing requirement for sustainable materials and eco-friendly chemical methods, the use of hybrid macromolecular materials based on polysaccharides and stimuli-responsive polymers as stabilizing and coating agents for AuNPs, represents a promising approach for the development of smart/responsive hybrid nanomaterials, that integrate their functionalities and properties [2, 3].
Inspired by these needs, a new biological/synthetic hybrid graft copolymer was obtained by grafting poly(acrylic acid) (PAA, synthesized via reversible addition-fragmentation chain transfer polymerization) to amylopectin (AMP). The attachment of PAA to the backbone of AMP was performed via a radical-mediated coupling reaction using the "*grafting to*" technique and the characterization of the resulting grafted copolymer was performed by ATR-FTIR and ^{1}H NMR spectroscopies, thermogravimetric analysis, dynamic and electrophoretic light scattering (DLS, ELS) measurements. Afterwards, the novel graft copolymer was tested as a reducing agent for the synthesis of AuNPs following an environmentally friendly procedure. The hybrid composites were prepared via an *in situ* process in aqueous solution using $HAuCl_4$ and AMP-*g*-PAA copolymer at different incubation temperatures, reaction duration, and inorganic/polymer weight ratios, without the addition of other reducing agents. By systematically studying the relationship between temperature and the ratio between initial components, it was found that higher temperatures increase the nucleation of AuNPs, decrease the aggregation tendency, and leads to the formation of more uniform composite nanostructures. Summarizing, the most stable colloidal nanocomposites were obtained at a ratio of 0.36 and a temperature of 60 °C for a 6 h reaction time, as shown by UV–vis, DLS, and STEM analysis. Based on the characterization results, the selected hybrid nanocomposites were further evaluated in terms of cytotoxicity, revealing a relative cell viability above 90% for all tested concentrations [2]. This investigation illustrates that the obtained composites represent a promising safety baseline for further investigation in biomedical applications.

Acknowledgements
This work was supported by a grant of the Ministry of Education and Research, CCCDI - UEFISCDI, through the project *Center of Excellence in water management, materials, by-products and waste valorisation for circular bioeconomy implementation*, project number PN-IV-P6-6.1-CoEx-2024-0056, contract 6CoEx/02.06.2026, and by CNCS-UEFISCDI, project number PN-IV-P1-PCE-2023-0738, within PNCDI IV.

References
1. Tepale N., Fernández-Escamilla V.V.A, González-Coronel V.J., Luna-Flores A, Aguilar J., Carreon-Alvarez C., Carreon-Alvarez A., Crystals. 2019, 9:612.
2. Bazarghideanu M.-M., Zaharia M.-M., Bucatariu F., Vasiliu A.-L., Mihai M, Pispas S., Polymers. 2026, 18(13):1636.
3. Abdulraheem M.I., Moshood A.Y., Gourkhede P.H., Xu L., Zang Y., Cadenas-Pliego G., Raghavan V., Hu, J., Polym. Bull. 2025, 5:1-39.

SEQUENTIAL COLUMN ASSEMBLY OF ALGINATE–COPPER HYBRID MATERIALS USING ION-EXCHANGE RESINS

Marius-Mihai ZAHARIA, Alina-Petronela MORARU, Florin BUCATARIU, Melinda-Maria BAZARGHIDEANU, Ana-Lavinia VASILIU, Marcela MIHAI

Petru Poni Institute of Macromolecular Chemistry, 41A Grigore Ghica Voda Alley, 700487 Iasi, Romania
zaharia.marius@icmpp.ro

Research into multifunctional hybrid materials that combine natural macromolecules and metal ions is a promising method for finding materials with controllable physicochemical properties. [1, 2] Additionally, the development of sustainable processes in the aqueous phase which allow us to recover and use chemical resources is of key importance for water management and the circular bioeconomy today. [3] Based on the above aspects, this research describes a column method which allows us to create polysaccharide-metal systems using sodium alginate (AlgNa), ion-exchange resins (IExR) and copper ions. To start with, AlgNa containing carboxylate groups was sorbed onto cationic and zwitterionic IExR in dynamic column conditions resulting in the formation of alginate-impregnated resin matrices. The charge density of the produced materials was measured using a particle charge detector (PCD) in order to understand the changes taking place during alginate sorption and its interaction with the resin functional groups. After that, the solution of copper ions passed through the alginate-loaded IExR columns, thus creating interaction between Cu^{2+} ions and the formed alginate/IExR matrices. The concentration of copper ions in the aqueous medium was measured by atomic absorption spectrometry (AAS) allowing us to quantify copper uptake.
The sequential method provides a controlled pathway to merge natural macromolecule with metal ion in an IExR matrix. The effective application of PCD along with AAS allows the characterization of the two stages of the sorption process, namely polysaccharide sorption followed by capture of metal ions. This dynamic column system also serves as a suitable model for continuous flow processes in liquid phase which may be further applied for water treatment technology, resource recovery, and making functional hybrid materials. The acquired results offer an understanding of interactions taking place between AlgNa, IExR, and Cu^{2+} ions, and also help in the development of preassembled natural macromolecule-metal combinations. The addressed method ensures usage of renewable materials, ion exchange processes, and metal ion recovery and opens prospects for development of multifunctional hybrid products with environmental, antimicrobial, and catalytic applications.

Acknowledgements
This work was financially supported by the grants of the Ministry of Education and Research, CNCS/CCCDI -UEFISCDI, projects numbers PN-IV-P1-PCE-2023-0738 and PN-IV-P6-6.1-CoEx-2024-0056, within PNCDI IV.

Reference
1. Gomez-Romero P., Pokhriyal A., Rueda-García D., Bengoa L.N., González-Gil R.M., Chem. Mater. 2024, 36(1):8-27.
2. Getya D., Gitsov I., Molecules. 2023, 28(16):6030.
3. Pandey A.K., Environ. Sci.: Water Res. Technol. 2025, 11(8):1822-1846.

A GREENER ROUTE TO GRAPHENE OXIDE: MICROWAVE-ASSISTED SYNTHESIS FROM COFFEE WASTE (GREEN SYNTHESIS) VS. THE HUMMERS METHOD

Alexandru VIŞAN[1], Roxana NICOLA[1], Ana-Maria LACRĂMĂ[1], Sorina ILIEŞ[1], Florica MANEA[2], Stefania Florina RUS[3], Elisabeta I. SZERB[1]

[1]"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223, Timişoara, România
[2]Politehnica University of Timisoara, Department of Applied Chemistry and Engineering of Inorganic Compounds and Environment, Timişoara, Romania
[3]National Institute for Research and Development in Electrochemistry and Condensed Matter, Str. Dr. A. Păunescu Podeanu 144, 300569 Timisoara, Romania
visan.alexandru@acad-icht.tm.edu.ro

The current research focuses on the synthesis of graphene oxide (GO) from renewable carbon sources, specifically, spent coffee grounds (SCGs), and includes a thorough comparison with the well-known process of GO synthesis based on mined graphite with the use of Hummers method. [1] Since this approach is both energy-consuming and ecologically harmful, finding alternatives becomes necessary when considering the modern importance of green nanotechnology. [2] In this experiment, GO is synthesized from biomass material via several-stage process involving SCGs. First, the material undergoes aerobic thermal treatment at 600 °C for two hours in order to conduct partial oxidation and carbonization of biomass. Next, crushing and ultrasonic treatment (15 minutes) take place. The formed carbon structure is activated with the help of 5% HCl solution at 90°C during two hours and the cleavage of carbon domains into nanocarbons was done by oxidative cutting using nitric acid as an oxidizing agent via microwave-assisted method. A sample of GO synthesized from commercial graphite via energy-consuming pretreatment of a 10 hours ultrasonic treatment with the use of a sonotrode, followed by a modified Hummers procedure, is selected for comparison.
Herein, the structural, chemical and technical aspects of the two approaches are evaluated (FT-IR, RAMAN, AFM, Electrochemical) and compared in order to analyze the advantages and drawbacks of the described methods. The proposed method of microwave-assisted nitric acid treatment dramatically decreases reaction time and excludes the use of hazardous heavy-metal oxidizers (MnO_2 and $KMnO_4$ used in the modified Hummers method). [1] The microwave-assisted nitric acid process provides a fast and eco-friendly method that is an improvement over the conventional Hummers method that requires the use of heavy metals. It is possible for such a method to be used for converting common agricultural waste, for example, spent coffee grounds (SCGs), into nanocarbons. The present study highlights the features of the new method of synthesis and compares the advantages and disadvantages of the proposed microwave-assisted treatment of biomass with the conventional graphite treatment.

Acknowledgements
This work was supported by Research Program No. 4 of the "Coriolan Drăgulescu" Institute of Chemistry, Timișoara, Romania.

Reference
1. Ramli R, Hidayat R., in Ikram M. (Ed.) Graphene - a wonder material for scientists and engineers, IntechOpen, London, 2023.
2. Mahmood F, Ali M, et al., Ind Crops Prod. 2025, 227:120830.

SUSTAINABLE PRODUCTION OF BIOACTIVE FLAVONOL GLYCOSIDES: OPTIMIZATION OF THE REACTION PARAMETERS

Livia DEVESELEANU-CORICI[1], Ildiko BUTĂ[1], Alina Ramona BUZATU[2], Alina MOGOŞANU[1], Costin-Ioan POPESCU[3], Liliana CSEH[1]

[1] *"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., Timisoara, Romania*
[2] *Victor Babeş University of Medicine and Pharmacy, Department of Biochemistry and Pharmacology, Timisoara, Romania*
[3] *Institute of Biochemistry of the Romanian Academy, Bucharest, Romania*
deveseleanulivia@gmail.com

Flavonoid glycosides have attracted increasing attention as high-value bioactive compounds due to their superior physicochemical properties and enhanced biological activities compared with their corresponding aglycones. [1, 2] Glycosylation improves aqueous solubility, chemical stability, and bioavailability, while frequently preserving or enhancing antioxidant, anti-inflammatory, antiviral, antimicrobial, and anticancer activities. [1] Among naturally occurring flavonols, myricetin is recognized for its exceptional therapeutic potential; however, its pharmaceutical and nutraceutical applications remain limited by its poor water solubility and low bioavailability. [3-4] Therefore, the development of sustainable and selective glycosylation strategies is essential to unlock the full potential of this flavonoid. Enzymatic glycosylation catalyzed by UDP-dependent glycosyltransferases (UGTs) represents an attractive alternative to conventional chemical synthesis, combining excellent regio- and stereoselectivity with high catalytic efficiency under environmentally benign reaction conditions. [5, 6]

In this work, recombinant UGTs were employed for the glycosylation of myricetin using UDP-glucose as the activated glycosyl donor. To establish an efficient and robust biocatalytic platform, the effects of the reaction parameters - including pH, temperature, enzyme loading, and UDP-glucose concentration - were systematically investigated. Furthermore, enzymatic kinetic studies were performed to characterize the catalytic behavior of the recombinant glycosyltransferase toward myricetin and to identify the optimal operating conditions for efficient glycoside synthesis. The optimized reaction conditions and kinetic characterization provide a comprehensive understanding of the catalytic performance of the recombinant UGT and constitute a fundamental step toward the development of sustainable enzymatic processes for flavonoid modification.

Acknowledgements
This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CCCDI - UEFISCDI, project number PN-IV-P7-7.1-PED-2024-2513, within PNCDI IV, and by the Research Program No. 4 of the "Coriolan Dragulescu" Institute of Chemistry, Timişoara, Romania.The authors also acknowledge the use of the RO-OPENSCREEN research infrastructure of the Institute (MySMIS code 127952, Contract No. 371/20.07.2020).

References
1. Lai X., Li X., Chen J., Liu X., Pan P., Zhou Y., Zhao G., Trends Food Sci. Technol. 2025, 165:105296.
2. Cunha M.-H., Ferrari I.B.S., Melo N.C., Carvalho L.M., Ortega M.M., Carvalho P.O., Antioxidants. 2026, 15(5):539.
3. Semwal D.K., Semwal R.B., Combrinck S., Viljoen A., Nutrients. 2016, 8(2):90.
4. Song X., Tan L., Wang M., Ren C., Guo C., Yang B., Ren Y., Cao Z., Li Y., Pei J., Biomed Pharmacother. 2021, 134:111017.
5. Li T., Nidetzky B., Enzyme Microb. Technol., 2026, 200:110916.
6. Ding J., Li X., Jin Z., Svensson B., Bai Y., Biotechnol. Adv., 2026, 89:108863.

CAN FERRIC-OXYL EXCITED STATES EXPLAIN ELONGATED IRON-OXYGEN BONDS IN HEME PEROXIDASE CATALYTIC INTERMEDIATES?

Maria LEHENE, Cezara ZAGREAN-TUZA, Adrian M.V. BRANZANIC, Radu SILAGHI-DUMITRESCU

Babeș-Bolyai University, Department of Chemistry, Str. Arany Janos Nr. 11, RO-400028 Cluj-Napoca, Romania
maria.lehene@ubbcluj.ro

The nature of the ferryl iron–oxygen bond in heme enzymes remains a topic of considerable interest. Recent time-resolved serial femtosecond X-ray crystallography (tr-SFX) studies on a dye-decolourising peroxidase revealed Fe-O bond lengths in Compounds I and II that are longer than expected for a classical ferryl Fe(IV)=O species. To investigate the origin of these structural features, density functional theory (DFT) calculations and QM/MM geometry optimizations were performed. The computational results reproduce the experimentally observed bond elongation and demonstrate that it does not arise from ferryl reduction or protonation to Fe(IV)-OH. Instead, the electronic structure is influenced by accessible excited states with significant ferric-oxyl (Fe(III)-O•) character, leading to partial single-bond character in the Fe–O interaction. These findings provide new insights into the electronic structure of ferryl intermediates and contribute to a more accurate interpretation of high-valent iron–oxo species in heme enzymes.

Acknowledgements
This study was supported by Romanian Ministry of Education and Research and grant PN-IV-PCB-RO-MD-2024-0515.

SYNTHESIS AND CHARACTERIZATION OF Cu SUPPORTED ON CeO_2 FOR CO_2 REDUCTION

Emanuel A. NKOTYA[1], Mihaela M. TRANDAFIR[1], Iuliana M. CHIRICA[1], Anca G. MIREA[1], Alexandra C. IACOBAN[1,2], Mihaela FLOREA[1,2] *

[1]Catalytic Materials and Catalysis, National Institute of Material Physics, Atomistilor 405A, Magurele, Ilfov, Romania
[2]International School of Doctoral Studies, University of Bucharest, Transilvania Street 6, 050067 Bucharest, Romania
mihaela.florea@infim.ro

Ceria has attracted sustained scientific interest for decades owing to its distinctive redox chemistry and its considerable oxygen storage capability. [1] It can be produced in a wide range of morphologies and particle sizes, and is already manufactured industrially for uses spanning polishing, electronics, glass production, and catalysis. Even so, reliably obtaining ceria-based materials that combine high surface area, high defect density, and good thermal stability remains an open problem. [2] Among the possible routes to valorize CO_2, its catalytic hydrogenation to methanol is particularly attractive: methanol is a key liquid platform chemical and an easily stored/transported energy carrier, making this reaction a promising way to couple CO2 mitigation with the production of a commercially valuable fuel and chemical feedstock. Building on this need and on our group's prior experience, the present study set out to validate a precipitation-based synthesis for Cu-doped ceria, scale it up at the laboratory level, and assess the resulting materials as catalysts for the reductive conversion of CO_2 into value-added products.
Samples were obtained via a modified co-precipitation method reported previously [2], with copper contents ranging from 0.5 to 2.5 %. Textural and structural properties were assessed by N_2 adsorption–desorption analysis, X-ray diffraction (XRD) to identify the crystalline phases present, and H_2-temperature-programmed reduction (H2-TPR) to evaluate the extent of reducibility. Specific surface areas were determined using the Brunauer–Emmett–Teller (BET) method, based on adsorption data collected over a relative pressure range (P/P0) of 0.01–0.995.
XRD confirmed that all samples retain the characteristic cubic fluorite structure of pure CeO_2. Copper doping was found to enhance the textural properties markedly: surface area rose from 66 $m^2 \cdot g^{-1}$ for undoped ceria to 105 $m^2 \cdot g^{-1}$ for the 2.5 %-Cu sample. This increase in surface area, together with the improved reducibility conferred by Cu incorporation, is consistent with the requirements for active CO_2-to-methanol catalysts, where a well-developed surface and accessible, readily reducible Cu–Ce sites are needed to promote CO_2 activation and hydrogenation toward methanol. These results therefore point to a beneficial role of Cu doping not only on the textural properties of ceria but also on its potential performance in CO_2 hydrogenation to methanol.

Acknowledgments
This work was supported by the Romanian Ministry of Education and Research and CCCDI-UEFISCDI through the project number PN-IV-P7-7.1-PED-2024-2346 (84/2025).

References
1. Dubey M., Wadhwa S., Mathur A., Kumar R., Appl. Surf. Sci. Adv. 2022, 12:100340.
2. Florea M., Matei-Rutkovska F., Postole G., Urda A., Neatu F., Pârvulescu V.I., Gelin P., Catal Today. 2018, 306.

NEW ASYMMETRIC CURCUMIN ANALOGUES: PH-RESPONSIVE BEHAVIOUR AND ANTIOXIDANT ACTIVITY

Alina MOGOSANU, Livia CORICI-DEVESELEANU, Liliana CSEH

"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223, Timişoara, Romania
alina.mogosanu23@gmail.com

Curcumin is a natural polyphenol widely investigated for its biological properties, including antioxidant, anti-inflammatory, and anticancer activities. However, its limited stability and poor bioavailability restrict its potential biological applications. [1, 2]
In this work, two new asymmetric curcumin analogues (Figure 1) were designed and synthesized to investigate the network of chemical reactions as a function of pH and antioxidant activity. The target compounds were synthesized through a two-step Claisen–Schmidt condensation between cyclohexanone and corresponding substituted aldehyde. The structures were confirmed by 1D and 2D NMR spectrometry, high-resolution mass spectrometry and elemental analysis.
The pH-dependent behaviour of the analogues was investigated by UV–Vis spectroscopy across the pH range 1–14. The compounds exhibited pronounced colour changes from red under acidic conditions to yellow under basic conditions with reversible structural transformations. The behaviour of these compounds mimics the behaviour of anthocyanin systems as has been demonstrated in previous studies performed by our group. [3]
Antioxidant activity was determined by DPPH radical-scavenging assay, yielding IC_{50} values of 63.7 µg/mL for A.4 and 21.8 µg/mL for A.5 compared with ascorbic acid 8.4 µg/mL.

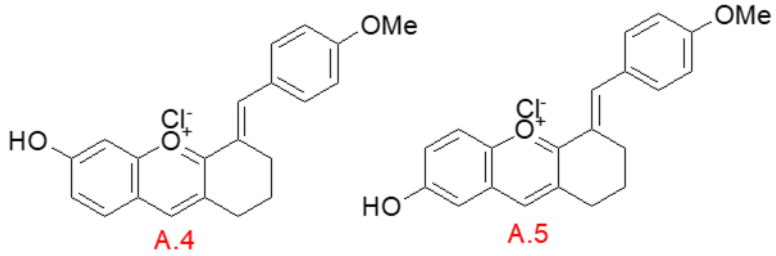


Figure 1. Structure of compounds

The results confirm the structures of the newly synthesized asymmetric curcumin analogues and demonstrate the successful isolation of their acidic forms with a purity exceeding 90%. The studies established the stable forms of the compounds at specific pH values, highlighting their pH-dependent structural transformations and associated optical properties. Furthermore, the synthesized compounds exhibited significant antioxidant activity.

Acknowledgements
This work was supported by Research Program No. 4 of the Coriolan Dragulescu" Institute of Chemistry, Timişoara, Romania, and by a grant of the Ministry of Research, Innovation and Digitization, CCCDI - UEFISCDI, project no. PN-IV-P7-7.1-PED-2024-2513, within PNCDI IV.

References
1. Nagargoje A.A., Panchgalle S.P., Siddiqui M.M., Shaikh M.H., More D., Shingate B.B., Archiv der Pharmazie. 2025, 358.
2. Kaur K., Al-Khazaleh A.K., Bhuyan D.J., Li F., Li C.G., Antioxidants. 2024, 13:1092.
3. Moro A.J., Parola A.J., Pina F., Pana A.-M., Badea V., Pausescu I., Shova S., Cseh L., J. Org. Chem. 2017, 82, 5301−5309

DEVELOPING SYNTHETIC PEPTIDES FOR IMMUNOAFFINITY CHROMATOGRAPHY

Andrei BĂRBOI[1,2], Alexandra CÂRLAN[1,2], Florentina PENA[3], Codruța POPESCU[1,2], Mihaela MATACHE[2,4], Adrian ȘALIC[1,4,5]

[1]*University of Bucharest, Faculty of Chemistry, Department of Inorganic and Organic Chemistry, Biochemistry and Catalysis, 90 Panduri Street, 050663, Bucharest, Romania*
[2]*Research Center of Applied Organic Chemistry, Department of Inorganic and Organic Chemistry, Biochemistry and Catalysis, Faculty of Chemistry, University of Bucharest, 90 Panduri Street, 050663, Bucharest, Romania*
[3]*Institute of Biochemistry, 296 Splaiul Independentei, 060031, Bucharest, Romania*
[4]*Faculty of Interdisciplinary Studies, University of Bucharest, Transilvaniei Street 6, 010798, Bucharest, Romania*
[5]*Harvard Medical School, Department of Cell Biology, LHRRB 401A, 240 Longwood Avenue, Boston MA, 02115, Boston, USA*
andrei.barboi@s.unibuc.ro

Efficient protein purification is essential for both functional analysis and biopharmaceutical applications, where the isolation of a specific protein from complex biological samples demands a high degree of selectivity while preserving protein yield, activity, and structural integrity. Among the various strategies available, immunoaffinity chromatography stands out as a highly efficient and specific method for the purification of recombinant proteins. In this technique, purified antibodies are immobilized onto a chromatographic support, allowing selective retention of the target protein during sample loading. Following removal of non-specifically bound contaminants, the captured protein can be recovered by applying elution conditions that maintain protein stability and functionality. [1]
In the present study, this strategy will be applied for the purification of recombinant proteins carrying the highly polar FLAG peptide tag. The corresponding anti-FLAG monoclonal antibodies were generated through hybridoma technology and their binding specificity was validated by immunofluorescence analysis. To facilitate both antibody purification and subsequent recovery of tagged recombinant proteins, peptide ligands were synthesized by solid-phase peptide synthesis (SPPS). [2] These included a cysteine-terminal version of the FLAG peptide designed for ligand immobilization as well as the soluble FLAG peptide intended for competitive elution of bound target proteins. The identity and purity of the synthesized peptides were confirmed by HPLC-MS.
The next step involves coupling the Cys-terminal peptides on an iodoacetyl-activated Sepharose matrix. The FLAG-cys peptides will be covalently attached through the reaction of their sulfhydryl groups with the reactive iodoacetyl groups from the matrix. [3] This strategy ensures optimal display of the peptide epitope, thereby enabling subsequent affinity capture of anti-FLAG antibodies needed for the generation of a robust chromatographic platform for the selective purification of tagged recombinant proteins.

Acknowledgements
This research was partially carried out and financed through ANC-UEFISCDI, PN-IV-P6-6.1-CoEx-2024-0088, TheraFast 9CoEx/2026. Romanian Ministry of Education and Research, PNRR/2022/C9/MCID/I8, project number CF 760056/23.05.2023, code 235/29.11.2022 is also aknowledged for partial funding.

References
1. Rodriguez E.L., Poddar S., Iftekhar S., Suh K., Hage D.S., et. al., J. Chromatogr. B. 2020, 1157:122332.
2. Behrendt R., White P., Offer J., J. Pept. Sci. 2016, 22:4-27.
3. Barredo-Vacchelli G.R., Giudicessi S.L., Martínez-Ceron M.C., Cascone O., Camperi S.A., Int. J. Pept. Res. Ther. 2021, 27:2905-2921.

SOLID PHASE SYNTHESIS OF PEPTIDES FOR SELECTIVE PURIFICATION

Alexandra CÂRLAN[1,2*], Andrei BĂRBOI[1,2], Florentina PENA[3], Codruța POPESCU[1,2], Mihaela MATACHE[2, 4], Augustin MĂDĂLAN[1,2], Adrian ȘALIC[1,4,5]

[1]University of Bucharest, Faculty of Chemistry, Department of Inorganic and Organic Chemistry, Biochemistry and Catalysis, 90 Panduri Street, 050663, Bucharest, Romania
[2]Research Center of Applied Organic Chemistry, Department of Inorganic and Organic Chemistry, Biochemistry and Catalysis, Faculty of Chemistry, University of Bucharest, 050663, 90 Panduri Street, Bucharest, Romania
[3]Institute of Biochemistry, 296 Splaiul Independentei, 060031, Bucharest, Romania
[4]Faculty of Interdisciplinary Studies, University of Bucharest, Transilvaniei Street 6, 010798, Bucharest, Romania
[5]Harvard Medical School, Department of Cell Biology, LHRRB 401A, 240 Longwood Avenue, Boston MA, 02115, Boston, USA
alexandra.carlan@s.unibuc.ro

Peptide synthesis is of exceptional importance due to its growing biomedical and bioengineering applications. Different properties can be encoded in the structures, enabling usage in drug development. For example, biomimetic peptides can be used directly as therapeutic agents, such being the case of GLP1 analogues [1], or they can exhibit self-assembling properties useful in drug delivery systems. [2]
The high affinity and specificity of certain biomolecules for peptides can be employed in affinity chromatography. A particular case is the antigen-antibody reaction, in which peptides can be either antigens for the purification of antibodies or tags for a protein of interest. [3]
We report the solid phase synthesis of peptides used for the purification of anti-protein C antibodies.

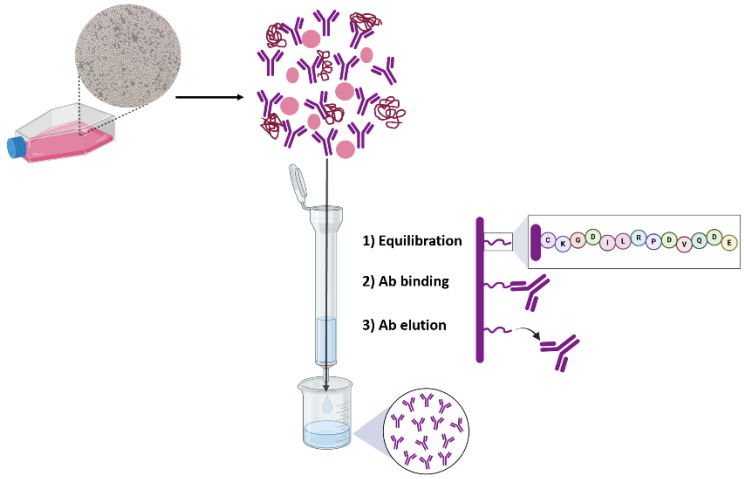


Figure 1. Affinity purification of monoclonal antibodies

Acknowledgements
This work was supported by a grant from the Romanian Ministry of Education and Research, PNRR/2022/C9/MCID/I8, project number CF 760056/ 23.05.2023, as well as ANC-UEFISCDI, PN-IV-P6-6.1-CoEx-2024-0088, TheraFast 9CoEx/2026.

References
1. Wang L., Wang N., et. al., Sig. Transduct. Target. Ther. 2022, 7:48.
2. Yang J., An H-W., Wang H., ACS Appl. Bio Mater. 2021, 4:24.
3. Kilgore R., Chu W., et. al., J. Chromatogr. A. 2023, 1687:463701.

SYNTHESIS AND INVESTIGATION OF NOVEL NICKEL-BASED METAL ORGANIC FRAMEWORKS

Diandra M. GHEORGHE[1], Anca G. MIREA[2], Iuliana M. CHIRICĂ[2], Augustin M. MĂDĂLAN[3], Codruța C. POPESCU[4], Mihaela MATACHE[4], Mihaela FLOREA[2], Dragoș M. CIUPARU[1]

[1]Petroleum-Gas University of Ploiești, 39 Bucharest Boulevard, 100680 Ploiești, Romania
[2]National Institute of Material Physics, 405A Atomiştilor Street, 077125 Măgurele, Romania
[3]University of Bucharest, Faculty of Chemistry, 90 Panduri Street, 050663 Bucharest, Romania
[4]University of Bucharest, Faculty of Chemistry, Research Centre of Applied Organic Chemistry, 90 Panduri Street, Bucharest, Romania
diandra-maria@upg-ploiesti.ro

Metal-organic frameworks (MOFs) represent a class of porous coordination polymers with exceptionally high surface area, thermal and chemical stability and a tailorable pore size that make them ideal for a wide range of applications. [1]

Herein we present synthesis and characterization of novel metal–organic frameworks using a quinoxaline-based multifunctional flexible ligand [2] and nickel ions. The successful formation of the MOFs was validated by single-crystal X-ray diffraction and powder X-ray diffraction (PXRD). FTIR spectroscopy further supported formation of the coordination framework, demonstrating the coordination of the nickel ions to the functional groups of the ligand. Thermogravimetric analysis revealed a multi-stage degradation profile, indicating the thermal robustness of the materials up to moderate temperatures. The porous nature of the synthesized materials was validated by N_2 adsorption–desorption isotherms, while CO_2 adsorption experiments at room temperature demonstrated measurable uptake capacities. [3]

Collectively, these results confirm the successful assembly of a thermally stable, structurally well-defined MOFs, and open the door for further exploration of this frameworks in gas sorption and separation applications.

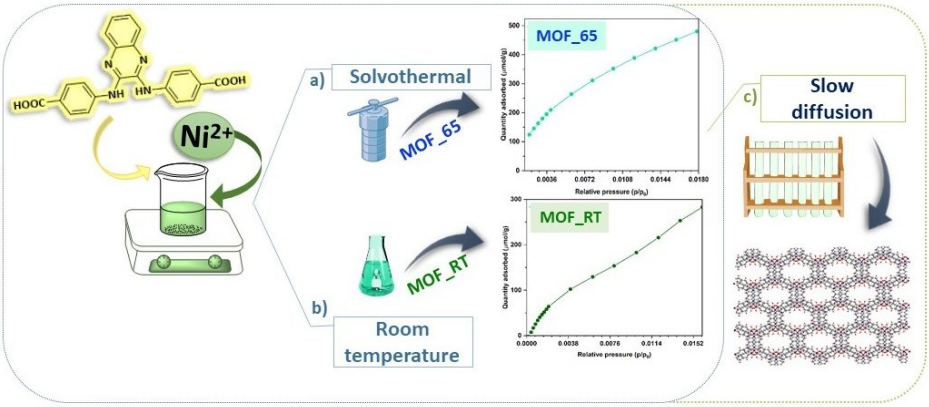


Figure 1. Synthesis of Ni-MOFs and their CO_2 adsorption capacities

Acknowledgements
This work was partially supported by grants of the Romanian Ministry of Research, Innovation and Digitization, PNRR/2022/C9/MCID/I8, project number CF 760056/23.05.2023, code 235/29.11.2022.

References
1. Katoch A., Goyal, N., Gautam S., Vacuum. 2019, 167: 287-300.
2. Zhu Y., Wang Y-M., Inorg. Chem. 2014, 53: 7692-7699.
3. Gheorghe D. M., Mirea A. G., Chirică I. M., Mădălan A. M., Popescu C. C., Matache M., Florea M., Ciuparu D., Synthesis. 2025, 57(24): 3660-3668.

SYNTHESIS AND CHARACTERIZATION OF AN AMPHIPHILIC Zn(II) COMPLEX WITH A NEW PHENANTHROLINE-BASED LIGAND

Raluca DANCIAR, Evelyn POPA, Elisabeta I. SZERB, Adelina-Antonia ANDELESCU*

"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223 Timişoara, Romania
andelescu.ade@gmail.com

Zn(II) is one of the most abundant metals in Earth's crust and in the human body performs several vital functions such as regulation of cellular metabolism and capacity to suppress apoptotic pathways. In this regard, scientists designed coordination complexes based on this metal center and *N*-donor ligands for their biological potential and emissive properties. [1, 2] Phenanthroline-type ligands exhibit numerous properties due to molecular rigidity and high chelating capacity, making them ideal candidates for obtaining new compounds with emissive properties. [3] In this paper, our group reports the synthesis of a phenanthroline-based ligand functionalized with amphiphilic chains and its coordination complex with Zn(II) (Zn_1, Figure 1).

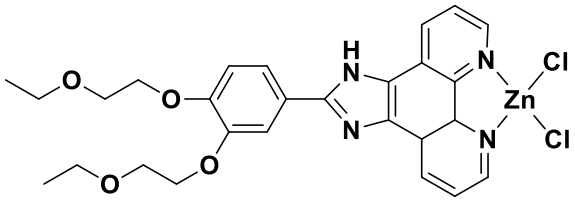


Figure 1. The proposed chemical structure of Zn_1

Zn_1 is highly soluble in organic solvents, such as DCM, EtOH and DMSO, which indicates inherent features for biological studies.
Also, Zn_1 and the ligand were structurally analyzed using FT-IR and NMR spectroscopic methods, and their purity was confirmed by elemental analysis. The photophysical properties of the new Zn(II)-based complex were investigated using freshly prepared dichloromethane solutions. Zn_1 has increased emission intensity and quantum yield compared to its respective ligand.

Acknowledgements
This work received financial support from the Romanian Academy through the research project "*Luminescent biocompatible coordination complexes based on d-block metals and derivatives of natural alkaloids as ligands for biomedical applications*", within the Romanian Academy–Vietnam Academy of Science and Technology Joint Research Project 2026–2027. The authors also acknowledge the support provided through Research Program No. 4 of the "Coriolan Dragulescu" Institute of Chemistry, Timisoara, Romania and the RO-OPENSCREEN research infrastructure of the Institute (MySMIS code 127952, Contract No. 371/20.07.2020).

References
1. Porchia M., Pellei M., Del Bello F., Santini C., Molecules. 2020, 25(24):5814.
2. Jomova K., Makova M., Alomar S.Y., Nepovimova E., Kuca K., Rhodes C.J., Alwasel S.H., Valko M., Chem. Biol. Interact. 2022, 367:110173.
3. Accorsi G., Listorti A., Yoosaf K., Armaroli N., Chem. Soc. Rev. 2009, 38:1690–1700.

SYNTHESIS AND CHARACTERIZATION OF A NI(II) SYSTEM BASED ON 2-CARBOXYETHYL(PHENYL)PHOSPHINIC ACID AND PIPERAZINE

Diana ANGHEL*, Vlad CHIRIAC*, Ghoeorghe ILIA

West University of Timisoara, Faculty of Chemistry, Biology, Geography, Department of Chemistry, 16 Pestalozzi Street, 300115 Timisoara, Romania
diana.anghel@e-uvt.ro and vlad.chiriac@e-uvt.ro

Phosphinic acids represent versatile ligands in coordination chemistry due to the ability of the phosphinate group to interact with metal centers through different coordination modes. [1] The incorporation of additional nitrogen-containing components may further influence the composition, organization, and physicochemical properties of the resulting materials. [2, 3]
This work reveals a new Ni(II)-containing system based on 2-carboxyethyl(phenyl)phosphinic acid (H_2CEPPA) and piperazine was synthesized and characterized.
The material was obtained under hydrothermal conditions using Ni(II), H_2CEPPA, and piperazine in an initial molar ratio of 1:1:0.5. The resulting solid was investigated by Fourier-transform infrared spectroscopy (FT-IR), Powder X-ray diffraction (PXRD), and Eemental Analysis (CHN). FT-IR analysis revealed changes in the characteristic vibrations associated with the phosphinate and carboxyl-containing ligand after reaction with Ni(II), while additional spectral features were consistent with the presence of the nitrogen-containing component in the obtained material. Elemental analysis confirmed the presence of nitrogen, supporting the incorporation of piperazine into the isolated solid. The experimental PXRD pattern showed a well-defined diffraction profile, indicating the formation of a crystalline phase distinct from the starting components.
The combined analytical results support the formation of a Ni(II)–phosphinate material containing piperazine and demonstrate the potential of H_2CEPPA for constructing multicomponent metal–organic systems. These findings provide a basis for further structural investigations and for exploring the influence of nitrogen-containing components on the organization and properties of metal phosphinate materials.

References

1. Bazaga-García M., Vílchez-Cózar Á., Maranescu B. Olivera-Pastor P., Marganovici M., Ilia G., Cabeza Díaz A., Visa A., Dalton Trans. 2021, 50(19):6539–6548.
2. Anghel D., Chiriac V., Vlascici D., Cernusca B.D., Ilia G., J. Chem. Res. 2026, 50.
3. Song X., Zhang Z., Ji Y., Chen D., Yang L., New J. Chem. 2025, 49(15): 6433–6442.

OPTIMIZATION AND MODELING OF TERNARY DYE ADSORPTION USING AN IRON OXIDE/CARBON NANOCOMPOSITE

Maria Andreea NISTOR, Liliana HALIP, Simona Gabriela MUNTEAN

"Coriolan Dragulescu" Institute of Chemistry, Romanian Academy, 24 Mihai Viteazu Blvd., 300223, Timisoara, Romania
nistor_andreea1990@yahoo.com

The presence of dyes in water, even at low concentrations, can adversely affect aquatic ecosystems by reducing light penetration and may pose risks to human health due to their toxic, mutagenic, and carcinogenic properties. [1, 2] Therefore, their efficient removal from wastewater is an important environmental priority. [3] Since real wastewater commonly contains mixtures of dyes rather than individual compounds, studying their simultaneous removal provides a more realistic assessment of treatment efficiency and applicability.

In this study, dye removal from a ternary system was investigated to develop an efficient and sustainable treatment process. Factorial design and Response Surface Methodology (RSM) were used to optimize adsorption conditions and maximize dye removal efficiency. [4]

A magnetic nanocomposite based on activated carbon and iron oxide (magnetite) was synthesized by the combustion method [5], characterized, and applied as adsorbent for the removal of dyes from ternary aqueous systems.

The influence of the main operational parameters, including solution pH and initial dye concentration, on the adsorption process was evaluated by considering four experimental factors (X_1–X_4). A series of factorial design experiments was performed using three representative dyes: Acid Orange 7 (AO7), Methylene Blue (MB), and Chromazurol S (ChS). The factorial design assessed the effects and interactions of the investigated variables, while Response Surface Methodology (RSM) was used to develop predictive models and optimize the adsorption process.

The optimal operating conditions were established based on contour plots and three-dimensional (3D) response surface representations generated for each pair of factors included in the model. High removal efficiencies were achieved for all three dyes, reaching values above 73% for AO7, 79% for MB, and 59% for ChS in the ternary system. Notably, these efficiencies were obtained under relatively mild operating conditions, namely the natural solution pH (6.91) and room temperature (25°C), highlighting the potential of the synthesized magnetic nanocomposite for practical wastewater treatment applications.

Furthermore, the regeneration and reusability of the magnetic nanocomposite were evaluated through six consecutive adsorption–desorption cycles, providing additional information regarding its stability and potential for repeated use.

Acknowledgments
This work was supported by Research Program No. 2 of the "Coriolan Dragulescu" Institute of Chemistry, Timisoara, Romania.

References
1. Khumalo S.P.G., Lokhat D., Chetty K., Chetty, L. (). Scientific Reports, 2022, 12:20009.
2. Athari M., Fattahi M., Khosravi-Nikou M., Hajhariri A., Scientific Reports, 2022, 12:20415.
3. Adane T., Adugna A.T., Alemayehu E., J. Chem. 2021, 1-14.
4. Nistor M.A., Halip L., Muntean S.G., Kurunczi L., Costișor O., Sustain. Chem. Pharm. 2022, 29:1-20.
5. Ianoș R., Păcurariu C., Mihoc G., Ceram. Int. 2014, 40:13649.

ADVANCED SPECTROSCOPIC STUDY OF PROTEIN BEHAVIOR AND PROTEIN-COMPOUND INTERACTIONS: A CASE STUDY ON SERUM ALBUMIN

Nicoleta ANDRIAN[1*], Radu SILAGHI-DUMITRESCU[1], Róbert TOTOS[1], Melinda KOVACS[2], Monica FOCȘAN[3]

[1]Department of Chemistry, Faculty of Chemistry and Chemical Engineering, Babeş-Bolyai University, 11 Arany Janos str., RO-400028 Cluj-Napoca, Romania
[2]INCDO-INOE 2000, Research Institute for Analytical Instrumentation, 67 Donath Street, RO-400293 Cluj-Napoca, Romania
[3]Nanobiophotonics and Laser Microspectroscopy Center, Institute for Interdisciplinary Research in Bio-Nano-Sciences, Babeş-Bolyai University, 42 Treboniu Laurian str., RO-400271 Cluj-Napoca, Romania
*nicoleta.andrian@ubbcluj.ro

This study investigates the effects of UV radiation on serum albumins (BSA, HSA, RSA) and highlights the formation of a unique chromophore.

UV radiation (254 nm) generates a well-defined chromophore at 310–320 nm in albumins [1], dependent on pH [2] and independent of salt concentration or buffer type. The chromophore persists after filtration and proteolytic digestion, indicating it is part of the polypeptide. Its formation involves local covalent modifications of aromatic and sulfur-containing residues, likely including tyrosine and cysteine, without detectable free radical generation.

Circular dichroism spectra reveal a progressive decrease in α-helical content upon irradiation, indicating that chromophore formation is accompanied by partial conformational rearrangement of the protein. MALDI-TOF-MS analyses indicate minor mass changes after irradiation, compatible with disulfide rearrangements and local chemical modifications, without major protein degradation. Quantification of free thiols with Ellman's reagent (DTNB) reveals an increase in accessible cysteine content upon irradiation, consistent with light-induced disulfide reduction, further confirmed by the formation of cobalamin–thiolate complexes upon UV irradiation in the presence of aquacobalamin.

These findings reveal a specific, light-induced modification mechanism in albumins, with implications for photobiology, biophotocatalysis, and protein chromophore design. The results highlight the need to reassess experimental conditions in protein studies and open new avenues for investigating the molecular mechanisms of photoinduced modifications. Furthermore, this work provides insight into protein stability, with potential applications in developing novel methods for biomolecule protection and stabilization.

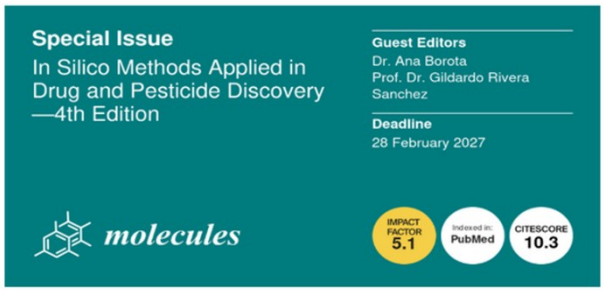
Acknowledgements
This study was supported by the Romanian Ministry of Education and Research through grant PN-IV-PCB-RO-MD-2024-0515 and by the World Federation of Scientists (WFS) through a National Scholarship.

1. Sozarukova M.M., Skachko N.A., Chilikina P.A., Novikov D.O., Proskurnina E.V., Molecules. 2023, 28:4646.
2. Zuorro A., Lavecchia R., Am. J. Biochem. Biotechnol. 2018, 14(4):247-254.

SPECIAL ISSUES & PUBLICATION OPPORTUNITIES

Special Issue · IJMS
Nature-Inspired and Synthetic Compounds: New Frontiers in Bioactivity and Drug Discovery

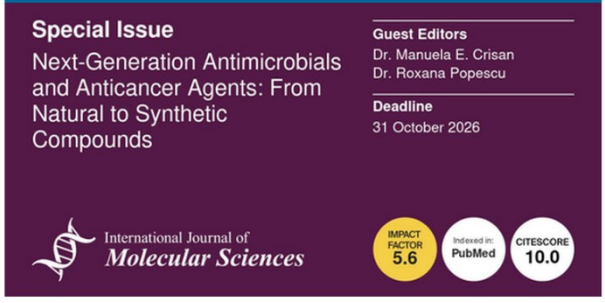
Special Issue · IJMS
In Silico Drug Design and Virtual Screening: The Latest Advances



Special Issue · Molecules
In Silico Methods Applied in Drug and Pesticide Discovery — 4th Edition

Special Issue · Molecules
Porous Materials for Environmental Pollutant Adsorption and Degradation

Special Issue · Sustainability
The Sustainable Development of New Materials and Products from Biobased and Biodegradable Polymers



Special Issue · IJMS
Next-Generation Antimicrobials and Anticancer Agents: From Natural to Synthetic Compounds

ROMANIAN ACADEMY
„CORIOLAN DRĂGULESCU" INSTITUTE OF CHEMISTRY
24 Mihai Viteazu Av., RO-300223,
Timişoara, Romania, phone: 0256-491818

ISSN: 2065-0760

Edited by
Alina BORA, Ildiko BUTĂ, Carmen CRETU, Andreea NISTOR