LAQV requimte

LABORATÓRIO ASSOCIADO
PARA A **QUÍMICA VERDE**

2020/2025 ACTIVITY REPORT & HIGHLIGHTS

CHEMISTRY – **A Key Player in Engineering a Sustainable World**

LAQV
2020-2025 ACTIVITY REPORT & HIGHLIGHTS

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DE ÉVORA

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01

About LAQV

VISION & MISSION

The **Laboratório Associado para a Química Verde | Associated Laboratory for Green Chemistry** is the Portuguese Research Centre for Sustainable Chemistry, hosted by the Network of Chemistry and Technology (REQUIMTE).

The **vision of LAQV is for a world in which Sustainable Chemistry is used as a powerful and dynamic tool** to tackle the societal, economic, and environmental challenges of modern life. Accordingly, **our mission is to initiate, advance, and promote the principles of Sustainable Chemistry** through a multiplicity of research, networking, training, and outreach activities.

LAQV aims at keeping a pivotal role in the Portuguese scientific system and at continuing to be an internationally recognized partner in all areas related to Sustainable Chemistry, a key component of an imperative World Sustainable Development.

Modern society relies on chemicals and chemical processes for its way of living. Concomitantly, it is well recognized by governments, industry, and the general public that a Sustainable Development is crucial to tackle the challenges of society. Therefore, a new way of thinking Chemistry has emerged, aiming the implementation of clean chemical reactions and processes that reduce the amount of materials, energy, costs, and risks.

Based on these principles, LAQV focuses its activity in six Thematic Lines aligned with the Research Agenda of the European Technology Platform for Sustainable Chemistry (SUSCHEM), the United Nations (UN) Sustainable Development Agenda, and the priorities of Horizon 2020 and Horizon Europe. The complementary proficiencies to stimulate innovation across these Thematic Lines are provided by eleven Research Groups that aggregate scientists who share similar backgrounds.

OBJECTIVES

Through 2025-2029, LAQV will pursue to:

- increase the research international impact in the Sustainable Chemistry field;
- make sure that more research outputs lead to economic and social outcomes, through co-operation with industrial partners and the creation of spin-offs;
- attract the best young researchers to be trained in the multiple topics supporting Sustainable Chemistry;
- seek industrial partners focused on implementing clean technologies and processes;
- share the principles of Sustainable Chemistry and research outputs with the general public, government, and industry, thereby increasing its presence in the community;
- assist stakeholders in making decisions on health and safety issues related to (bio)chemical products or processes, through increased participation in regulatory bodies.

LAQV is a research-based organization fully integrated in the international environment. Therefore, LAQV works to contribute for the advancement of Science and to increase their, especially onto the international Green Chemistry community. As a University-based research centre, improving training at PhD level is a second key goal, and intimately linked to the previous one. Fulfilling these two core objectives will also enable LAQV to pursue: a) collaboration with industry/ technology transfer; b) start-up launching, and c) participation in public awareness activities.

HISTORY

The Associated Laboratory for Green Chemistry is part of the Network of Chemistry and Technology (REQUIMTE), created in 1996 by researchers from the Universities of Porto and NOVA of Lisbon. In the present configuration, LAQV spreads out from the two initial universities to include the University of Aveiro, Coimbra, Évora, Trás-os-Montes e Alto Douro, the Polytechnic Institute of Porto, and small sites all over the country. The distribution over the Portuguese territory empowers an improved scientific and technologic capacity and an internal synergy of resources and interactions with stakeholders.

1996

REQUIMTE, the Network of Chemistry and Technology, was created as a partnership of the University of Porto and NOVA University of Lisbon.

2001

REQUIMTE was officially recognised by the Portuguese Minister of Science and Higher Education as host to the **Associated Laboratory for Green Chemistry - LAQV.**

2003

REQUIMTE was formally chartered as a non-profit scientific organization.

2015

REQUIMTE reached the dimension of around 200 researchers and took the strategic decision to split-up. Chemistry-oriented researchers remained at LAQV and those with a strong Biology focus formed a new centre (UCIBIO).

2018

LAQV@ REQUIMTE classified as **excellent** by the Portuguese Foundation of Science and Technology (FCT).

2020

LAQV@ REQUIMTE partnered with VICARTE and got renewa of the Associated Laboratory status.

2024

LAQV@ REQUIMTE classified as **excellent** by the Portuguese Foundation of Science and Technology (FCT).

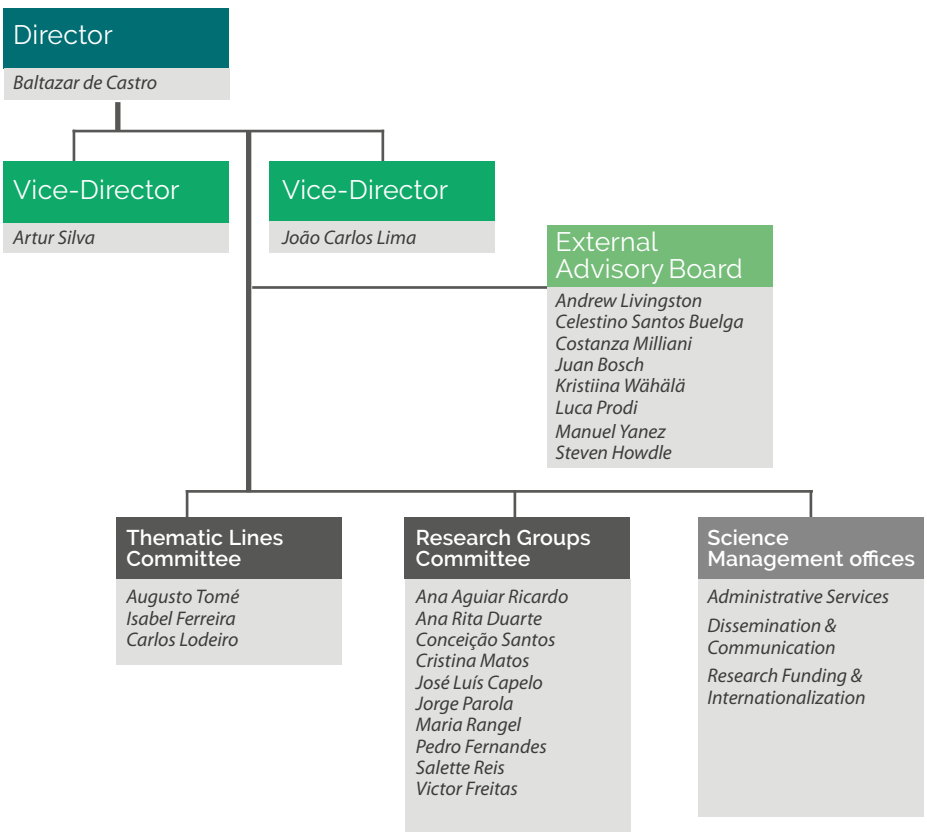
GOVERNANCE

LAQV is managed through a simple and efficient governance structure, with well-defined responsibilities and clearly allocated tasks, which has ensured the smooth implementation and successful execution of its activities since 2001.

The model includes a Board of Directors, composed of a director (University of Porto) and two vice-directors (Universities of Aveiro and NOVA University of Lisbon). The inclusion of representatives from the different poles of the research unit ensures the overall executive management of LAQV. The Board of Directors is elected by the Scientific Council, which comprises all integrated PhD holders of LAQV, that also elect the coordinating committee of this council.

The Board of Directors nominates two Research Committees to support the management of LAQV at a scientific level: the Multidisciplinary Lines Committee and the Research Groups Committee, composed of the coordinators of each Multidisciplinary Line and Research Group, respectively.
The Board of Directors are also supported by the External Advisory Board, constituted of 6 renowned specialists in Sustainable Chemistry.

The governance of LAQV is also supported by administrative services, which manage both human resources and financial aspects of the R&I&D projects, and a Science Management & Communication Office, whose many activities rely on science dissemination, communication, and outreach activities; support on grants and awards applications; and IT support.



SCIENTIFIC ORGANIZATION

The research activity of LAQV is organized in three Thematic Lines, aligned with national and international public policies, the SUSCHEM Research Agenda, EU Horizon 2020 and Horizon Europe, and UN Sustainable Development Agenda. The lines work as driven vectors in which Chemistry and Chemical Engineering play a crucial role, and include:

A. Sustainable Chemistry and Technology
B. Food Chemistry and Technology
C. Chemistry for Health and Wellbeing

The complementary proficiencies to stimulate innovation across the Thematic Lines are provided by ten Research Groups which aggregate scientists from various research labs who share similar backgrounds:

1. Molecular synthesis
2. Chemistry and Bioactivity
3. Omics and Analytical Development
4. Environmental chemistry
5. (Bio)Chemical process engineering
6. Cultural heritage and responsive materials
7. Materials for sustainability and wellness
8. Nanoplatforms for Life
9. Food Quality and Technology
10. High Performance Computing in Molecular Modelling

FACTS & FIGURES

→ Our active community in December 2025

356
Senior Researchers

129
Other doctorate Researchers

29
Post-doctoral fellows

329
PhD students

89
Other researchers (research grantees, technicians, MSc Students)

932 members... From 29 different countries.

→ Our numbers in 2020-2025

6827
Indexed publications

170051
Citations*

462
Research Projects in execution

95 M€
Funding

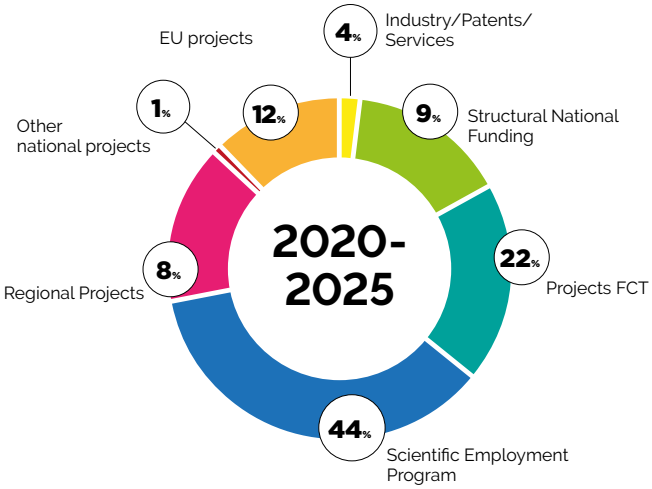
46
Patents

46%
International Coauthoring

333
PhD dissertations

1064
MSc dissertations

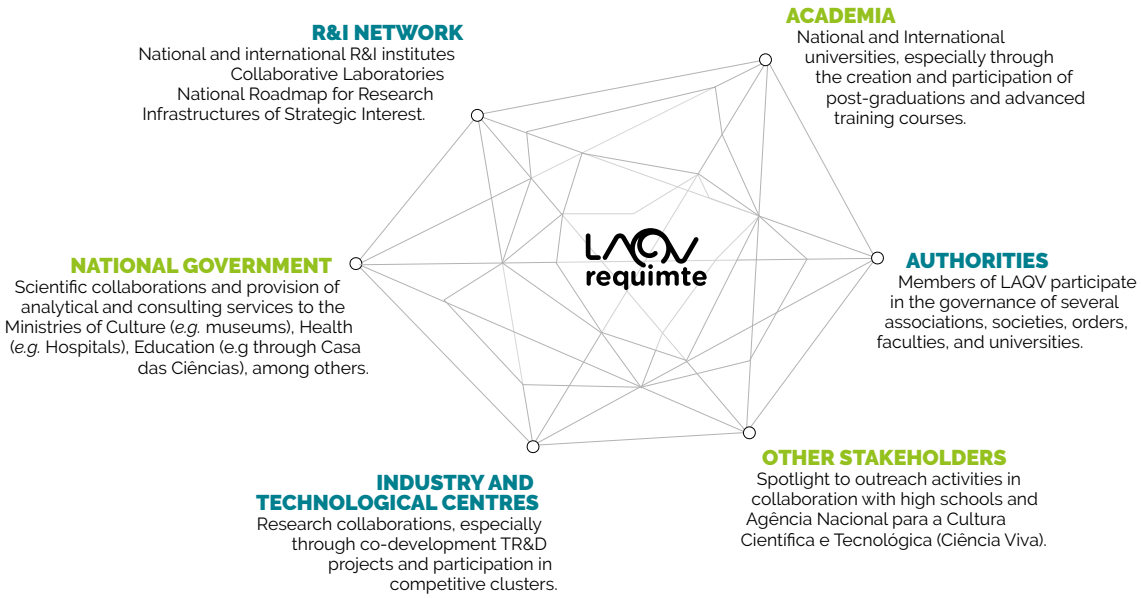
* total number of citations in 2020-2025 for all the publications published since the beginning of LAQV



TOTAL

95M€

→ LAQV is integrated in a scientific, intersectoral, and technology hub



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02

Thematic Lines

LAQV - ORGANIZATION 2025-2029

LAQV has, as Main Management Institution, REQUIMTE, an organization of the Universities of Aveiro, Nova Lisbon, and Porto, which has the legal status of a non-profit private Association. The General Assembly of REQUIMTE brings together the Rectors of the three Universities, guaranteeing that the operations of REQUIMTE research sites are aligned with the research plans of the Universities.
LAQV@REQUIMTE past achievements have been based on its vision of enhancing scientific relevance by fostering interdisciplinarity, diversity and integration of contributions from different institutions and locations. The vast experience of LAQV in managing inter-university scientific endeavors over the past two decades will be instrumental to smoothly integrate the contributions of new research sites into the mainstream of LAQV activities. This management approach is founded on large Research Groups of about 30 senior researchers with similar backgrounds. These groups are effectively a federation multiple collaborating research laboratories, and represent the first front of research coordination.

LAQV researchers are organized in ten Research Groups:

1. Molecular Synthesis
2. Chemistry and Bioactivity
3. Environmental Chemistry
4. Omics and Analytical Development
5. Cultural Heritage and Responsive Materials
6. (Bio)Chemical Process Engineering
7. Materials for Sustainability and Wellbeing
8. Nanoplatforms
9. Food Quality and Technology
10. High-Performance Computing in Molecular Modelling

The coordinator of each group is expected, through intensive networking, to define a research strategy aligned with the key vectors and the vision of LAQV, which will focus on (a) procurement of funding from competitive sources; (b) participation in doctoral programs; (c) establishment of collaborative programs with industry and (d) promotion of science dissemination programs. Identification of key areas for hiring new researchers and of promotions of key researchers starts at this level. The activities are carried out at the research labs, which reflect diversity in location and/or specific interests.
The strategic scientific plan now comprises three thematic lines, taken as interdisciplinary research areas that will promote collaboration of research labs and research groups.

The primary responsibility of the management team (see below) will be to steer research activity of the ten Research Groups towards integrated goals along the following Thematic Lines:

A. Sustainable Chemistry and Engineering;
B. Food Chemistry and Technology;
C. Chemistry for Health and Well-being

The choice of these research vectors has clearly been inspired by internationally defined agendas for sustainable development, such as the UN Sustainable Development Agenda or the research agenda of SUSCHEM, the European Chemical Industry platform. This definition of thematic lines is primarily used as an internal management tool. It will be utilized to drive research activities towards achieving the defined objectives, encouraging LAQV researchers to align their efforts in order to enhance their international impact. The main task of management will be to design a system of incentives, through resource allocation, to encourage research labs to cluster around specific areas of the thematic lines, hence creating critical mass to enhance the chances of obtaining new funding.
LAQV is governed by an Executive Board featuring a Director, two Vice-Directors, and three Deputy Directors representing the Universities of Aveiro, Porto, and NOVA Lisbon. This leadership team is elected by a Scientific Council comprising all doctorate members of the laboratory.

The Scientific Council, due to the number of researchers, functions through three smaller Committees: the elected Coordinating Committee of the Scientific Council, and the Thematic Lines Committee and the Research Groups Committee, which consists of their respective coordinators.

The Executive Board designates the coordinators for each Thematic Line and Research Group, and depends on the guidance of the Coordinating Committee of the Scientific Council and Thematic Lines Committee to establish and execute the strategic vision of LAQV, including budget, personnel, research incentives, and new contracts.
The Research Groups Committee provides guidance to the Executive Board on overseeing research activities, developing training programs, establishing collaborative projects with other organizations, namely industries and research and health institutions, and also on ways to promote societal awareness of Chemistry as a fundamental player in the contemporary world.
LAQV integrates researchers from six Management Institutions and several Participating Institutions. Out of the total of more than 350 integrated researchers of LAQV, around 50% have contracts as professors with the Universities of Aveiro, NOVA Lisbon, and Porto, the sole associates of REQUIMTE, and with the Universities of Coimbra and Évora and from the Polytechnic University of Porto, whose participation is governed by collaboration agreements with REQUIMTE.

SUSTAINABLE CHEMISTRY AND TECHNOLOGY

Thematic Line Coordinator:
Augusto Tomé

Research Groups that contribute to the Thematic Line:

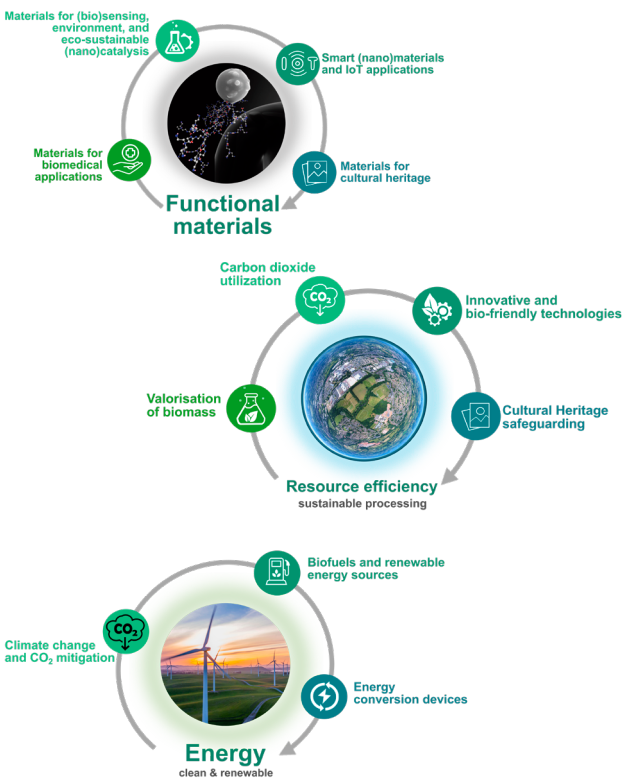
- Molecular Synthesis
- Materials for Sustainability and Wellness
- Bio(chemical) Process Engineering
- Environmental Chemistry
- Chemistry and Bioactivity
- Cultural Heritage and Responsive Materials

The research line Sustainable Chemistry and Technology aims at addressing some of the most pressing global challenges we face today, ranging from environmental degradation to resource depletion and public health concerns prioritizing environmental and societal well-being throughout chemical processes by minimizing the environmental impact of chemical production and product lifecycles.

New approaches are required to meet the needs of the present without compromising the ability of future generations to reach their own needs. Key principles include the reduction of production and emission of pollutants by using renewable and non-toxic materials, development of cleaner production methods, renewable energy integration and carbon capture technologies, thereby minimizing exposure risks for workers, consumers, and communities. Attaining this general goal requires solid interdisciplinary research, only possible by conjugating knowledge across disciplines from Chemistry, Biochemistry, Materials Science & Engineering and Environmental and Biomedical Sciences. Interdisciplinary research helps to identify opportunities for improvement and optimization of processes in a lifecycle perspective, i.e., from raw materials extraction to end-of-life disposal.

This research line integrates various research groups of LAQV-REQUIMTE that are committed to develop collaborative work aiming to offer to the community innovative molecules, materials and processes attained via sustainable approaches that fall within the principles of Green Chemistry. The research line Sustainable Chemistry and Technology deals with a diversity of key topics centered in the development of new synthetic methods (including catalytic transformations and alternative solvents) and exploitation of natural resources for innovative and novel molecules, using biomass in a biorefinery perspective for the design of advanced functional, smart and responsive (nano) systems, as well as molecular imprinted systems with supercritical fluids and for conservation and restoration of cultural heritage; to environmental protection (including air, soil, water quality and pollution control, water and soil remediation, waste valorization); exploring alternative energy sources reducing reliance on fossil fuels and lowering greenhouse gas emissions; coupled with modelling and optimization of separation processes, and computational systems and artificial intelligence for chemical and biological technology.

Within the Sustainable Chemistry and Technology research line we are committed to addressing environmental challenges and advancing to a more sustainable future. By integrating principles of green chemistry, catalysis, materials science, energy efficiency, and life cycle assessment, this field is driving innovation toward cleaner, safer, and more environmentally friendly chemical processes and products.



FOOD CHEMISTRY AND TECHNOLOGY

Thematic Line Coordinator:
Isabel Ferreira

Research Groups that contribute to the Thematic Line:

- Food Quality and Technology
- Bio(chemical) Process Engineering
- Chemistry and Bioactivity
- Environmental Chemistry
- Omics and Analytical Development

Food Chemistry and Technology thematic area is committed to contribute to a food environment that facilitates healthy and sustainable choices, promoting sustainable diets that mitigate life-threatening diseases. At the same time, it is aimed to stepping up the fight against food waste throughout the whole food chain, particularly at retail and consumer levels. Achieving these goals involves enhancing food quality, ensuring authenticity, and effectively controlling allergens, additives, natural toxins, and chemical contaminants. It will also involve the optimization of advanced food processing methods and the development of novel processed products to enhance both nutritional and sensory characteristics of food, while maintaining high levels of safety and traceability. Additionally, research activities are directed towards the conservation of natural resources, promoting sustainable procedures and technologies to minimize food losses and waste, and implementing circular economy principles across the entire food system to reduce its environmental impact. Understanding the mechanisms underlying the protective effects of nutrients and bioactive compounds and reducing the incidence of non-communicable diet-related diseases are also crucial areas of investigation of this thematic area.

These research objectives are aligned with the overarching strategy of establishing connections between fundamental and applied food science to protect and enhance food quality and safety, which is in line essentially with cluster 6 of Pillar II from the Horizon EU program structure. To achieve this, the thematic line encompasses three primary research fields: 1) Food Composition, Properties & Processes; 2) Healthier & Safe Foods; and 3) Food Sustainability. Research vectors span various domains such as Food (Bio)Chemistry and Quality Control, Mechanisms of Food Perception, Technological Properties of Foods, Advanced Traceability Technologies to Combat Food Fraud, Dietary Shift toward Healthier Food Choices, Bioaccessibility, Absorption and Bioactivity, Functional Ingredients for Microbiota, Emergent Dietary Allergens, Food Chain Contaminants, Valorization of Novel Food Sources and By-Products, Green and Sustainable Methods for Food Ingredients Extraction and Preservation, Innovative Protein & Fat Sources, and Animal Feed and Precision Nutrition.

These research domains are in line with the Food 2030 EU's research and innovation policy framework, supporting the transition towards sustainable, healthy, and inclusive food systems, essential for achieving the United Nations' Sustainable Development Goals, the policy objectives of the Farm-to-Fork Strategy ("Our food, our health, our planet, our future"), and the EU Green Deal.

CHEMISTRY FOR HEALTH AND WELLBEING

Thematic Line Coordinator:
Carlos Lodeiro

Research Groups that contribute to the Thematic Line:

- Molecular Synthesis
- Materials for Sustainability and Wellness
- Food Quality and Technology
- High-Performance Computing in Molecular Modelling
- Chemistry and Bioactivity
- Omics and Analytical Development
- Nanoplatforms for Life

This thematic line focus lays the foundation for addressing major global dilemmas of the 21st century, offering constructive guidance to individuals, societies and countries by translating conceptual models and research into practical devices and practices. By integrating clinical, communal, and societal perspectives, this multidisciplinary approach contributes to enhancing economic, social, and environmental dimensions, essential for sustainable development.

To fully realize these concepts, our line employs effective integrated approaches and interventions, tackling significant health challenges through interdisciplinary and multidisciplinary research.

With backgrounds spanning Chemistry, Biochemistry, Materials Science & Engineering, Biomedical Sciences, Clinical Sciences, and Entrepreneurship Development, we collaborate across distinct research groups within LAQV-REQUIMTE to establish strategic frameworks. These frameworks, embracing Sustainable & Green Chemistry principles, collectively foster supportive environments for health, paving the way for a sustainable and adaptable journey.

Health & Wellbeing aligns closely with our vision for better life. With scientific knowledge transfer and technological valorization as our ultimate objectives, our multidisciplinary approach focuses on four key areas: Diagnosis and Prognosis, New Treatments, Environmental Control-Toxicology and Healthier Food.

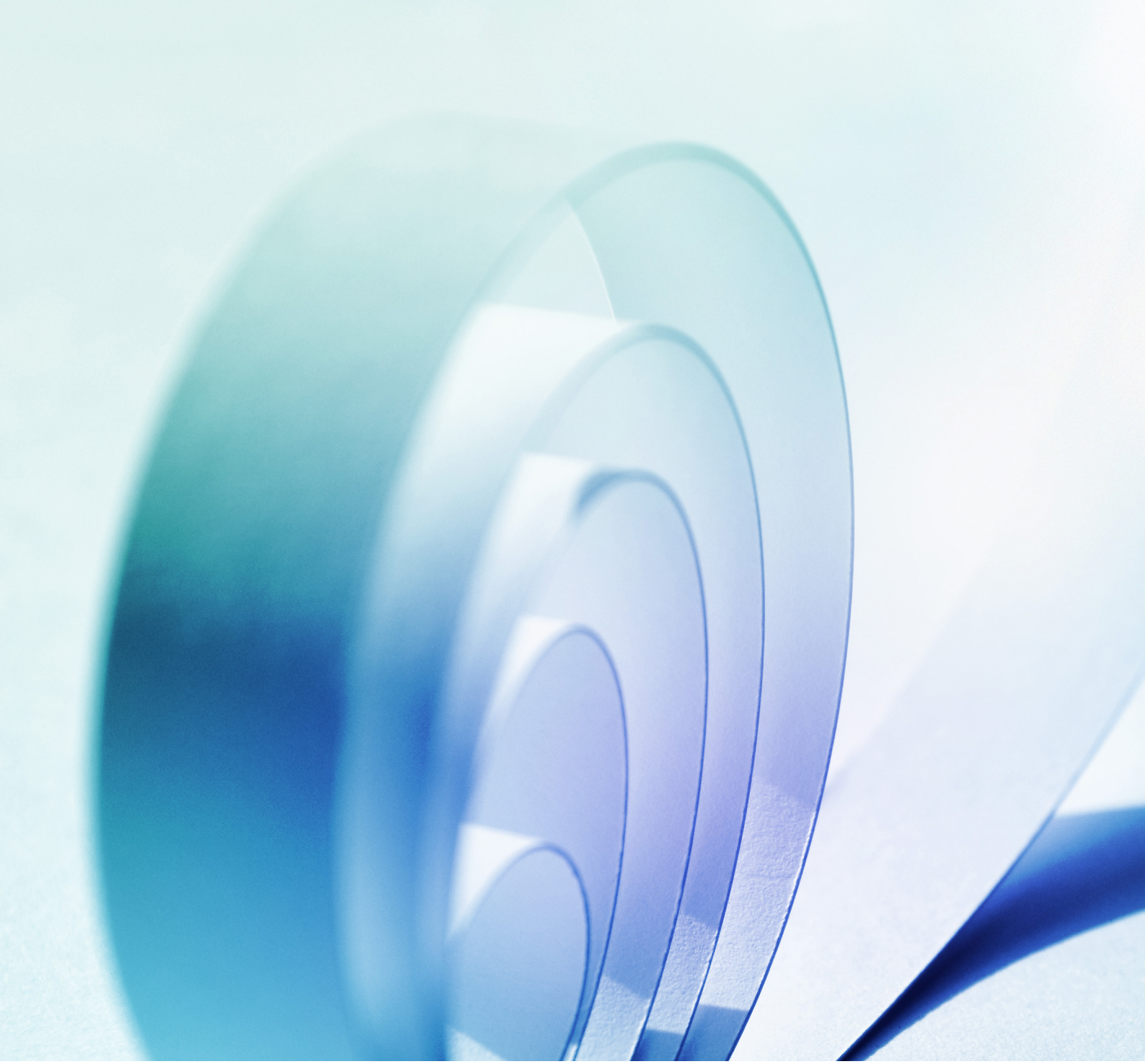
By leveraging cutting-edge technologies including Mass Spectrometry and Nanotech we aim to provide accurate and timely diagnoses, enabling early intervention and personalized treatment strategies to reduce treatment cost and pain.

In addition to diagnostics, we are committed to exploring Novel Compounds and Nano(Materials) for the treatment of various illnesses. We seek to identify and develop therapeutics that are effective, safe, and targeted to specific disease mechanisms. Our goal is to improve patient outcomes and quality of life through the development of innovative treatment modalities.

Our research extends to Designing Methodologies and Advanced Treatments for analyzing hazardous chemicals in the environment. By developing sensitive and selective Analytical Techniques, we aim to identify and quantify environmental contaminants, assess their impact on human health, and develop strategies for mitigating exposure.

Lastly, we are dedicated to Analyzing Health Impact of Food Additives and Food Sources to promote a better quality of life. Through comprehensive analyses, we aim to ensure the safety and nutritional quality of food products, identify potential health risks associated with food additives, and promote sustainable and healthy food choices.

Overall, this research line is committed to advancing health and well-being through the development of novel analytical solutions, therapeutics, and methodologies, addressing key challenges in disease diagnosis, treatment, environmental health, and food safety.



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03

Research Groups

MolSyn
MOLECULAR SYNTHESIS

CHEMBIO
NATURAL PRODUCTS CHEMISTRY AND BIOACTIVITY

OAD
OMICS & ANALYTICAL DEVELOPMENT

EnvChem
ENVIRONMENTAL CHEMISTRY

BCPE
(BIO)CHEMICAL PROCESS ENGINEERING

Charm
CULTURAL HERITAGE AND RESPONSIVE MATERIALS

MatSusWell
MATERIALS FOR SUSTAINABILITY AND WELLNESS

NanoPlat
NANOPLATFORMS

4FOOD
FOOD QUALITY AND TECHNOLOGY

Computing
HIGH PERFORMANCE COMPUTING IN MOLECULAR MODELLING

MolSyn

MOLECULAR SYNTHESIS

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

Group Coordinators:

Artur Silva
Maria Rangel

The Molecular Synthesis group integrates organic, inorganic, physical, and biological chemists whose common interest is to create molecules. Molecules are synthesized because they are needed. Either as simple molecules, as units to produce complex structures, or even to prove a scientific hypothesis – molecules are key players in everyday life. Research is focused on the design of Molecules and Materials for biomedical, agricultural, environmental, energy and food applications, and improvement of Synthetic Methods granting the sustainable chemistry concept.

Several classes of molecular frameworks such as hydroxypyridinones, porphyrins, carbohydrates, terpenoids, amino acids, alkylaminophenols, cyclitols, benzimidazoles, calcitriol derivatives, coelenterazine derivatives, and peptides are functionalized with several chemical groups to produce molecules whose physicochemical properties are finetuned according to the application in view. Examples are fluorescent chelators to monitor and sensing metal ions in body fluids and natural waters, anticancer, antimalarial, antimicrobial, antiparasitic, and novel anti-inflammatory drug candidates.

Peptides, carbohydrates, porphyrin, and conjugated based dyes assembled on coumarin, acenaphthylene, diketopyrrolopyrrole and xanthene scaffolds are preferential frameworks to produce innovative [Bio]materials with potential applications in Biomedical Engineering, [Bio] sensing, Catalysis, Separation, and Cleaner Energies.

RESEARCH OBJECTIVES [2025-2029]

The Molecular Synthesis group will pursue work focused on the design and synthesis of new Molecules and Materials. We intend to strengthen the design of new molecules with application in the fields of sustainable agriculture and forestry, marine and inland water research, and clean and efficient energy production.

The development of innovative methods for chemical synthesis or computational design and study of relevant target molecules will continue. Additionally, we intend to reinforce the development of new synthetic routes using green chemistry procedures for the most common types of chemical reactions performed within the group.

Cellulose, peptides, carbohydrates, porphyrin, and conjugated based dyes assembled on coumarin, acenaphthylene, diketopyrrolopyrrole and xanthene scaffolds are preferred frameworks to produce innovative [Bio]materials with potential applications in Biomedical Engineering, [Bio]sensing, Catalysis, Separation, and Cleaner Energies.

The group benefits from the synergy between organic chemistry teams across LAQV poles, enhancing expertise in organic synthesis, both in developing new classes of molecules and materials and new synthetic methodologies, including asymmetric synthesis. Focus will be given to molecules for chemo- and bio-sensing, photodynamic tumors therapy, or the photodynamic inactivation of protozoa, bacteria, viruses, and fungi. Green processing approaches will also be expanded, including Ohmic Heating (ΩH), an advanced thermal method that improves yields, selectivity, and reaction times in synthetic routes.

RESEARCH TEAM

SENIOR RESEARCHERS

Ana Margarida Silva

Ana S. M. Gomes

António Santos

António Teixeira

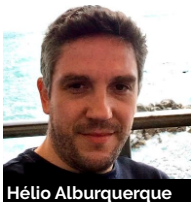
Artur Silva

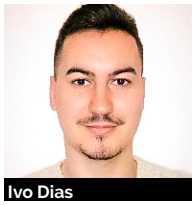
Augusto Tomé

Baltazar de Castro

Catarina Ramos

Clara Gomes


Hélio Alburquerque

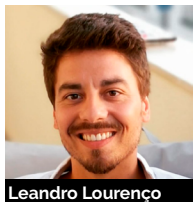

Ivo Dias

Joana Sousa

José Cavaleiro

José Enrique Borges

Krasimira Petrova


Leandro Lourenço

Luísa Amaral

Luisa Ferreira

Maria Rangel

M. Graça Neves

M. João Araújo

M. Luisa do Vale

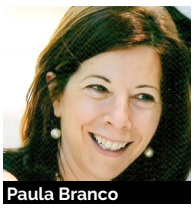
M. Manuel Marques

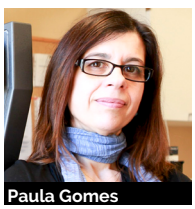
M. Manuela Pereira

Mário Simões

Nuno Candeias

Nuno Moura


Paula Branco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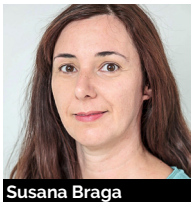
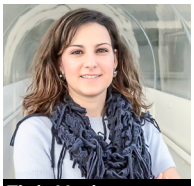
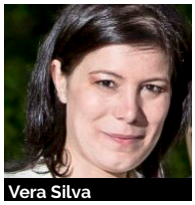

Susana Braga


Tânia Moniz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RESEARCH THEMES/ MOLECULES

Chemical synthesis of a wide diversity of molecules for:

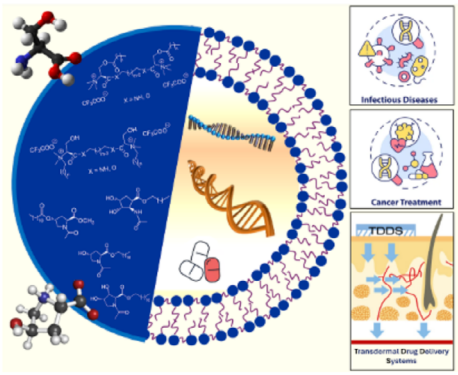
BIOMEDICAL APPLICATIONS

A broad portfolio of molecules has been chemically synthesized for advanced biomedical applications. The work integrates organic synthesis, coordination chemistry and photochemistry to produce functionally diverse compounds with targeted biological activities.

1. Molecular Probes and Imaging Agents
Design of chromophoric and fluorescent probes to support imaging of protein aggregates, lipid accumulation, and fungal cells, enabling early detection and visualization of disease-related processes.

2. Antioxidant, Anticancer, and Anti-inflammatory Agents
Oxygen- and nitrogen-based heterocyclic molecules showing antioxidant, anticancer, and antidiabetic potential.
Amphiphilic antioxidants derived from betulinic acid and phenolic derivatives displaying dual antioxidant and cytotoxic activity, particularly against brain and prostate cancers.
Steroid hybrids of quinoline and chromenol[xanthone] that inhibit protein aggregation and Alzheimer's-related targets such as A peptides and AChE.

3. Photodynamic Therapy (PDT) and Photoinactivation (PDI)
The classes of porphyrins, chlorins, corroles, and phthalocyanines have been used to: Synthesize cationic porphyrins and phthalocyanines that act as efficient photosensitizers against resistant bacteria (e.g., MRSA, E. coli, C. albicans), viruses, and cancer cells. Study structure–activity relationships to enlighten relevant substituent effects (-functionalization, axial units, cationic charge). Apply advanced strategies that include graphene oxide hybrids, fluorinated derivatives in polymer matrices, and metallated Ru/Ir complexes to optimize light-induced cytotoxicity.



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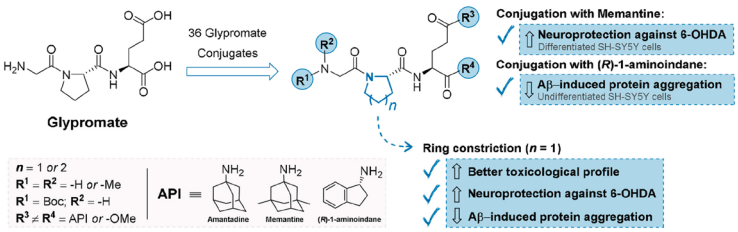
RESEARCH THEMES/ MOLECULES

Chemical synthesis of a wide diversity of molecules for:

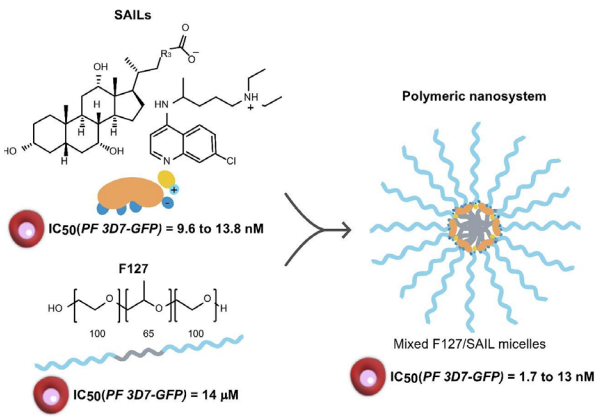
■ BIOMEDICAL APPLICATIONS (CONT.)

4. DNA Interaction and G-Quadruplex Targeting
Cationic and multicharged porphyrinic or phthalocyanine ligands which selectively stabilize G-quadruplex DNA structures, relevant for anticancer mechanisms and biosensing. Novel derivatives such as Ag(II)-TMPyP and diketopyrrolopyrrole compounds that show promising selectivity.

5. Antimicrobial and Antiviral Compounds
Several compounds to target bacteria, fungi, and viruses using photosensitization, phenolic scaffolds, antimicrobial peptides, and sugar/peptide hybrids have been prepared. Notably, glycosyl flavonoids exhibit anti-coronaviral activity, and cationic corroles demonstrate potent antibacterial action.



6. Peptides, Ionic Liquids, and Neuroactive Compounds
Bioactive and wound-healing peptides, including ionic liquid conjugates, showing high potential for topical treatment of skin infections and diabetic ulcers.
Neuroprotective peptides and spiropyrazolone heterocycles aimed at treating neurodegenerative disorders such as Parkinson's disease.
Positive allosteric modulators of dopamine D2 receptors and dopaminergic neuroprotectants that further expand neurological applications.



7. Metal Complexes and Chelators
Ru, Ir, and Zn porphyrinic complexes, alongside iron chelators, are designed to tackle melanoma, iron-related diseases, and metabolic disorders like diabetes.

8. Nature-Inspired and Hybrid Molecules
Marine, plant, and bacterial-derived compounds inspired the synthesis of bioactive analogues with cytotoxic, antimicrobial, and antioxidant effects, bridging natural product chemistry and synthetic optimization.

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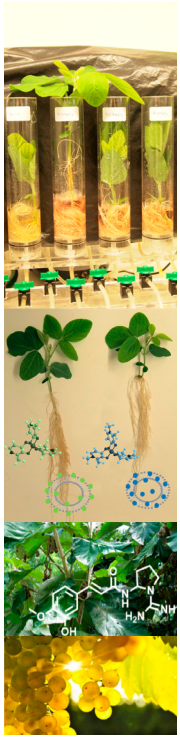
RESEARCH THEMES/ MOLECULES

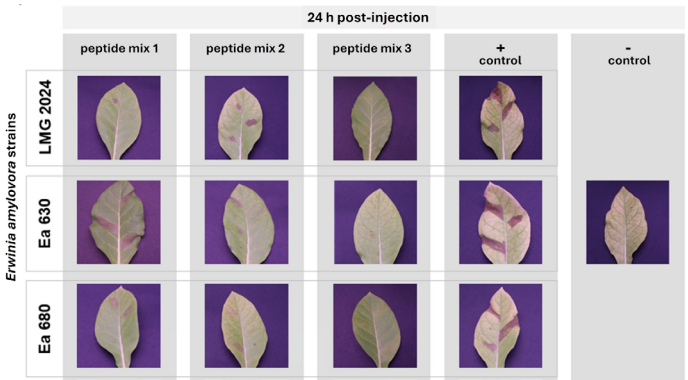
Chemical synthesis of a wide diversity of molecules for:



AGRICULTURAL, ENVIRONMENTAL AND FOOD APPLICATIONS

Tailored molecular structures, especially porphyrins, chelators, dyes, peptides, and hybrid materials, to address practical problems in water and wastewater treatment, agricultural protection and crop resilience, sensing and analytical materials, food and wine applications and sustainable chemistry and catalysis have been prepared. The following examples illustrate more specific applications:

- Photodynamic inactivation was explored for wastewater disinfection, including SARS-CoV-2 model systems, with adjuvants such as hydrogen peroxide improving antiviral efficiency.
- Antimicrobial photodynamic treatment was also applied to food and agricultural pathogens, including Alicyclobacillus acidoterrestris, Lasiodiplodia theobromae, and Pseudomonas syringae in crop sanitation.
- Porphyrin-functionalized solids, silica-based adsorbents, and supramolecular hybrid materials were designed for heavy-metal removal, water purification and potential antimicrobial agents.
- The shikimic acid pathway was explored as a source for sustainability research.
- Organometallic molecules were advanced as catalysts for CO2 functionalization and other chemical reactions.
- Peptides and proteins of relevance in wine properties were studied in depth.
- Gas chromatography–mass spectrometry electroantennographic detection for insect olfaction.
- Titanium- and zinc-based nanomaterials were used to reduce plant stress and heavy-metal toxicity, supporting more resilient agricultural systems.
- Chelators of the 3,4-pyridinone class for iron supplementation in plants and design of new iron fertilizers to address IDC.
- Metal ion chelators for iron speciation and quantification in natural waters.
- Molecules for sensing and stabilization work included imine ligands and ferrocene-based mercury sensors, rhodamine/rosamine dyes for metal ions and biogenic amines, and cellulose-based materials for wine protein stabilization.



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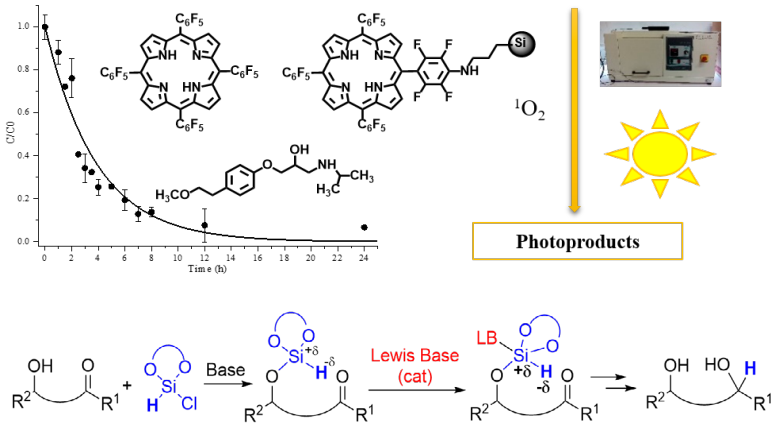
RESEARCH THEMES/ MOLECULES

Chemical synthesis of a wide diversity of molecules for:

CATALYSIS

- Homogeneous and heterogeneous oxidation of alkenes, alkanes, catechol, 3,5-di-tert-butylcatechol, monoterpenes, organosulfur compounds
- Photodegradation of metoprolol using a porphyrin as photosensitizer under homogeneous and heterogeneous conditions
- Advances in photocatalytic degradation of organic pollutants in wastewaters: harnessing the power of phthalocyanines and phthalocyanine-containing materials
- Substituted azaindoles were synthesized by a C-N/Heck reaction catalysed by CALB/PdNPs hybrids
- The sustainable synthesis of imines was achieved from primary alcohols and (Hetero)Aromatic Amines catalysed by Mn-complexes
- Homogeneous oxidation of indole to afford indigo dye
- Novel chlorosilane for metal-free Lewis bases-catalyzed hydrosilylation of aldehydes and reductive amination of alkylphenol ketones
- Chiral molybdenum-based complexes for catalytic epoxidation of olefins
- Synthesis of ortho isomeric Mn(III) N-alkyl- and alkoxyalkylpyridylporphyrins—enhancers of hyaluronan degradation induced by ascorbate and cupric ions.



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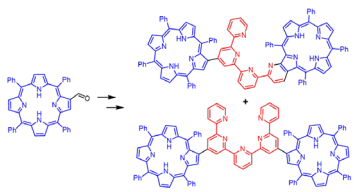
RESEARCH THEMES/ METHODS

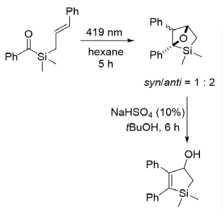
Development of innovative methods for the chemical synthesis or computational design and study of relevant target molecules

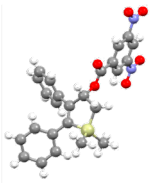
SYNTHETIC APPROACHES

- Design and synthesis of porphyrins for supramolecular systems
- Design and synthesis of porphyrin–fullerene donor–acceptor conjugates for energy transfer
- Design, synthesis and optical properties of porphyrin-oligopyridine triads
- Synthetic access to new porphyrinoids from 2-nitro-5,10,15,20-tetraphenylporphyrin and an arylacetonitrile

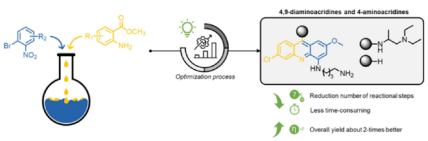


- Synthesis of nitroindazolylacetonitriles via vicarious nucleophilic substitution and tautomeric switching mediated by anions
- Autooxidative aerobic synthesis of densely functionalized thioethers
- Unprecedent silacyclopentenols via photocycloaddition of acyl silanes
- Short preparation of bacterial natural products from abundant quinic acid
- Ohmic heating-assisted synthesis and characterization of Zn(II), Cu(II) and Pd(II) complexes of heterocyclic–fused chlorins
- Irradiation of gold nanoparticles successfully immobilized in situ with mercapto corroles under reductive conditions revealed a coalescence effect without significant ligand detachment.





- Synthesis, spectroscopic properties and singlet oxygen generation of a new beta-functionalized porphyrin–rosamine conjugate
- The dual behaviour of -vinylporphyrins in the presence of ,'- dioxothiones
- New triazine bridged triads based on BODIPY-porphyrin systems with extended absorption, efficient energy transfer and upconverted emission for application in sensing and imaging.
- Synthesis of analogues of the green fluorescent protein chromophore for bioimaging applications
- Design, synthesis and optical properties of triarylpyridines
- Multicomponent synthesis of luminescent iminoboronates
- Design, synthesis and optical properties of difluoroborate complexes
- Mechanistic studies by combined use of UV photoelectron spectroscopy and computational methods



- Development and optimization of synthetic routes towards 4-amino- and 4,9-diaminoacridines
- Design, synthesis and optical properties of benzimidazole-based N,O difluoroborate complexes
- Use of light to generate nucleophilic carbene from acylsilanes, triggering formation of highly functionalized cyclopentenes.
- Exploring the shuffle ability of silyl ether protecting groups to identify opportunities in total synthesis
- Development of a new methodology for the synthesis of symmetric 3,5-Disubstituted Nitrobenzenes, without resorting to the classic nitration agentsagents and harsh conditions.
- Developing of an one-pot methodology for the synthesys of aromatic aminopropyl lactams as potential anticancer agents.

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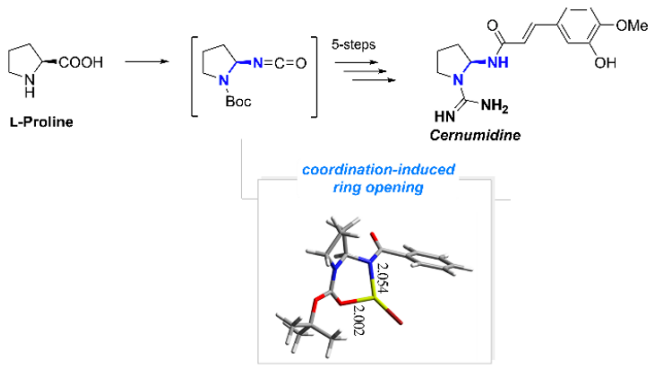
RESEARCH THEMES/ METHODS

Development of innovative methods for the chemical synthesis or computational design and study of relevant target molecules

SYNTHETIC APPROACHES (CONT.)

- One-pot synthesis of amides
- Chemoenzymatic synthesis of complex carbohydrates
- Synthetic routes towards novel 4,9-diaminoacridine antimalarials, and picocyanobacteria-derived metabolites
- Ohmic heating as an emerging concept in organic synthesis and their application in the synthesis of bioactive compounds
- Design and synthesis of efficient solid fluorophores with potential application in luminescent materials
- Cycloaddition reactions for creating improved porphyrin-based photosensitizers
- Aza-michael addition reactions – unprecedented sapphyrin derivatives
- Development of coumarin-based chromophores with diverse heterocyclic-π-bridge for DSSC applications.
- Synthesis of sulfonamides mediated by a PEG-supported hypervalent iodine reagent.
- Novel hypervalent iodine(III) reagents bearing transferable primary amines were synthesized and applied on the Electrophilic - Amination of Stabilized Enolates
- Naturally occurring carbohydrate esters - development of sustainable synthetic methods, computational studies, synthesis scale-up, and novel applications
- Synthesis and transformations of vinyl- and styrylpyrazoles for bioactivity studies
- Ionic liquids and ohmic heating in combination for Pd-catalyzed crosscoupling reactions towards the sustainable synthesis of flavonoids
- Ohmic-heating assisted synthesis of C-glycosylquinolones and related derivatives for cancer therapy
- Enantioselective total synthesis and anti-inflammatory potential evaluation of a natural alkaloid and derivatives containing an hybrid aminal core.
- Total synthesis of galactose-based phosphotriesters and their modulation of human neutrophil oxidative burst toward novel anti-inflammatory agent development.



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RESEARCH THEMES/ MATERIALS

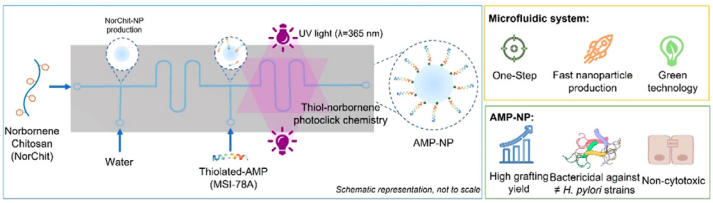
Use of molecular synthesis tools towards development of innovative [bio]materials with potential applications in Biomedical Engineering, Drug Delivery, Separation Techniques and Cleaner Energies

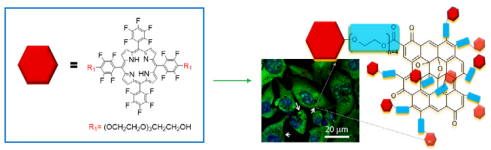
- Biomedical engineering: biomaterials for DNA targeting, drug delivery, antimicrobial surfaces, and cancer therapy. Examples include graphene oxide–porphyrin hybrids for G-quadruplex detection, photoactive porphyrin and 2-hydroxyethyl methacrylate (HEMA) materials with bactericidal properties, peptide-tethered antimicrobial coatings for bone implants and wound dressings, and graphene-based delivery systems for cationic porphyrin photosensitizers against bladder cancer cells. It also includes graphene oxide and porphyrin hybrids for imaging and biosensing, with interest in light-harvesting systems.

- Imaging: fluorescent and photoactive materials for biological visualization. It includes graphene oxide, graphene quantum dots, and other graphene derivatives covalently linked to porphyrins, gold nanorods doped with porphyrin macrocycles for fluorescent microcapsules, GQD–phthalocyanine nanosensors for ds-DNA, and coumarin dyes used as labels for bacterial cell membranes. These systems are designed to improve imaging performance in both cellular and microbial contexts

- Sensing: selective molecular sensors for chemical detection. A key example is a highly emissive pyrrolidine-fused-chlorin anchored on nanoporous TiO2 films for the selective detection of the TATP explosive. This theme shows the use of tailored chromophores and hybrid materials for high-sensitivity recognition of specific analytes.

- Separation and cleaner energies: functional materials for photocatalysis, hydrogen generation, solar energy conversion, and filtration. It includes graphitic carbon nitride sensitized with porphyrins for visible-light photocatalysis, -cyclodextrin-derived holey C-doped g-C3N4 nanosheets for hydrogen generation, all-organic fluorophores for luminescent materials, coumarin, diketopyrrolpyrroles, porphyrin and acenaphthylene-based chromophores for dye-sensitized solar cells, and synthetic cellulose derivatives for the separation of positively charged compounds.





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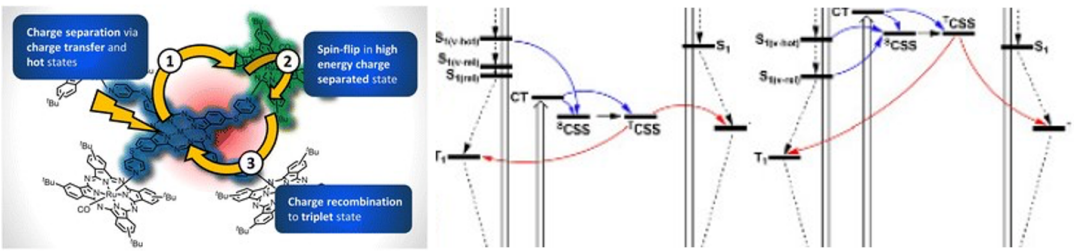
HIGHLIGHTS

UNIQUE ASSEMBLIES OF THIOPYRIDYL-PHTHALOCYANINES AND RUTHENIUM PHTHALOCYANINES; VIBRATIONALLY-HOT EXCITED STATES THAT POWER SPIN-FLIPS IN CHARGE-SEPARATED STATES

Controlling molecular architecture of well-organized organic building blocks and linking their functionalities with the impact of solar-light converting systems constitutes a grand challenge in materials science. Strong absorption cross-sections across the visible range of the solar spectrum as well as fine-balanced energy- and redoxgradient are all important features that pave the way for either funneling excited state energy or transducing charges. In light of this, we used thiopyridyl-phthalocyanines (PcSPy) and ruthenium (tert-butyl)- phthalocyanines (RuPc) as versatile building blocks and demonstrated the realization of a family of multi-functional PcSPy-RuPc (Figure 1) by means of axial coordination. Sizeable electronic couplings between the electron donors and acceptors in PcSPy-RuPc govern ground-state as well as excited-state reactivity. Time-resolved techniques, in general, and fluorescence and transient absorption spectroscopy, in particular, helped to corroborate a rapid charge separation next to a slow charge recombination. Key to these charge transfer characteristics are higher lying, vibrationally hot states of the singlet excited states in parallel with a charge transfer state and the presence of several heavy atom effects that are provided by ruthenium and sulfur. As such, our advanced investigations confirm that rapid charge separation evolves from both higher lying, vibrationally hot states as well as from a charge transfer state, populating charge separated states, whose energies exceed those of the singlet excited states. Charge recombination involves triplet rather than singlet charge separated states, which delays the charge recombination by one order of magnitude .

Unique Assemblies of Thiopyridyl-Phthalocyanines and Ruthenium Phthalocyanines; Vibrationally-Hot Excited States That Power Spin-Flips in Charge-Separated States

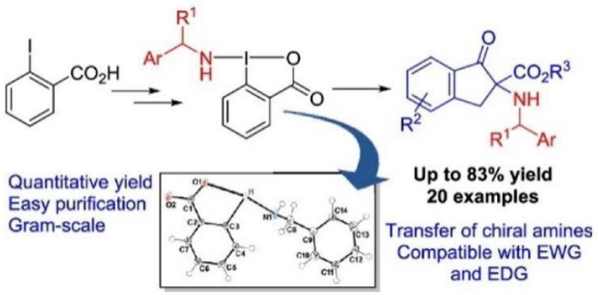
Nanoscale, 2022, 14, 13155-13165



HIGHLIGHTS

SYNTHESIS OF NOVEL HYPERVALENT IODINE REAGENTS WITH A PRIMARY TRANSFERABLE AMINE AND APPLICATION ON THE ELETROPHILIC ALFA-AMINATION OF BETA-KETOESTERES

New primary-amine-bearing hypervalent iodine reagents were successfully synthesized on the gram scale and were obtained in near-quantitative yields. The transfer of primary amines to model carbon nucleophiles using these new reagents was tested, with amination products being obtained in up to 83% yield. A chiral version of the reaction is also described, albeit with preliminary results.



The reaction mechanism was studied with ESIMS studies and DFT calculations. The possible transferable groups using hypervalent iodine reagents are expanded to include primary amines. These new compounds emerge as both powerful and versatile reagents for group transfer reactions, highlighting the ongoing he growth of hypervalent iodine chemistry.

Hypervalent Iodine(III) Reagents with Transferable Primary Amines: Structure and Reactivity on the Electrophilic - Amination of Stabilized Enolates.

Org. Lett. 2022, 24, 776 - 781

SYNTHESIS OF SULPHONYL HYDRAZIDES ENABLE BY HYPERVALENT IODINE REAGENTS

New primary-amine-bearing hypervalent iodine reagents were successfully synthesized on the gram scale and were obtained in near-quantitative yields. The transfer of primary amines to model carbon nucleophiles using these new reagents was tested, with amination products being obtained in up to 83% yield. A chiral version of the reaction is also described, albeit with preliminary results.
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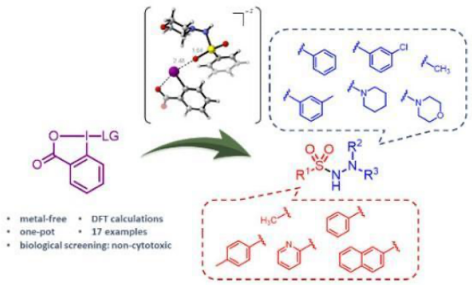
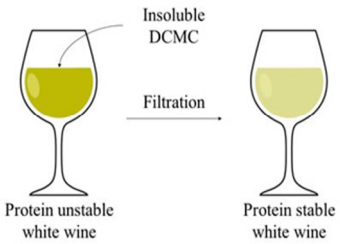


Practical Synthesis and Biological Screening of Sulfonyl Hydrazides

Org. Biomol. Chem. 2023, 21, 2118

HIGHLIGHTS

DEVELOPMENT OF A SUSTAINABLE ALTERNATIVE – A CELLULOSE DERIVATIVE - TO BENTONITE ON WHITE WINE PROTEIN STABILIZATION



DCMC as a Promising Alternative to Bentonite in White Wine Stabilization. Impact on Protein Stability and Wine Aromatic Fraction.

Molecules 2021, 26, 6188

Compound, method of production and uses thereof WO2019/197884A1

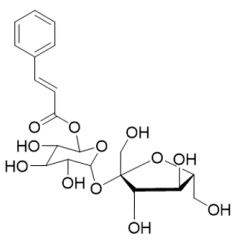
This work describes an improved and greener methodology to replace bentonite on white wine protein stabilization. Dicarboxymethyl cellulose (DCMC) is a recently described by us cellulose-derived polymer which is negatively charged at the wine pH and presents the capacity to adsorb positively charged substances and wine proteins. DCMC was applied to wines, prepared from cultivars that are generally known to produce high protein instability. The efficacy of DCMC when compared with that of bentonite in decreasing the hazing potential of white wines, promote protein removal, preserve the phenolic content and pH, the slight calcium depletion and predictable changes in the wine aromatic fraction allowed us to propose DCMC as a sustainable alternative to bentonite fining in white wine protein stabilization.

SCALE-UP STUDIES OF THE SYNTHESIS OF PHENYLPROPENOID SUCROSE ESTER

Phenylpropenoid saccharide esters, methods and uses thereof.

Patent No. WO2020183442 A2 2020, March 16

Phenylpropenoid sucrose esters are constituents of herbs like Scrophularia ningpoensis, which have been used in traditional Chinese medicine and are known to have many therapeutic effects, including antioxidative and antiaging. A market study over the antiaging cosmetics shows that the market has been growing at a steady 5% over the period from 2017-2020 and is valued at 38.62 billion USD in 2020. Until now, the only known method for obtaining the title substances was extraction from raw plant material, which is a very low yielding process. We have developed a method to synthesize the target compound by using a selective esterification method like the Mitsunobu's reaction, with much higher yield. The objective of this research is to evaluate whether it is possible to obtain the natural esters by synthesis on a larger scale (10kg per batch) and if it will be profitable. In the scope of this work, we have performed several experiments - using a mole ratio of 1:2 between the sucrose and other reagents yielded 25% conversion of sucrose. The time to complete a batch is about 48 hours and the bottleneck of the process is the reaction time, which is at least 24 hours. The next step will be a further scale-up of the process. Calculations of the dimensions, time, energy, and materials consumption of an industrial installation are being performed.



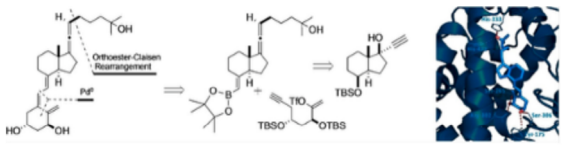
6-*O*-cinnamoyl sucrose, Sibirioside A

Veronicastrum Sibiricum

HIGHLIGHTS

CONFORMATIONALLY RESTRICTED ANALOGUES OF VITAMIN D

Calcitriol derivatives (Vitamin D receptor ligands) have potential for the treatment of hyperproliferative diseases and disorders related to the immune system. Looking for side-chain conformational requirements of vitamin D analogs for selective biological activity, a new active vitamin D analog that has conformationally restricted mobility at the side chain and adopts a similar structure than the natural hormone 1,25-dihydroxyvitamin D3 in the binding pocket was designed by docking and synthesized. The highlights of the synthesis include a Pd0-catalyzed cascade and an orthoester-Claisen-rearrangement for the formation of the trienic system and the allenic side-chain, respectively.



Design, Synthesis, Evaluation and Structure of Allenic 1,25-Dihydroxyvitamin D3 Analogs with Locked Mobility at C-17.

Chem. Eur. J. 2021, 27, 13384–13389

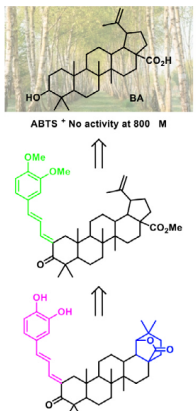
DEOXYGENATIVE DIVERGENT SYNTHESIS

Finding synthetic transformations that maximize the full potential of abundant natural compounds is a timely challenge in the panorama of sustainability. Notwithstanding the many methods available for the defunctionalization of polyols, few promote selective deoxygenations and provide molecules with the right degree of functionalization prone for further manipulations. A new concept for organic synthesis that is based on the selective deoxygenation of natural polyols for preparation of fragments of reasonable complexity has been explored. The controlled deoxygenation of quinic acid resorting to boranes-catalyzed hydrosilylation reaction has been showcased. The methods explored have been optimized for regioselectivity, allowing the synthesis of new chiral fragments of great potential use in total synthesis from a common quinic acid-derived precursor. The borane-catalyzed hydrosilylation for cleavage of C(sp3)-O bonds of a cyclitol was studied for the first time, and the reaction mechanism unraveled through computational studies.

Deoxygenative Divergent Synthesis: En Route to Quinic Acid Chirons.

Org. Lett. 2020, 22, 8370-8375

AMPHIPHILIC ANTIOXIDANTS BASED ON THE FUNCTIONALIZATION OF BETULINIC ACID WITH POLYPHENOLIC FRAGMENTS



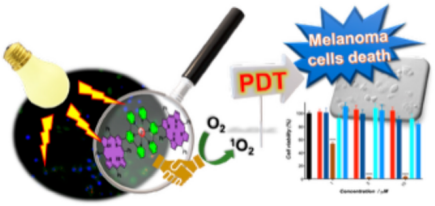
This work aimed at the valorization of biomass derived compounds by their transformation into new added-value compounds with enhanced antioxidant properties. In this context, polyhydroxylated compounds derived from (E)-2-benzylidene-19,28-epoxyoleanane-3,28-diones were prepared, starting from natural betulinic acid (BA) and using a two-step methodology. The synthesized compounds were designed to have specific substitution patterns at C-2 of the triterpene scaffold, allowing the establishment of a structure-activity relationship. In particular, their radical scavenging ability was evaluated using the 2,2-diphenyl- 1-picrylhydrazyl (DPPH•) and 2,2'-azino-bis(3-ethylbenzothiazoline- 6-sulphonic acid) (ABTS•+) assays. The most efficient scavenger was 19,28-epoxyoleanane-3,28-dione derivative bearing a catechol moiety and an ,,,-diunsaturated carbonyl system at C-2, which was more active than -tocopherol used as positive control and the pristine BA in the ABTS•+ assay.

Functionalization of Betulinic Acid with Polyphenolic Fragments for the Development of New Amphiphilic Antioxidants

Antioxidants 2021, 10, 148

HIGHLIGHTS

β-MODIFIED PORPHYRIN BEARING TERPYRIDINE UNITS AS LIGANDS TO PREPARE IRIDIUM AND RUTHENIUM COMPLEXES WITH IMPROVED PHOTOSENSITIZING PROPERTIES TOWARDS CANCER CELLS



Ruthenium and iridium complexes bearing porphyrin moieties: PDT efficacy against resistant melanoma.

Dyes Pigments 2022, 205, 110501

Tetrapyrrolic macrocycles, namely porphyrins and reduced analogues, exhibit an excellent ability to act as photosensitizers (PS) in photodynamic therapy (PDT). Also, ruthenium and iridium complexes, mainly containing pyridine ligands, have been highlighted as potential PS for PDT, due to their photochemical and photophysical properties. The combination of porphyrin derivatives with iridium or ruthenium ions may create singular features and, consequently, improve the PDT effect. In this paper, we report the and photophysical characterization of symmetrical and unsymmetrical ruthenium and iridium complexes of -functionalized porphyrin derivatives bearing terpyridine ligand units. The synthesized porphyrin derivatives bearing attached ruthenium or iridium terpyridine units display appropriate photophysical properties to act as PS through a photodynamic process, namely high singlet oxygen quantum yields. The ruthenium and iridium porphyrin complexes' efficiency was evaluated against B16F10 cells, selected as a model of resistant melanoma cells, by using MTT assays. The PDT outcome in this melanotic cell line shows that the symmetrical iridium bis(porphyrin-terpyridine) complex exhibits high photodynamic activity at lower concentrations due to the high values of singlet oxygen quantum yield and cellular uptake found. The PDT performance displayed by this complex induces a melanoma cancer cellular death higher than 96% at concentrations ranging from 2.5 to 10 μM with a light irradiation of 5 J cm−2. The symmetrical iridium bis(porphyrin-terpyridine) complex displays an astonishing photodynamic activity against B16F10 cells, even when compared with porphyrin complexes (PS) described in the literature, using both lower PS concentration and total light dose, and subcellular localization near the nucleus. Moreover, also, the non-symmetrical ruthenium (porphyrin-terpyridine)-terpyridine complex exhibits a great photodynamic effect against B16F10 cancer cells inducing a cellular death at 10 μM ranging from 84 ± 2.0% to 89 ± 2.7%, depending on the total light-dose delivery. The modification of the porphyrin moiety at one of the -pyrrolic positions with ligand-type moieties to coordinate transition-metal ions leads to porphyrin complexes with improved PS activity when compared with other extensively studied meso-tetraarylporphyrin derivatives.

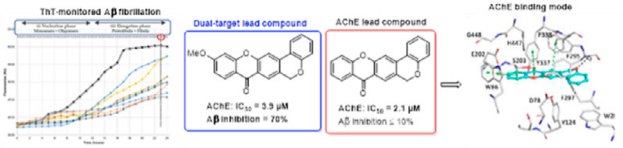
HIGHLIGHTS

CHROMENO[3,4-B]XANTHONES AS FIRST-IN-CLASS ACHE AND Aβ AGGREGATION DUAL-INHIBITORS

Following the multi-target directed ligands (MTDLs) concept, chromeno[3,4-b]xanthones were designed, synthesized, and evaluated as first-in-class acetylcholinesterase (AChE) and Aβ aggregation dual-inhibitors. The core structure of chromeno[3,4-b]xanthones emerged as AChE lead with IC50 of 2.1 μM, whether the methoxy-substituted derivative stood up as AChE and Aβ aggregation dual-inhibitor with IC50 of 3.9 μM and 70% inhibition, respectively. The molecular docking showed that most of the compounds bound to AChE through hydrogen bonds with residues of the catalytic triad and π-stacking interactions between the main scaffold and the aromatic residues present in the binding pocket.

Chromeno[3,4-b]xanthones as First-in Class AChE and Aβ Aggregation Dual Inhibitors

International Journal of Molecular Sciences 2021, 22, 4145

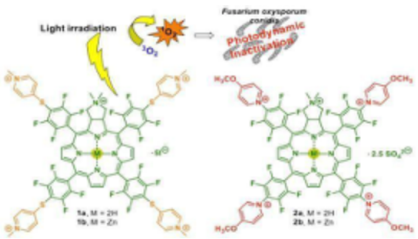


IN VITRO PHOTODYNAMIC TREATMENT OF FUSARIUM OXYSPORUM CONIDIA THROUGH THE ACTION OF THIOPYRIDINIUM AND METHOXYPYRIDINIUM CHLORIN DYES

Antimicrobial photodynamic inactivation (PDI) has been explored as an innovative therapeutic and phytosanitary approach because it can be used to inactivate microbial vegetative forms and spores, without significant development of resistance to photosensitization and collateral damage to host tissues. The objective of this study was to assess the photodynamic antifungal/sporicidal activity of quaternized chlorins (Chls) with thiopyridinium or methoxypyridinium substituents. Free-base and zinc(II) thiopyridinium or methoxypyridinium Chls (1a, 1b, 2a, and 2b, respectively) were prepared and tested on Fusarium oxysporum conidia. The PDI tests were conducted with photosensitizer (PS) concentrations of 100, 25, 15 and 5 μM, under white light exposure at an irradiance of 50 mW.cm−2, applied during 60 min (light dose of 180 J.cm−2). A high PDI efficiency, corresponding to inactivation to the detection limit, was observed with all the molecules. The free-base thiopyridinium chlorin 1a was the most effective PS, requiring the lowest concentration and the shortest irradiation time, for the complete inactivation of conidia (15 μM, 15 min, 45 J.cm−2). Complete inactivation was also achieved with the other chlorins but a higher concentration (100 μM) of PS and, in the case of chlorin 1b, a longer irradiation period (30 min, 90 J.cm−2), were required. Because of the low concentrations and small energy doses required to inactivate resistant biological forms such as fungal conidia, these chlorins can be regarded as potent antifungal photodynamic drugs.

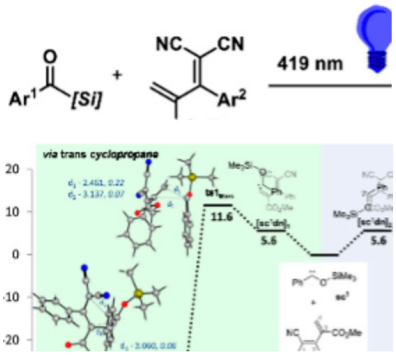
A versatile strategy for effective photoinactivation of fusarium oxysporum conidia

Photochem. Photobiol., A, 2022, 432, 114081



HIGHLIGHTS

USING VISIBLE LIGHT TO SYNTHESIZE HIGHLY FUNCTIONALIZED CYCLOPENTENES



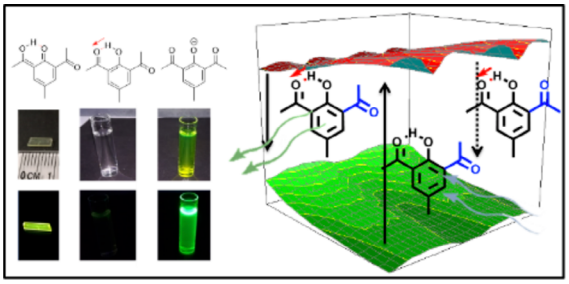
Functionalized Cyclopentenes via the Formal [4+1] Cycloaddition of Photogenerated Siloxycarbenes from Acyl Silanes.

Journal of Organic Chemistry 2022, 87 (14), 8910-8920

Acylsilanes are a particular class of organosilanes firstly synthesized in 1957 and characterized by presence of a silicon atom bonded to a carbonyl group. Early studies were mostly devoted to their unusual spectroscopic properties, mainly credited to the inductive release of electrons from the silicon atom to the carbonyl group. Much is currently known about the reactivity of acylsilanes, but it is still surprising that siloxycarbenes derived from photolysis of acylsilanes have been scarcely used in the context of preparative organic synthesis.
In this work we presented the preparation of functionalized cyclopentenes through an unexplored cyclopropanation/vinyl cyclopropane rearrangement starting from benzoylsilanes.
We demonstrated that electron-withdrawing dienes, useful in the inverse-electron-demand Diels-Alder reaction, react with siloxycarbenes to deliver cyclopentenes. Upon formation, the vinyl cyclopropane undergoes a well-known ring expansion to cyclopentene, providing an entry for the formal 4+1 cycloaddition of a carbene to a diene. The formation of the siloxycarbene and further formation of the cyclopentene was achieved solely by use of visible light (419 nm) at room temperature, avoiding use of metals or other catalysts, and the mechanism of the transformation was elucidated by density functional theory studies.

EXCITED-STATE (INTRAMOLECULAR) PROTON TRANSFER IN ORGANIC LUMINESCENT DYES

Understanding the different pathways followed by organic dyes when they absorb and emit light is the first step toward the design of efficient, tunable and stable luminophores. The transfer of protons in the excited state is a particular challenge, as it modulates the photo-physical properties of the dyes and depends on many internal and external factors. Here, series of dyes were designed to favor the Excited-State (Intramolecular) Proton Transfer (ESIPT), synthesized and characterized: chalcones, triarylpyridines and phenols, decorated with peripheral substituents to tune their luminescence color and intensity. The ESIPT can be favored or restricted, depending on both the substituents and the environment of the dyes: solvent (polarity, proticity, viscosity, pH), solid or crystalline state. All these observations have been rationalized using DFT and td-DFT calculations, to model the molecular orbitals and determine the energy of the vertical transitions. The study of these luminescent dyes paves the way toward their application in sensing and emissive devices, and as ratiometric molecular probes for biological imaging.



Unsymmetrical 2,4,6-Triarylpyridines as Versatile Scaffolds for Deep-Blue and Dual-Emission Fluorophores

ChemPhotoChem 2020, 4, 5312-5317.

Single-Benzene Fluorophore with Enhanced Emission: Insights into Photophysical properties through Proton Transfer Mapping

Chem. Eur. J. 2025, 31, e202501178.

Excited-State Proton Transfer in Luminescent Dyes: From Theoretical Insight to Experimental Evidence

Chem. Eur. J. 2023, e202301540.

Influence of the Intramolecular Hydrogen Bond on the Fluorescence of 2-ortho-Aminophenyl Pyridines

Chem. Eur. J. 2022, e202201844.

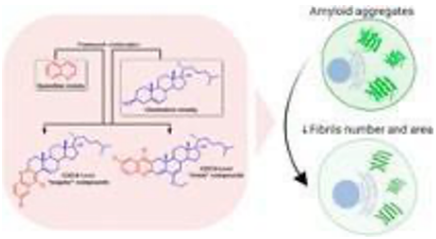
Push-pulling induces the excited-state intramolecular proton transfer in 2'-aminochalcones

Dyes Pigm. 2022, 202, 110275

HIGHLIGHTS

STEROID-QUINOLINE HYBRID MOLECULES FOR INHIBITION AND REVERSION OF PROTEIN AGGREGATION

Acylsilanes are a particular class of organosilanes firstly synthesized in 1957 and characterized by presence of a silicon atom bonded to a carbonyl group. Early studies were mostly devoted to their unusual spectroscopic properties, mainly credited to the inductive release of electrons from the silicon atom to the carbonyl group. Much is currently known about the reactivity of acylsilanes, but it is still surprising that siloxycarbenes derived from photolysis of acylsilanes have been scarcely used in the context of preparative organic synthesis. In this work we presented the preparation of functionalized cyclopentenes through an unexplored cyclopropanation/vinyl cyclopropane rearrangement starting from benzoylsilanes. We demonstrated that electron-withdrawing dienes, useful in the inverse-electron-demand Diels- Alder reaction, react with siloxycarbenes to deliver cyclopentenes. Upon formation, the vinyl cyclopropane undergoes a well-known ring expansion to cyclopentene, providing an entry for the formal 4+1 cycloaddition of a carbene to a diene. The formation of the siloxycarbene and further formation of the cyclopentene was achieved solely by use of visible light (419 nm) at room temperature, avoiding use of metals or other catalysts, and the mechanism of the transformation was elucidated by density functional theory studies.

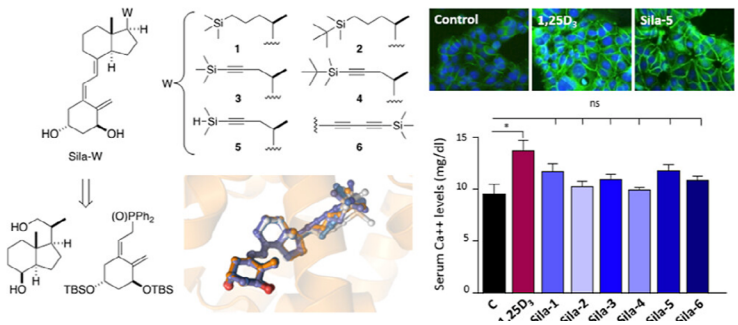


Steroid–Quinoline Hybrids for Disruption and Reversion of Protein Aggregation Processes.

ACS Medicinal Chemistry Letters 2022, 13, 443-448

FIRST SILA-ANALOGUES OF VITAMIN D

Incorporating silicon bioisosteres into pharmacological structures is a strategy to enhance drug therapeutic potential. Six secosteroidal analogues of the natural hormone 1,25-dihydroxyvitamin D3 (1,25D3) were designed with silicon as a C25 side-chain isostere and synthesized via the Wittig–Horner approach from Inhoffen-Lythgoe diol. Crystal structures revealed that the sila-containing side chains form additional interactions that stabilize the active conformation of the vitamin D receptor (VDR). These analogues show similar VDR binding and transcriptional activity as 1,25D3 but with reduced hypercalcemic effects and, when combined with chemotherapy, significantly inhibit cell proliferation.



First Sila-Vitamin D Analogues: Design, Synthesis, Structural Analysis and Biological Activity.

J. Med. Chem. 2024, 67, 23, 21505–21519.

VITAMIN D COMPOUNDS, METHOD OF PRODUCING SAID COMPOUNDS AND USES THEREOF

International Patent Application: PCT/IB2022/052839; WO/2023/161688

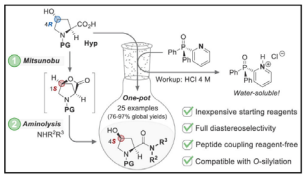
Portuguese Patent (Granted): 117825

Spanish Patent (Granted): P202330169

HIGHLIGHTS

A SUSTAINABLE METHODOLOGY IN PEPTIDE SYNTHESIS FOR APPLICATION IN MEDICINAL CHEMISTRY

This work presents a diastereoselective, efficient, and peptide coupling reagent-free methodology for the synthesis of cis-4-hydroxy-L-prolyl amides.



Telescoped One-Pot Strategy for the Assembly of cis-4-Hydroxy-L-Prolyl Amides.

ACS Sustainable Chem. Eng. 2024, 12, 46, 16986−16998

Synfacts

Using a two-step telescoped one-pot protocol, these amides are prepared directly from readily available trans-4-hydroxy-L-proline. The key transformations involve stereoinversion of trans-4-hydroxy-L-proline via an intramolecular Mitsunobu reaction, followed by lactone aminolysis, enabling the formation of amide bonds with a variety of nucleophiles, including primary, secondary, and aromatic amines, amino alcohols, amino acid derivatives, and dipeptides in high overall yields (76-97%, 25 examples) without isolation of intermediates.

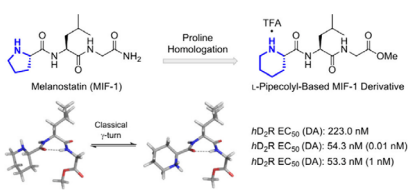
This methodology is easily scalable and can be extended to a three-step, one-pot synthesis by incorporating an O-silylation step, demonstrating superior efficiency, higher atom economy, and reduced waste compared to traditional disconnected approaches. The practical value of this approach is highlighted by the formal synthesis of a bioactive compound exhibiting antiamnesic properties, showcasing its potential utility in medicinal chemistry and peptide-based drug development. This work was highlighted in Synfacts (DOI: 10.1055/a-2496-8950), underscoring its significance in contemporary peptide synthesis.

MELANOSTATIN CONJUGATES WITH AMANTADINE AS ANTI-PARKINSON LEADS

Melanostatin (MIF-1) is a naturally occurring neuropeptide acting as a positive allosteric modulator (PAM) of dopamine D2 receptors (D2R), offering therapeutic potential for central nervous system disorders related to dopaminergic dysfunction, including depression, addiction, restless legs syndrome, tardive dyskinesia, and Parkinson's disease. In this work, a new series of MIF-1 analogues was synthesized using L-pipecolic acid as an L-proline surrogate and pharmacologically evaluated in functional assays at the D2R. Among them, methyl L-pipecolyl-L-leucylglycinate (compound 9) demonstrated superior activity, increasing dopamine potency ~4.1- and ~4.2-fold at 0.01 and 1 nM, respectively. In silico studies showed that compound 9 preferentially adopts a -turn, indicating that neither the C-terminal carboxamide nor a type II -turn is required for PAM activity. Toxicological assays in human dopaminergic SH-SY5Y cells revealed no significant toxicity up to 100 µM. This work was highlighted by the American Peptide Society (https://americanpeptidesociety.org/research/allosteric-turns/) and was awarded the IACOBUS Papers 2025, underscoring its significance in peptide-based neuropharmacology.

Proline Homologation in Melanostatin Neuropeptide: Discovery of Potent Modulators of the Dopamine D2 Receptors.

ACS Med. Chem. Lett. 2025, 16, 8, 1437−1444



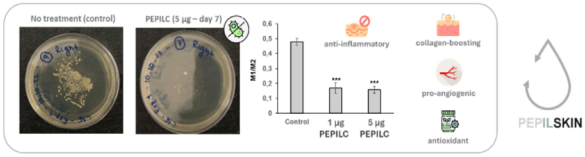
American Peptide Society

PROGRAMA IACOBUS

HIGHLIGHTS

BEYOND ANTIMICROBIALS: A MULTIMODAL PEPTIDE–IONIC LIQUID CONJUGATE FOR DIABETIC FOOT ULCERS

Diabetic foot ulcers (DFU) are a severe complication of diabetes, frequently leading to chronic wounds, amputation, and increased mortality. Their treatment is compromised by persistent inflammation, impaired angiogenesis, and poor tissue regeneration. To address these challenges, we developed peptide - ionic liquid conjugates (PEPILC) as multifunctional topical agents. The most promising PEPILC demonstrated potent broad-spectrum antimicrobial activity and significant collagenesis inducing effects in vitro. Upon topical application in wounds on diabetic mice, PEPILC accelerated healing through a multimodal action, encompassing anti-inflammatory, antioxidant, pro-angiogenic, antimicrobial, and collagen-stimulating effects. Overall, the treatment enhanced wound maturation while protecting the lesion from infection. Protected by a patent application, the PEPILC technology is being broadened in application scope and advanced for clinical translation towards skin-related disorders under the name PEPILSKIN.



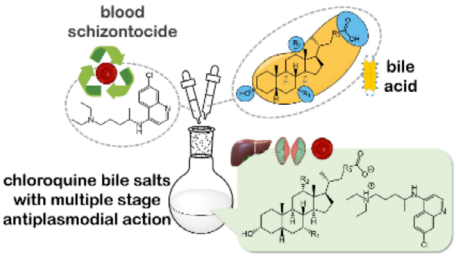
Enhancement of wound healing in diabetic mice by topical use of a peptide-ionic liquid conjugate.

The International Journal of Biochemistry & Cell Biology 2025, 180, 106753

International Patent Application: PCT/IB2022/052839; WO/2023/161688

"SEASONING" DRUGS: BILE ACID-DERIVED GUMBOS AS MULTISTAGE ANTIPLASMODIALS

The development of new antimalarial drugs prioritizes cost-effective multi-stage antiplasmodial agents, for higher efficacy and lower propensity to elicit drug-resistant parasites. Following up on our long-term research towards the rescue of classical antimalarial aminoquinoline drugs, we have developed new organic salts by acid-base pairing of those drugs with natural bile acids. The novel compounds, which belong to the so-called Group of Uniform Materials Based on Organic Salts (GUMBOS), were active in vitro against the three developmental stages of malaria parasites in the human host, namely, hepatic, erythrocytic and gametocyte stages. These findings pave a new pathway for drug rescuing, with impact much beyond antimalarial drug discovery. This work was featured in the front cover of the August 2024 issue RSC Medicinal Chemistry, upon invitation by this journal.



"Seasoning" antimalarial drugs' action: chloroquine bile salts as novel triple-stage antiplasmodial hits.

RSC Medicinal Chemistry 2024, 15, 2657-2662

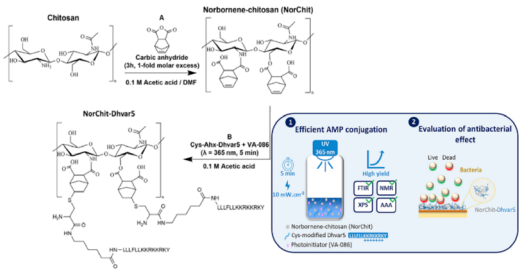
HIGHLIGHTS

COMBINING TWO NOBEL-PRIZED CHEMISTRIES TO CREATE PEPTIDE-GRAFTED BIOMATERIALS WITH ANTIBACTERIAL PROPERTIES AND BEYOND

Thiol–Norbornene Photoclick Chemistry for Grafting Antimicrobial Peptides onto Chitosan to Create Antibacterial Biomaterials.

ACS Applied Polymer Materials 2022, 4, 5012-5026

From Merrifield's revolutionary solid-phase peptide synthesis to the transformative click-chemistry innovations of Sharpless, Meldal, and Bertozzi, these landmark advances reshaped the molecular sciences by enabling rapid, reliable, and biocompatible construction of complex molecules, forging a deep and lasting integration between Chemistry and the Life&Health Sciences and providing foundational technologies that continue to drive modern biomedical discovery and production. We are using these two Nobel-prized chemical approaches for the covalent grafting of antimicrobial peptides onto FDA-approved biomaterials, envisaging new topical treatments, as dressings or hydrogels, to tackle skin and soft tissue infections. In this connection, the highly efficient thiol-norbornene photoclick chemistry was successfully applied for peptide grafting onto norbornene-modified chitosan in aqueous medium under mild conditions. Ultra-thin films of the peptide-grafted material showed significant antibacterial activity. This chemical approach enables fast and easy fabrication of diverse functional biomaterials for multiple therapeutic applications, which can be tailored by a sensible choice of the bioactive peptide or peptides that is or are to be grafted onto the biopolymer.

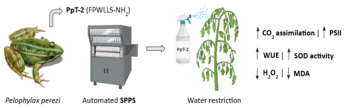


NATURAL ANTIOXIDANT PEPTIDE PPT-2 ENHANCES TOMATO TOLERANCE TO DROUGHT

Bioprospecting a Natural Antioxidant Peptide for Tomato Biostimulation Under Water Limitations: Physiological Approach.

Journal of Plant Growth Regulation 2025, 44, 2569-2582

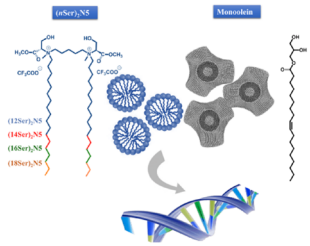
Drought is becoming one of the most severe constraints on agriculture, reducing photosynthesis, increasing oxidative stress, and threatening global food security. As conventional solutions such as irrigation, breeding, or chemical inputs become insufficient or environmentally costly, interest has grown in natural biostimulants, particularly small bioactive peptides of natural origin, which can display signaling or antioxidant functions. In this context, the peptide PpT-2, previously isolated from the skin secretion of Pelophylax perezi amphibians, and shown to suppress the generation of reactive oxygen species in cellular systems, was synthesized by solid-phase peptide synthesis and explored as a potential biostimulant to enhance the resilience tomato plants (Solanum lycopersicum) to water scarcity. Foliar application of PpT-2 at 150 mg/L in tomato plants alleviated the negative effects of water restriction by improving CO_2 assimilation, PSII efficiency, and water-use efficiency (WUE), while strongly reducing oxidative stress markers such as H_2O_2 and malondialdehyde (MDA). The peptide also enhanced superoxide dismutase (SOD) activity, reinforcing antioxidant defenses, with no effect on the morphological parameters of tomato plants, indicating a targeted physiological effect. Overall, the study highlights the potential of natural peptides as promising, eco-friendly biostimulants capable of strengthening tolerance to drought, through improved photosynthetic performance and effective reduction of oxidative stress.



HIGHLIGHTS

CATIONIC SERINE-BASED GEMINI SURFACTANT: MONOOLEIN AGGREGATES AS PROMISING NANOCARRIERS FOR GENE THERAPY APPLICATIONS

Cationic gemini surfactants have emerged as potential gene delivery agents as they can co-assemble with DNA due to a strong electrostatic association. Commonly, DNA complexation is enhanced by the inclusion of a helper lipid, which also plays a key role in transfection efficiency. In this connection, we investigated the DNA complexation ability of mixtures of the serine-based gemini surfactants (nSer)2N5 with monoolein (MO) as a helper lipid. The gemini surfactants:MO aggregates were non-cytotoxic up to 35-90 μM, with higher MO content and longer surfactant chain length seemingly promoting higher cell viability. DNA was efficiently complexed and compacted by all gemini surfactant/MO systems, which are therefore disclosed as promising gene delivery vectors.

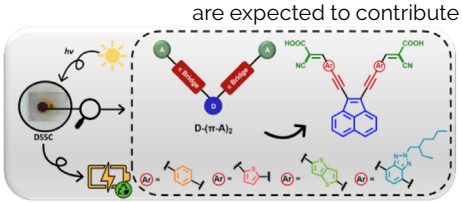


Cationic Serine-Based Gemini Surfactant:Monoolein Aggregates as Viable and Efficacious Agents for DNA Complexation and Compaction: A Cytotoxicity and Physicochemical Assessment.

Journal of Functional Biomaterials 2024, 15:224

DEVELOPMENT OF ACENAPHTHYLENE-BASED CHROMOPHORES FOR DSSC APPLICATION

Dye-sensitized solar cell (DSSCs) have attracted considerable interest due to their lower fabrication costs compared to conventional silicon-based solar cells, the flexibility in molecular design of sensitizers, and their relatively high energy conversion efficiencies. In this context, and aligned with European policy goals aimed at achieving net-zero carbon emissions by 2050, DSSCs are expected to contribute significantly to renewable electricity generation. This study focuses on the development of a series of di-branched, and the dianchoring diethynylacenaphthylene-based dyes, employing as π-bridges phenyl, thiophene, benzotriazole and thieno[3,2-b]thiophene rings, and their application as sensitizers in DSSCs.

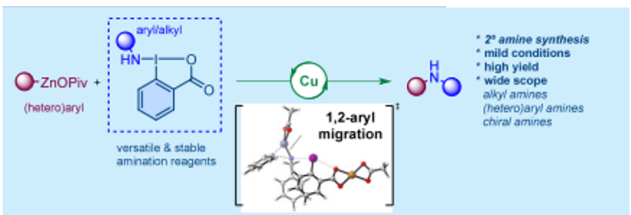


Acenaphthylene-Based Chromophores for Dye-sensitized Solar Cells: Synthesis, Spectroscopic Properties, and Theoretical Calculations.

ACS Omega, 2024, 9(12), 14627–14637.

COPPER-CATALYZED ELECTROPHILIC AMINATION OF ARYL AND PYRIDYLZINC PIVALATES MEDIATED BY N-BASED HYPERVALENT IODINE(III) REAGENTS

A new Cu-catalyzed electrophilic amination of rapidly prepared, air-stable polyfunctional organozinc compounds was developed using hypervalent iodine reagents bearing transferable aryl/alkyl amines. This procedure allows access to a wide range of aryl, heteroaryl, and alkyl amines, showing excellent functional group tolerance. The mechanism of the reaction was investigated using density functional theory calculations..



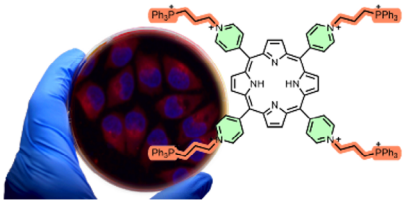
Copper-Catalyzed Electrophilic Amination of Aryl and Pyridylzinc Pivalates Mediated by N-Based Hypervalent Iodine(III) Reagents.

Org. Lett. 2025, 27, 9914–9919

HIGHLIGHTS

PORPHYRIN-TRIPHENYLPHOSPHONIUM CONJUGATES AS PROMISING TOOLS FOR A DUAL APPROACH AGAINST CANCER

This work describes the development of multicharged porphyrin-triphenylphosphonium conjugates as selective G-quadruplex (G4) stabilizers targeting telomeres and oncogene promoters (MYC, KRAS). Octa- and hexa-cationic derivatives arose as the most promising, representing the first report of porphyrins with more than four positive charges evaluated for G4 stabilization. Spectroscopic assays and molecular dynamics simulations confirmed high G4 affinity and selectivity over double-stranded DNA, with ligands binding via 5'-end stacking. Hexacationic derivative showed preference for MYC while octacationic favored KRAS. The biological efficacy was validated by PCR stop assays, where the conjugates effectively blocked Taq polymerase activity through G4 stabilization. Furthermore, these ligands exhibited exceptional singlet oxygen (1O2) generation, surpassing the standard H2TMPyP by 30%, and maintained this activity even when bound to DNA. In vitro studies in metastatic melanoma cell lines (A375 and SK-MEL-28) revealed efficient nuclear internalization and significantly higher cytotoxicity compared to non-tumorigenic keratinocytes. Highly charged porphyrins-phosphonium conjugates emerge as a lead candidate for a dual therapeutic approach, combining G4-mediated oncogene regulation with Photodynamic Therapy (PDT) to selectively compromise tumor cell proliferation.

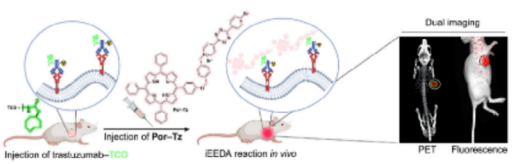


Oncogenic and telomeric G-quadruplexes: Targets for porphyrin-triphenylphosphonium conjugates.

Int. J. Biol. Macromol. 2024, 277, 134126

POSITRON EMISSION TOMOGRAPHY AND OPTICAL IMAGING TO MONITOR BIOORTHOGONAL DIELS-ALDER CLICK CHEMISTRY OF TRASTUZUMAB WITH A PORPHYRIN

The treatment of skin disorders may be seriously hampered by other existing co-morbidities, such as ischemia, neuropathy, immune system dysregulation, and chronic inflammation. All these increase the risk of infection that, in turn, worsens the overall situation, giving rise to a vicious cycle that is hard to break. This is a common scenario in non-healing wounds affecting, e.g., diabetic and/or bedridden elderly patients, whose life quality and expectancy are put at stake. Thus, treatments are needed that both promote an effective clearance of microbial pathogens, including of multidrug resistant isolates whose
prevalence is spiraling worldwide, and fast healing.
We have recently developed new constructs that meet these conditions in vitro and in vivo, and which result from linking short cosmetic peptides to antimicrobial ionic liquids, by means of “click” chemistry. Besides showing wound-healing and antimicrobial activity when used topically on wounds in type 1 diabetic mice, the novel peptide-ionic liquid conjugates display antioxidant, anti-inflammatory, pro-collagen, and pro-angiogenic actions in vivo. This unprecedent chemotype is now under later stage preclinical investigations, envisaging its future clinical translation.

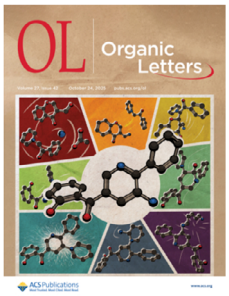


Positron Emission Tomography and Optical Imaging to Monitor Bioorthogonal Diels–Alder Click Chemistry of Trastuzumab with a Porphyrin

Bioconjugate Chem. 2025, 36, 1013

HIGHLIGHTS

SYNTHESIS AND META-AMINATION OF PYRIDINES VIA MULTICOMPONENT CASCADE REACTION



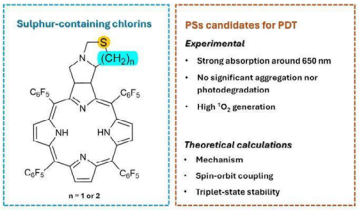
Synthesis and meta-Amination of Pyridines via Multicomponent Cascade Reaction

Org. Lett. 2025, 27, 11757–11763

Pyridines are the most frequently employed nitrogen heterocycle in approved drugs. The electronically biased resonance forms of pyridine pose significant challenges for the preparation of meta-substituted derivatives, compared to the much more attainable ortho- and para-substituted isomers. Despite the most modern strategies for functionalization of pyridines, such as temporary dearomatization and the use of Zincke imine intermediates, both fail when it comes to the installation of the NH2 group at the meta-position. A new multicomponent reaction (MCR) platform was developed for the one-pot synthesis and meta-amination of pyridines, using readily available feedstock like 3-formylchromones, pyridinium salts and NH4OAc. The reaction proceeds through the regioselective in-situ assembly of a [1,3-bipyridin]-1-ium intermediate, which, upon aminolysis, enables the access of meta-aminopyridines. The method offers broad scope (>20 examples), good functional group tolerance, and scalability in batch and flow procedures. Synthetic utility is demonstrated through conversion into 3-halo, 3-hydroxy, and 3-thiopyridines, expanding the access to meta-substituted pyridines through peripheral editing of the unprotected amino group.

SULPHUR-CONTAINING PYRROLIDINE-FUSED CHLORINS AS POTENTIAL CANDIDATES FOR PHOTODYNAMIC THERAPY: EXPERIMENTAL AND THEORETICAL PHOTOPHYSICAL EVALUATION

Organic & Biomolecular Chemistry (2025) 23, 8212–8222.



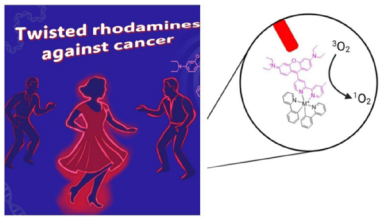
Two novel sulphur-containing pyrrolidine-fused chlorin derivatives were synthesized through a 1,3-dipolar cycloaddition reaction of meso-tetrakis(pentafluorophenyl)porphyrin with azomethine ylides generated in situ from paraformaldehyde and either cysteine or L-thiazolidine-4-carboxylic acid, yielding Chlor-SH_trans and homocysteine to produce Chlor-CSH_trans. The synthesized chlorins were structurally characterized using various techniques, including nuclear magnetic resonance, absorption and fluorescence spectroscopies and mass spectrometry. Density functional theory calculations confirmed that the trans isomer is the most stable for both chlorins, corroborating nuclear magnetic resonance findings. The reaction mechanisms were elucidated, revealing the potential formation of multiple products from the interaction of formaldehyde units with the amino acids cysteine or homocysteine. Chlor-CSH_trans exhibited enhanced stability, potentially due to the formation of a six-membered ring. In dimethylformamide, Chlor-CSH_trans demonstrated a slightly higher molar absorption coefficient at 650 nm, but a lower fluorescence quantum yield compared to Chlor-SH_trans. Interestingly, Chlor-SH_trans showed enhanced singlet oxygen production, attributed to a higher value of spin-orbit coupling and higher triplet state stability. Neither chlorin exhibited significant aggregation or photodegradation at the studied concentrations, indicating promising properties for photodynamic applications.

HIGHLIGHTS

METAL COMPLEXES WITH A TWIST: MODIFIED RHODAMINES AS A PROMISING THERANOSTIC APPROACH FOR COMBATING CANCER

Dalton Trans. (2025) 54, 9472–9482

Rhodamines have been recognized for their exceptional optical properties, making them suitable for detection, imaging, and disease diagnosis. However, their use as photosensitizers in Photodynamic Therapy (PDT) has been limited by their low singlet oxygen production and limited tissue penetration. The development of rhodamine-metal complexes has overcome these limitations, offering a promising new approach for cancer treatment. These complexes in combination with structural and optical tuning of rhodamines, have been engineered to enhance tumour cell selectivity, improve reactive oxygen species (ROS) generation, and mitochondrial-targeted delivery. Notably, a variety of metal ions, including iridium(III), ruthenium(II) and platinum(II/IV) can form complexes with bright rhodamines with excellent optical responses and remarkable ROS generation. These breakthroughs have the potential to improve cancer diagnosis and therapeutic applications. Photophysical properties, photostability, and targeting agents, particularly in the near-infrared (NIR) range, will be discussed, with a focus on their applications in cancer detection, localization, and cytotoxicity.



TARGETED STRATEGIES TO ADDRESS INTRACELLULAR INFECTIONS.

Antimicrobial resistance is a major global health challenge, responsible for approximately 1.27 million deaths annually, highlighting the urgent need for alternative therapeutic strategies. Given the essential role of iron in bacterial metabolism, iron deprivation has emerged as a promising non-antibiotic approach to infection control.

This work aimed to develop macrophage-targeted nanocarriers to shuttle iron chelators into bacteria and fight intracellular bacterial infections by means of Fe deprivation.

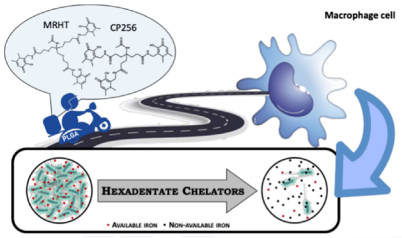
Previous work demonstrated that rhodamine-derived hexadentate 3,4-hydroxypyridinone chelators effectively inhibited bacterial proliferation, particularly the intramacrophagic growth of Mycobacterium avium. However, toxicity associated with the rhodamine moiety motivated the development of safer chelators lacking this structural unit.

Nanoparticle-based delivery systems offer a powerful strategy to overcome the limitations of non-encapsulated chelators. Direct administration is hindered by their high affinity for biological iron and cell membranes, which can limit macrophage uptake. Encapsulation within functionalized nanoparticles is expected to promote targeted delivery to infected macrophages, enabling efficient iron scavenging within phagosomes.

Encapsulation of two chelators into nanoparticles was achieved, their biocompatibility was assessed, and surface functionalization to enhance macrophage uptake was explored. The results demonstrated efficient encapsulation and improved cellular internalization. As far as we know, this represents the first report on the encapsulation of 3,4-hydroxypyridinones into nanoparticles for antibacterial applications.

A Macrophage-Targeted Strategy to Address Intracellular Infections.

Journal of Drug Delivery Science and Technology, 2026, 115, 107645.

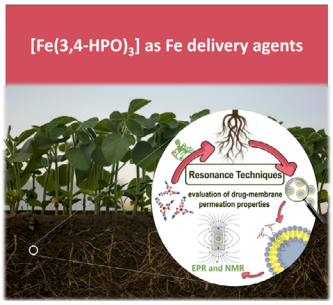


HIGHLIGHTS

DESIGN OF FE FERTILIZERS TO ADDRESS IRON DEFICIENCY CHLOROSIS

Ligands of the 3-hydroxy-4-pyridinone (3,4-HPO) class are eligible to formulate new Fe fertilizers for Iron Deficiency Chlorosis (IDC). The 3-hydroxy-4- pyridinone Fe-chelates, [Fe(mpp)3], [Fe(dmpp)3], and [Fe(etpp)3], are able to provide Fe and prevent IDC as shown in a model of Soybean (Glycine max L.) plants grown in hydroponic conditions and supplemented with Fe-chelate.

Results regarding the effectiveness of the [Fe(3,4-HPO)$_3$] chelates to prevent IDC demonstrate that: (a) all three chelates are able to deliver Fe to plants and (b) their efficacy is dependent on the ligand following the order [Fe(mpp)$_3$]> [Fe(dmpp)$_3$]> [Fe(etpp)$_3$]. Chelate [Fe(mpp)$_3$] provides the best effect as shown by the morphological, physiological, and gene expression parameters while [Fe(etpp)$_3$] shows the poorer performance. From EPR biophysical studies using spin probes and liposomes, prepared from a soybean lipid extract, we hypothesize that the distinct efficacy may be related with the different preferential location close to the surface or on the hydrophobic region of the lipid bilayer.



An experiment using artificial soil allowed establishment of the timeline, methodology and procedure of Fe supplementation for plant growth in agricultural soil. Results showed that foliar application of chelate [Fe(mpp)3] has a longer lasting effect than the commercially available products, induces efficient root responses and produces fruits with an increased Fe content. Concomitantly, application of the Fe chelate promotes a better uptake of other nutrients by the plant.

Plants treated with nanofertilizers, prepared by encapsulation of [Fe(dmpp)$_3$] chelate in polymeric nanoparticles, showed an improvement in morpho-physiological and genetic traits and an increase in relevant gene expression. The results illustrate the potential of the developed nanofertilizers as a seed-soaking agent, promoting plant growth, reducing IDC, and activating molecular-level iron availability responses.

A combined physiological and biophysical approach to understand the ligand-dependent efficiency of 3-hydroxy-4-pyridinone Fe-chelates.

Plant Direct, 2020, 4, e00256

Foliar application of 3-hydroxy-4-pyridinone Fe-chelate [Fe(mpp)3] induces responses at the root level amending iron deficiency chlorosis in soybean.

Physiologia Plantarum, 2021, 173, 235-245

NMR and EPR study of the interaction of tris(3-hydroxy-4-pyridinonato) Ga(III) complexes with liposomes that mimic plant membranes.

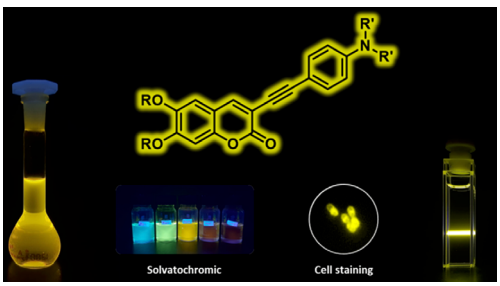
Biophysical Chemistry, 2023, 298, 107021.

Novel polymeric nanoparticles as nanofertilisers for alkaline iron-deficient conditions.

Plant and Soil, 2025, 514, 1263-1283.

SUCCESSFUL MEMBRANE LABELLING OF S. PNEUMONIAE BY COUMARIN DYES PRESENTING ELECTRON-DONATING AMINOPHENYL GROUPS.

Three new coumarin dyes with an inverse push-pull architecture were synthesized and showed similar absorption behavior while a positive solvatochromic response was present in their emission spectra in different solvents. They present no toxic in bacterial membrane staining experiments, with two of them effectively labelling S. pneumoniae. One of the dyes performed similarly to Nile Red, while the other possessed a more selective distribution. Future work will explore how structural changes affect dye behavior across different bacterial membranes.

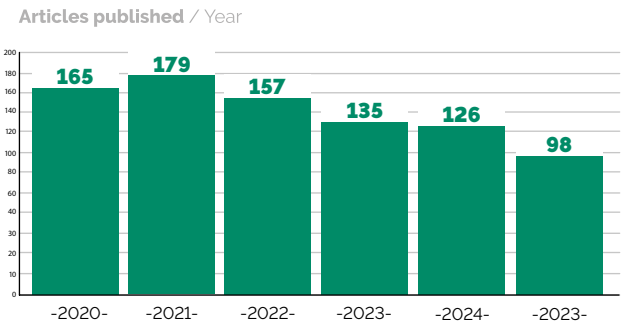


Synthesis of inverse push-pull coumarin dyes and their application as solvatochromic probes and labelling agents for bacterial cell membranes

Dyes Pigm., 2024, 228, 112204

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION



H-index: **45**

860 articles*
15313 citations

***01/2020-12/2025**
From WOS core collection

FUNDED PROJECTS *(Representative projects)*

- **MYCOPEPTALKING – Optimizing Antimicrobial Peptides using cutting-edge strategies to combat infections caused by non-tuberculous mycobacteria.**
  PTDC/BIA-MIC/3458/2020. April 2021 – March 2024; participated by Paula Gomes and Ana Gomes (team members). Total funding: € 249,984.88
- **AMAZING – AMAZonian snake toxins: creatING value from bioresources**
  CIRCNA/BRB/0281/2019; September 2020 – February 2024; led by Paula Gomes (PI) and participated by Cátia Teixeira and Ana Gomes (team members). Total funding: € 298,857.55
- **Marine Chemiluminescence as a Broad Spectrum Anticancer Therapy with Enhanced Tumor Selectivity and Activity**
  MPTDC/QUI-QFI/2870/2020. January 2021 – June 2024; led by José Enrique Borges (local PI). Total funding: € 249,496.16
- **DrosuGreen - Controlling the quarantine pest Drosophila suzukii through epidemiological studies and new green biocontrol techniques**
  PTDC/ASP-PLA/4477/2020. March 2021 – February 2025; participated by Paula Gomes and Cátia Teixeira (team members). Total funding € 249,654.62)
- **SMASK – Smart Mask with colorimetric biosensor for SARS-CoV-2 contamination and humidity**
  POCI-01-02B7-FEDER-070241. November 2020 – November 2021; participated by Ricardo Ferraz (team member). Total funding € 202,624.29
- **KIWIBOL – Looking Beyond KIWIfruit ESCA Complex to Define a PeptaiBOL-based Strategy to Disease Control**
  PTDC/ASP-PLA/2440/2021. April 2022 – March 2025; initially led by Cátia Teixeira, then by Maria João Araújo (PIs); participated by Paula Gomes (team member). Total funding: € 234,932.00
- **NovInDog - New Functional Ingredients for Dog Food: A Sustainable Approach**
  POCI-01-0247-FEDER-047003. February 2021 – June 2023; participated by Paula Gomes and Ricardo Ferraz (team members). Total funding € 585,041.96
- **STOP.SUZUKII - Operational tool to improve blueberry production and combat damage caused by Drosophila suzukii**
  POCI-01-0247-FEDER-047034. January 2021 – June 2023; participated by Paula Gomes and Cátia Teixeira (team members) Total funding: € 625,186.72
- **VINEPROTECT - Ecological survey for the biological management and protection of Mediterranean vineyards in the face of climate change**
  PRIMA/0011/2021. March 2022 – March 2026; participated by Paula Gomes and Cátia Teixeira (team members). Total funding € 216,833.00
- **A peptide-decorated anti-microbial and pro-healing hyaluronic acid dressing to promote diabetic wound healing**
  EFSD Lilly European Diabetes Research Programme 2022. January 2024 – December 2024; led by Paula Gomes (local PI) and participated by Ana Gomes (local team member). Total funding € 100,000.00
- **Smart4Vir - Smart surfactant-based nanovectors for RNA anti-viral therapeutics**
  2022.05543.PTDC. February 2023 – July 2026; participated by Luísa do Vale and Bárbara Sampaio (team members). Funding REQUIMTE € 64,305.96
- **DynaPro - Probing Dynamic Chirality to the Rescue of Melanostatin in Parkinson's Therapy**
  2022.01175.PTDC. March 2022 – December 2024; led by Ivo Dias (PI). Total funding: € 49,997.55,
- **Ionic liquid-modified peptidomimetics as a key tool towards in situ forming hydrogels for the topical treatment of diabetic foot ulcers**
  2023.12331.PEX. January 2025 – June 2026; led by Ana Gomes (PI), participated by Paula Gomes (team member). Total funding: € 50.000,00,
- **Pep2mer - Pep2mer: Melanostatin Peptide-Peptoid Hybrids: A Tailored Pharmacological Strategy to Tackle Parkinson's Disease**
  2023.14440.PEX. January 2025 – June 2026; led by Ivo Dias (PI). Total funding: € 50,000.00,
- **PepTRAP - An Innovative Pharmacological Approach to Tackle Parkinson's Disease**
  BIP PROOF 2024/2025. January 2025 – December 2025; led by Ivo Dias (PI). Total funding: € 10,000.00
- **PEPILSKIN - PEPtides Ionic Liquids for SKIN**
  BIP PROOF 2024/2025. January 2025 – December 2025; led by Ricardo Ferraz (PI). Total funding € 10,000.00,
- **LitCure - Lithocholic Acid Derivatives for Application in Triple-Negative Breast Cancer Therapy**
  BIP PROOF 2025/2026. January 2026 – December 2026; led by Ivo Dias (PI). Total funding: € 10,000.00,
- **Silanol - Silanol-Based Lithocholic Acid Derivatives as Super Agonists of Vitamin-D Receptor for Application in Breast Cancer Therapy**
  COMPETE2030-FEDER-00881500. September 2025 – August 2028; led by José Enrique Borges (PI). Total funding: € 212,461.92

GROUP IN NUMBERS

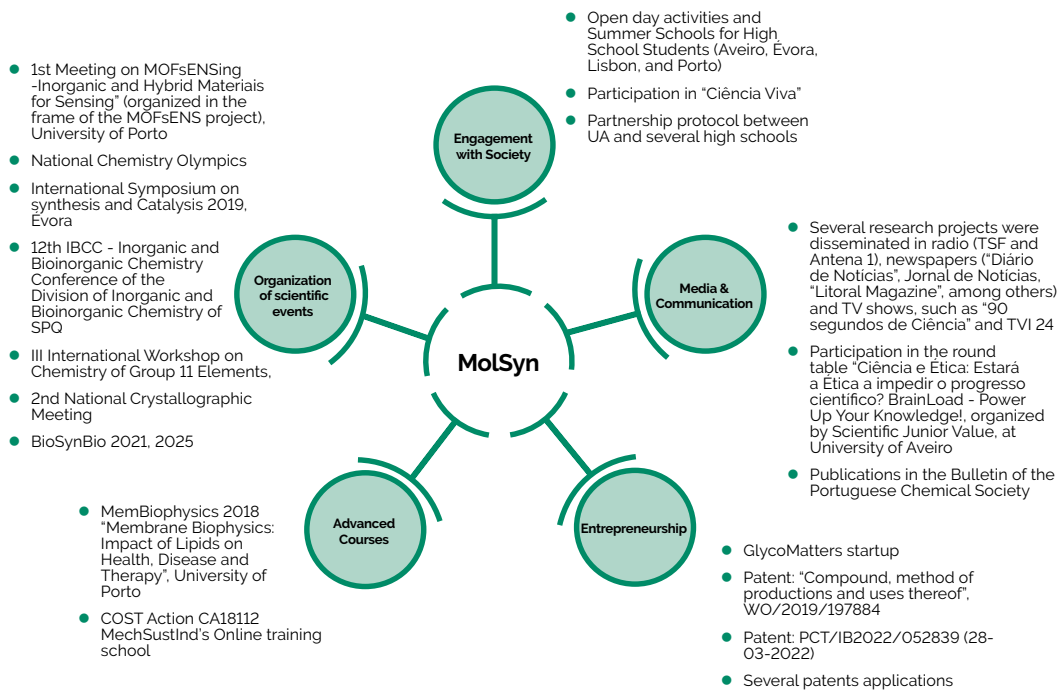
FUNDED PROJECTS *(Representative projects)*

- **INPEPTICIDE – INvesting in natural PEPTIdes as biopestiCIDEs to control the American grapevine leafhopper.**
  COMPETE2030-FEDER-00673200. October 2025- September 2028; led by Paula Gomes (PI), participated by Maria João Araújo, Ricardo Ferraz and Renato Pereira (team members). Total funding: € 212,498.64
- **Plastics To Nanomaterials: From waste bottles to MOF nanomaterials in a sustainable approach – Plas2Nano**
  Funded by Fundação para a Ciência e a Tecnologia, PI: Ana M. G. Silva (REQUIMTE), Amount: 49.502,38 €
- **One-pot bimetallic catalyzed synthesis of challenging N-heterocycles**
  PTDC/QUI-QOR/0712/2020, April 2021 – March 2025, Maria Manuel Marques (PI). Total Funding: € 247.034,00
- **PAGE – Protein aggregation across the lifespan**
  Centro-01-0145-FEDER-000003, Centro2020, Artur Silva (PI). Funding: € 569,787.00. Total Funding: € 1,598,206.47
- **MOFsENS – Synthesis of metal-organic frameworks as optical gas sensors**
  M-ERA.NET, Ana Margarida Silva (Local PI). Funding: € 177,732.00. Total funding: € 533,625.00
- **Organic Redox Mediators for Energy Conversions**
  PTDC/QUI-QOR/7450/2020. March 2021- December 2024, Principal investigator: Paula Branco. Total Funding: € 248.344,28
- **Smart Ligands for Manganese Catalysis**
  PTDC/QUI-QIN/0359/2021. April 2022 – December 2025. Co-PI: Maria Manuel Marques. LAQV funding: € 47,000.00
- **Novel C-glycosylated oxygen and nitrogen heterocyclic compounds as potential epigenetically active immunestimulatory anticancer agents**
  PTDC/QUI-QOR/29767/2017. Artur Silva (PI). Total Funding: € 239,581.00
- **Hi2E-Synth - Synth: Hypervalent iodine to expand the chemical space and access synthetic N-containing molecules**
  FCT.2022.04623.PTDC. April 2023 – March 2027, Principal investigator: Maria Manuel Marques. Total funding: € 200.000,00
- **CellMembrane - HORIZON-EIC-2023-PATHFINDEROPEN-01**
  March 2025 – November 2026. Principal investigator: Ricardo Chagas and Luisa Ferreira (co-PI).Total Funding: € 489 785.00
- **Resilcrops - Interreg Atlantic - EAPA_0100/2024 - Harnessing Circular Economy to Improve Crop Resilience in the Atlantic Area**
  October 2025 – September 2028. Ricardo Chagas (co-PI). Total funding: € 387.000,00
- **Aero2Cycle - Hydrid aeropils for CCU**
  November 2025 – October 2028. Ricardo Chagas (co-PI). Total funding: € 209.896,00,
- **ACHIEVE -Development of orthogonal synthetic methodologies to obtain cellulose derivatives with differentiated structure and properties**
  2022.02917.PTDC, Luisa Ferreira (PI). Funding: € 49 977,21,
- **CAR T-Matters - Transforming the CAR T-cell therapy landscape in Portugal**
  February 2025 – January 2028, Florbela Pereira (Coord at LAQV). Funding: € 282274,08 (Joint Budget UCIBIO/LAQV),
- **DCMatters**
  LISBOA2020, Nº 47212 (2021-2023), July 2021 – June 2023. Florbela Pereira (Coord at LAQV). Funding: € 413,200.00 (Joint Budget UCIBIO/LAQV).
- **ProDGNE**
  EJPRD/0001/2020 (2021-2024), April 2021 – March 2024. Florbela Pereira (Coord at LAQV). Funding: € 250,000.00 (Joint Budget UCIBIO/LAQV),
- **Funcionalização estéreo-seletiva e aumento de complexidade de ácido quínico por transferência de hidrogénio e oxidação**
  Nuno Candeias 1AQ+i/PTDS/QUI-QOR/1131/2020 162 139.95€.
- **MuTaTher-AD**
  2022.06064.PTDC Artur Manuel Soares da Silva. Entidade Coordenadora: Universidade de Aveiro Data de Início: 01-02-2023 Data de conclusão: 31-01-2026, Custo total elegível UA: 243,546.46€.
- **Domando radicais pela libertação do potencial sintético de bis(silil)peróxidos**
  BiSiPe4Tame/COMPETE2030-FEDER- 00753500 Nuno Candeias. Data de Início: 15-07-2025 Data de conclusão: 14-07-2028. Custo total elegível UA: 206 712.0€.
- **Sensibilizadores de ftalocianina baseados em sistemas de impulso-atração para células solares de perovskita**
  eDyeCell/COMPETE2030-FEDER-00799000 Leandro Lourenço. Data de Início: 01-10-2025 Data de conclusão: 29-09-2028. Custo total elegível UA: 249 998.4€.
- **GERMINAR - Novel Functional Food products to Reach Nutrient Needs: from Nano-Enriched Plant Sprouts to Salads and Fruit-based products**
  project 15854 (COMPETE2030-FEDER-00696700), COMPETE, September 2025- August 2028, Principal investigator: Tânia Moniz, ~206k€.
- **eQuaNTI: An enzymatic assay for the determination of blood serum non-transferrin-bound iron**
  2022.06328.PTDC, FCT, January 2023- July 2024, Principal investigator: André Silva, Co-PI: Baltazar de Casto, ~50k€.
- **NANOFERTIL - Cellulose-based iron nanofertilizers for sustainable growth of soybean plants**
  EXPL/QUI-QIN/0411/2021, FCT, January 2022- December 2023, Principal investigator: Tânia Moniz, Co-PI: Baltazar de Castro, ~50k€.

INTERNATIONAL COOPERATION AND NETWORKING

- COST action CA23111 "SNOOPY - Searching for Nanostructured or pOre fOrming Peptides for therapY" (2024-2028) - Vice-chair
- Bilateral Cooperations with Brazil, Morocco, Algeria and France,
- International Cooperation with several research centres and universities from: Algeria, Austria, Brazil, Ecuador, France, Germany, Italy, Macau, Spain, United Kingdom, United States of America, Finland, Bulgaria and Canada.
- COST ACTIONS 17104, 18132, 18112 (Grant Awarding Coordinator, Gender Balance Coordinator, Core Group member), CA21101, CA22107 (Communication team, Gender Balance representative and Compound Tracker) and CA22147 (WG1 and WG3 member, EU4MOFs Round Robin Test: MOF characterization – co-coordinator)
- PRIMA Project: VINEPROTECT (Project-PRIMA/0011/2021)
- Project Erasmus Mundus Joint Master "ChEMoinformaticsplus - Artificial Intelligence in Chemistry" (Project 101050809
- Bilateral Cooperation Portugal-France: Project FCT- PHC-Pessoa 2019-2021 "Big data exploration of the chiral chemical space with new molecular descriptors"
- Bilateral Research Programme with the project "Plastics to Sensors: Recycling PET plastic waste into nanomaterials for optical sensors development" Institutions involved REQUIMTE UPorto and Liverpool John Moores University (UK), funded by FCT and PARSUK
- IACOBUS programme participation in diffferent editions
- EFSD Lilly Europeand Diabetes Research Programme
- European Peptide Society (EPS) Mobility Grants Programme
- Fullbright and FCT/PARSUK programmes

DISSEMINATION & OUTREACH



LABORATÓRIO ASSOCIADO
PARA A **QUÍMICA VERDE**

CHEMBIO

NATURAL PRODUCTS CHEMISTRY AND BIOACTIVITY

OVERVIEW & OBJECTIVES

Group Coordinators:

Conceição Santos

RESEARCH OVERVIEW

The Chemistry and Bioactivity (CHEMBIO) group comprises the expertise of a wide interdisciplinary team working in synergy towards the common goal of discovering, characterizing, and valorizing new chemical entities, whether naturally occurring, modified, or synthesized through (hemi)synthesis, and their application in health, agri-food, and other biotechnological fields. The group evaluates new candidate products for structure, bioactivity, and biosafety. We use multidisciplinary tools from chemistry, biology, and health sciences. Among natural sources, we highlight products from plant, algae, and animal origins. We study biochemical signaling and networking that regulate compound bioactivity in cells and in holobiont's homeostasis.

The CHEMBIO group gathers analytical and (in) organic chemistry, biochemistry, pharmacy, phytochemistry, microbiology, molecular biology, biotechnology, and biology experts from several institutions. In particular, our expertise includes diagnosis, imaging, genomic and transcriptomic profiling of target organisms, as well as proteomic analysis of pharmacological and health processes. This expertise is directed toward the discovery, characterization, and application of bioactive compounds, focusing on: (i) the prevention and treatment of human diseases (cancer, diabetes, as well as inflammatory and neurodegenerative disorders), and (ii) innovation in agri-food processes and environmental safety, (iii) the understanding of holobiont's networking and homeostasis, (iv) the development of biotechnological processes for product valorization and sustainable applications.

Researchers are organized into research teams that share top infrastructures and know-how among their laboratories. CHEMBIO's expertise and recognition is further reinforced by active participation in international networks of excellence, enabling high-impact, interdisciplinary collaborations that translate fundamental knowledge into innovative solutions for global challenges in health, biotechnology, and the agri-food sector.

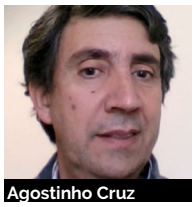
RESEARCH OBJECTIVES [2025-2029]

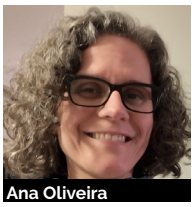
The major research objectives of the Chemistry and Bioactivity Group are:

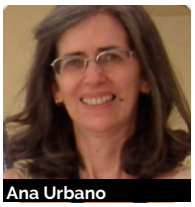
- Development and application of chemical and instrumental methods for the study of natural matrices;
- Development of green hemi-synthetic processes for obtaining novel bioactive molecules;
- Chemical, biological, and pharmacological characterization of natural and (semi-) synthetic compounds, with a focus on drug discovery for cancer, metabolic, inflammatory, and neurodegenerative disorders;
- Elucidation of mechanisms linking bioactive compounds to the modulation of key pathophysiological pathways
- Design and development of plant-based strategies nature-inspired nanoparticles and delivery systems, including in vitro and in vivo evaluation of their bioactivity and biosafety for applications in agri-food and health;
- Investigation of the impact of emerging stressors, including nanoparticles and endocrine-disrupting chemicals, on cellular metabolism and biochemical pathways in the context of metabolic diseases, using relevant biological models;
- Discovery and mechanistic validation of natural compounds, as protective agents against xenobiotic-induced redox and inflammatory imbalance;
- Exploit new bioactive compounds on microbiota taxa and their impact on microbiota homeostasis;
- Develop biotechnological solutions (e.g., SynComs), based on compatibilities and bioactivity of microbiota taxa.

RESEARCH TEAM

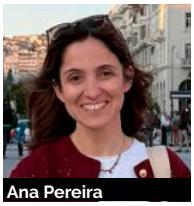
SENIOR RESEARCHERS


Agostinho Cruz

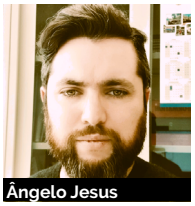

Ana Oliveira

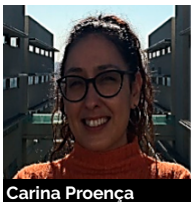

Ana Urbano

Ana Canadas Sousa


Ana Pereira

Andreia Gonçalves


Ângelo Jesus


Carina Proença

Carlos Monteiro

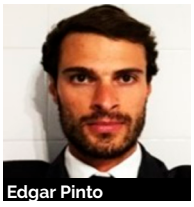
Carmen Pereira

Cláudia Pinho

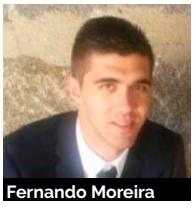
Conceição Santos

Diana Pinto

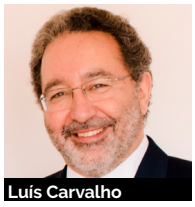
Diana Silva


Edgar Pinto

Eduarda Fernandes


Fernando Moreira

Lucília Saraiva


Luís Carvalho

Manuela Morato

Marcelo Catarino

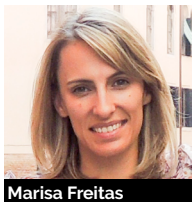
Jennifer Fadoni

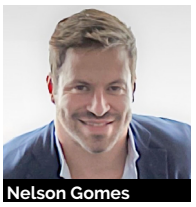
Marlene Santos

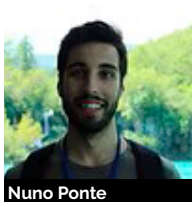
M. Amparo Faustino

M. Paula Marques

Maria Ramos Silva


Marisa Freitas

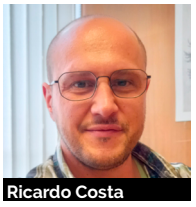

Nelson Gomes


Nuno Ponte

Patrícia Pereira

Patrícia Valentão

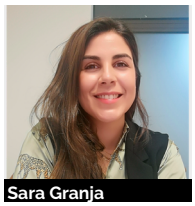
Paula B. Andrade


Ricardo Costa

Romeu Videira

RESEARCH TEAM

SENIOR RESEARCHERS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Sílvia Coimbra

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Mariana Lucas
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Ricardo Ferreira
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Rui Gonçalves

RESEARCH THEMES/
IDENTIFICATION, ISOLATION AND MODIFICATION OF BIOACTIVE NATURAL PRODUCTS

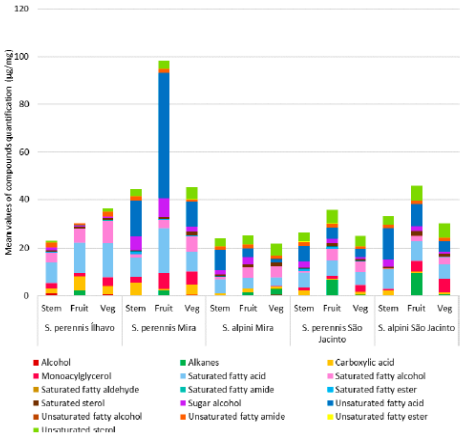
The exploration of natural products has historically been one of the most successful strategies for discovering new drugs, offering fundamental chemical structures that act as direct drugs or as templates for synthetic development. The CHEMBIO group enhances this strategy by combining ethnomedicinal knowledge with cutting-edge analytical technologies.

CHEMBIO methodology is based on metabolic profiling and detailed chemical characterization (using advanced techniques such as HPLC-DAD-ESI/MSn, UHPLC-ESI/QTOF/MS), GC-MS, FTIR, and RMN/EPR, supported by other techniques like imaging and omics.

This process ensures the authenticity and safety of natural matrices — crucial for human nutrition and therapeutics — and allows the identification of novel chemical scaffolds.

By establishing experimental evidence between chemical constituents (such as alkaloids, sterols, and phenolics) and their biological properties, the group prioritizes compounds with high pharmacological potential. As example, we highlight ethonotanical studies grounded on global collaboration networks — spanning regions such as Europe, Africa, South America, Europe, and Asia — the group investigates taxa organisms (eg plants) used in folk medicine, but which are still underexplored in terms of their bioactive constituents and potential in controlling chronic diseases such as cancer, diabetes, and neurodegenerative disorders.

In this way, CHEMBIO researchers remain at the forefront of developing and validating chromatographic and omics' applied to diverse sources, from terrestrial and marine organisms to agro-industrial waste. This multidisciplinary approach, which ranges from structural elucidation to pharmacological evaluation, allows the consolidation of a robust platform for innovation in new drugs, functional foods, and cosmetic formulations, transforming ancestral knowledge and biodiversity into high-impact scientific solutions.



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RESEARCH THEMES/
DRUG DISCOVERY FOR HUMAN HEALTH

ANTICANCER DRUG DISCOVERY

Drug discovery from natural sources and hemi-synthetic molecules is a pivotal theme to BIOCHEM, and covers the evaluation and mechanisms of action of molecules with potential use in cancer. We develop studies on

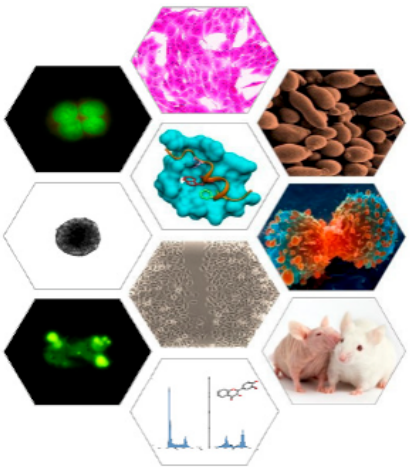
• Assessing the anticancer effects of small molecules on the impact upon mitochondrial function/status, caspase-activating capacity, p53 activity and expression, calcium dynamics, and chromatin status.

• model systems like the Saccharomyces cerevisiae (has a high degree of conservation of cellular processes and molecular pathways to human cells) are powerful models to study human proteins and molecular mechanisms underlying the pathobiology of human diseases. If the gene encoding the protein of interest is conserved in yeast, its function can be directly studied in this model, but if the gene has no orthologues in yeast, its study is still possible by heterologous expression. This so-called humanized yeast model is widely used by our group for biological and pharmacological studies of human proteins with a key role in cancer. Previous yeast models, and new yeast strains with humanized genes, will be constructed and used in association with yeast cell-based as approaches to discover new therapeutics for cancer.

• Osteosarcoma research, with focus on the cytotoxic and cytostatic actions of polyphenolic compounds, including drug combination, and the study of cell cycle regulation.

• 2D and 3D immortalized and patient-derived cancer cells and xenograft mice.

• Cytotoxicity evaluation of newly designed polynuclear metallodrugs (Pt-, Pd-, Ni-based) with biogenic polyamines, on human cancer cells, and mice. Metabolic impacts are measured by vibrational spectroscopy, microRaman, microFTIR (including synchrotron radiation), and neutron scattering (INS, QENS).



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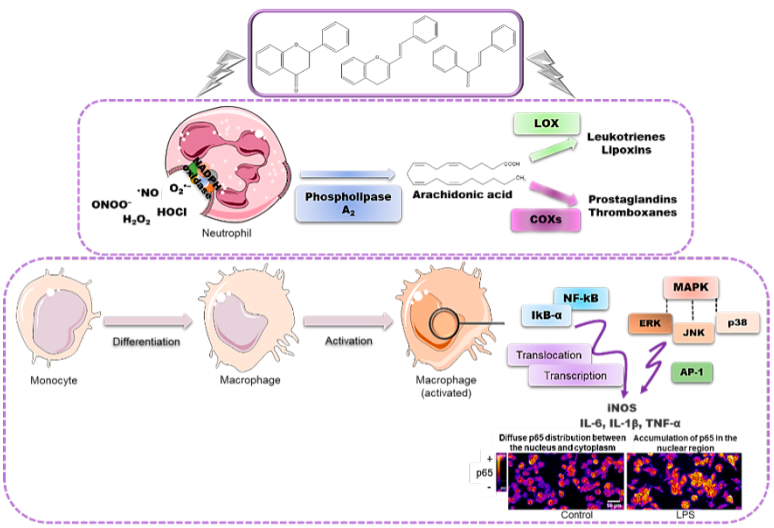
RESEARCH THEMES/
DRUG DISCOVERY FOR HUMAN HEALTH

ANTI-INFLAMMATORY DRUG DISCOVERY

In physiological conditions, inflammation is a tightly regulated and self-limiting process. However, impaired resolution and persistent activation of inflammatory pathways underlie a wide range of pathological conditions, affecting virtually all organ systems. These include classical autoimmune diseases (e.g., rheumatic diseases and psoriasis), as well as metabolic disorders such as diabetes, inflammatory bowel disease, cardiovascular diseases, and neurodegenerative disorders.

Despite the availability of anti-inflammatory therapies, current pharmacological options are often associated with significant side effects and remain insufficient to curb the growing incidence and prevalence of chronic inflammatory conditions. In this context, researchers within the CHEMBIO group have been actively engaged in the identification and development of novel bioactive compounds capable of modulating inflammatory responses, particularly through the regulation of redox homeostasis. Natural and synthetic molecules have been evaluated on their ability to modulate key targets in the inflammatory process, including enzymes (e.g. NADPH oxidase, lipoxygenases, elastase), and cellular signaling cascades (e.g. nuclear factor NF-kB and MAPK pathways) with a key role in the expression of pro-inflammatory mediators such as interleukins, TNF- and inducible nitric oxide synthase (iNOS).

To study the impact of naturally-derived and synthetic compounds on the crosstalk between oxidative stress and inflammation, researchers use several cellular models (human, murine) and non-cellular systems as research tools, gathering biochemical, functional, and molecular/omics complementary tools.



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RESEARCH THEMES/
DRUG DISCOVERY FOR HUMAN HEALTH

RETHINKING METABOLIC DISEASES: THE ROLE OF NUTRITION AND BIOACTIVE COMPOUNDS

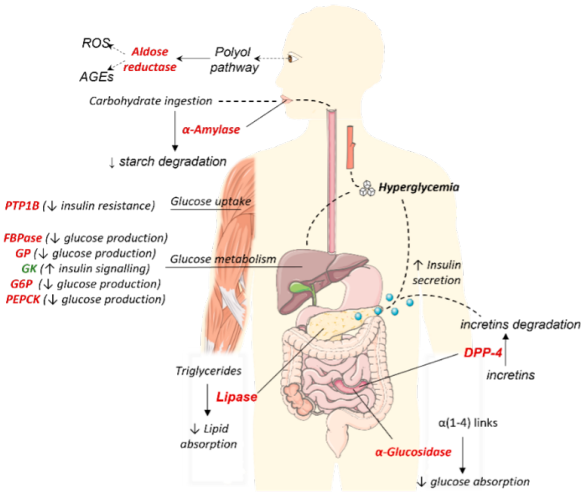
Nutritional functions are associated with metabolic diseases, including diabetes and obesity, some of which are leading causes of disability and death worldwide. These conditions are influenced by nutritional and lifestyle factors shaping metabolic risk and disease progression. BIOCHEM researchers are integrated into international networks that contribute to a better understanding of disparities in risk factors and disease burden across populations. Dysregulation of glucose and lipid metabolism, such as excessive hepatic glucose production and impaired insulin signaling, plays a central role in metabolic dysfunction. These alterations are closely linked to dietary patterns and nutrient exposure, reinforcing the importance of nutrition in the onset and progression of metabolic diseases.

Despite therapeutic advances, current pharmacological options remain limited in efficacy and are often associated with adverse effects, highlighting the need for safer and more effective strategies.

The group integrates a strong nutritional research component, focusing on the role of diet and bioactive food compounds in the prevention and management of metabolic diseases, bridging molecular mechanisms with real-life dietary exposure. Polyphenols emerge as promising multitarget agents capable of modulating key pathways involved in metabolic diseases. We focus on the study of polyphenols, targeting relevant enzymes and pathways such as -glucosidase and pancreatic lipase (regulation of carbohydrate and lipid absorption), DPP-4 (incretin metabolism), and PTP1B (insulin signaling), as well as cellular pathways involved in glucose uptake and metabolic homeostasis.

Their bioactivity has been evaluated using in vitro and in vivo models, demonstrating the ability to improve glycaemic control, modulate lipid metabolism, and enhance insulin sensitivity.

To further support drug discovery efforts, research also includes the design and synthesis of polyphenol-based compounds aimed at enhancing bioactivity and targeting multiple pathways involved in metabolic disorders.



Legend:
AGEs: Advanced glycation end-products
DPP-4: Dipeptidyl peptidase-4
FBPase: Fructose 1,6-bisphosphatase
GK: Glucokinase
G6P: Glucose 6-phosphate
GP: Glycogen phosphorylase
PEPCK: Phosphoenolpyruvate carboxykinase
PTP1B: Protein tyrosine phosphatase 1B
ROS: Reactive oxygen species
inhibition
activation
insulin

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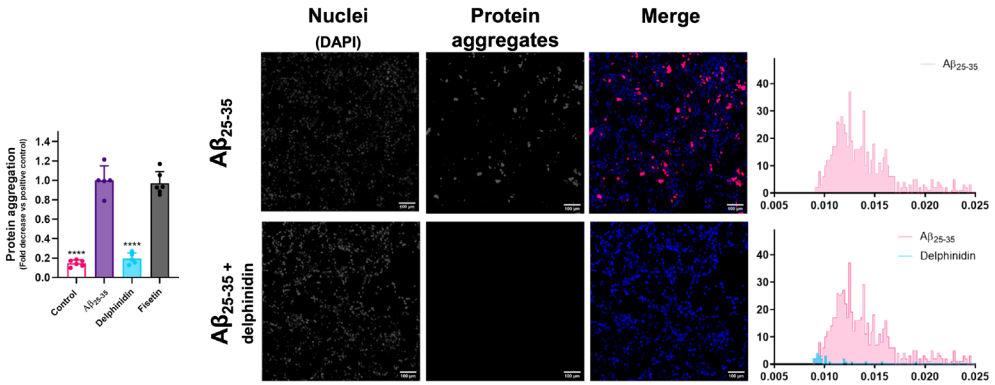
RESEARCH THEMES/
DRUG DISCOVERY FOR HUMAN HEALTH

NEUROLOGICAL DISORDERS AND DRUG DISCOVERY

The group is focused on the initial events of brain degeneration in the context of diseases like Parkinson's and Alzheimer's (PD and AD). Cell-based and murine models of PD and AD have been used to investigate the molecular mechanisms underlying the role of endoplasmic reticulum stress, the unfolded protein response and the cellular processes involved in proteostasis. Some attention has also been given to the functional organization of the mitochondria and overall cellular fitness. Large libraries of natural molecules were evaluated for their ability to counter or prevent some of the events ultimately resulting in protein aggregation. The best-performing molecules were then evaluated in a neuronal model of A-induced proteotoxicity, which allowed the identification of several small molecules capable of countering these pathological events.

The development of lipid-based nanocarriers for oral and nasal administration and delivery of phytochemicals to selected cellular targets is also under investigation.

Other studies related to social and biochemical/functional disorders, including addiction and violence-associated conditions, are also being pursued by researchers in the group. In parallel, advanced biomaterial-based delivery systems, including dissolvable polysaccharide microneedles for neuronal imaging and minimally invasive therapeutic administration, are under development as emerging translational strategies for human health applications.



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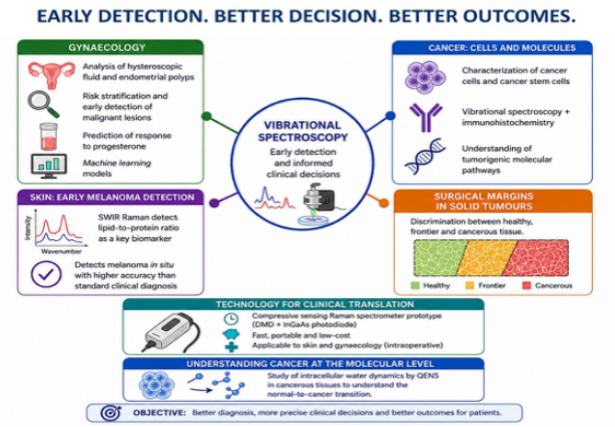
RESEARCH THEMES/
MOLECULAR PATHOLOGY AND DIAGNOSIS

Early diagnosis of pathology through the detection of disease-induced variations in the vibrational profile of human cells and tissues is a central research thread, with applications spanning gynaecological oncology, dermatology and transplant medicine.

Biomarkers of malignancy are identified by microRaman, microFTIR, AFM-IR and synchrotron-based FTIR, complemented by coherent anti-Stokes Raman spectroscopy (CARS) for real-time visualisation of specific vibrational modes in liver graft rejection. In the endometrial cancer context, this approach is being applied to hysteroscopic fluid and fresh polyp tissue sections from asymptomatic postmenopausal women, aiming at the risk-stratification of endometrial polyps and early detection of malignant endometrial lesions, as well as the prediction of responsiveness to progesterone-based treatment-objectives pursued through two independent machine learning classification models. Endometrial cancer cell lines and cancer stem cells enable a more complete characterisation of tumorigenic molecular pathways through vibrational spectroscopy and immunohistochemical analysis.

Assessment of safe surgical margins in solid tumours is equally pursued, where discrimination between healthy, cancerous and frontier tissue regions is sought.

In the field of pigmented skin lesions, Raman spectroscopy in the short-wave infrared (SWIR) has demonstrated the ability to detect the lipid-to-protein ratio as a key spectral biomarker for early-stage melanoma, including in situ cases, outperforming standard clinical diagnosis. Building on this, a prototype compressive sensing Raman spectrometer — incorporating a digital micromirror device and a single-channel InGaAs photodiode — is under development, targeting translation to the clinics with fast, low-cost and portable operation, applicable both to pigmented skin lesions and to gynaecological screening in an intraoperative setting. Finally, the dynamical profile of intracellular water is investigated by quasi-elastic neutron scattering (QENS) measurements on cancerous human tissues, aiming at a deeper understanding of the normal-to-cancer transition at the molecular level.



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RESEARCH THEMES/
EMERGING ENVIRONMENTAL STRESSORS: FROM BIOLOGICAL MECHANISMS TO BIOACTIVITY AND SAFETY

We investigate agrifood systems' health through the lens of host-microbiome interactions, focusing on signaling pathways and the identification of novel bioactive molecules capable of restoring microbiome homeostasis and improving host performance. This is achieved by integrating genomic, transcriptomic, and metabolomic approaches to understand the dynamic responses of both host and microbiome under (a)biotic stress conditions.

The group explores the discovery, characterization, and safety of emerging compounds across multiple biological systems (animals, plants, soil, and aquatic environments), with particular emphasis on the:

• Bioactivity and toxicological profiling of nanoparticles (NP) in diverse matrices and organisms;

• Impact of environmental contaminants, including endocrine-disrupting chemicals (EDCs), on biological systems, microbiome composition, and ecosystem health, and contribution to metabolic diseases;

• Role of biomolecules (e.g., proteins) in regulating plant and microbial growth and reproduction;

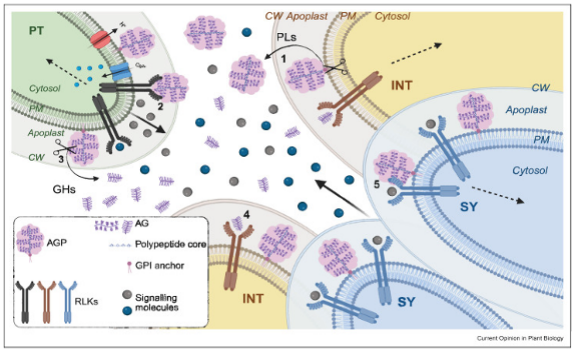
• Application of antimicrobial peptides (AMP) and microorganisms as Biocontrol Agents to manage pests;

• Development of innovative solutions, such as NP or microbial-derived extracts, to enhance crop resilience (e.g., drought tolerance) and support environmental remediation;

• Assessment of bioactivity, ecological safety, and resistance acquisition, with new (nano)compounds

• Effects of emerging compounds on microbiome dynamics and overall environmental safety.

Aligned with the One Health framework, we develop sustainable biotechnological solutions that address interconnected challenges in agrifood systems, environmental health, and human well-being. This includes strategies to mitigate antimicrobial resistance, improve crop productivity/yield for sustainable agricultural practices. We also explore mitigation strategies against the adverse effects of NP, through the use of bioactive compounds such as flavonoids, targeting oxidative stress, inflammatory signaling, and metabolic dysregulation of crops in sustainable systems



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97 Biotechnology Advances 2023, 68, 108223. doi: 10.1016/j.biotechadv.2023.108223

98 Sci. Total Environ., 2024, 912, 168664. doi: 10.1016/j.scitotenv.2023.168664

99 Sci. Total Environ., 2024, 945, 173815. doi: 10.1016/j.scitotenv.2024.173815

100 Nature Plants 10 11 (2024): 1607-1609. doi: 10.1038/s41477-024-01818-5

101 Current Opinion in Plant Biology 88 (2025): 102800. doi: 10.1016/j.pbi.2025.102800

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103 Aquaculture 596 (2025): 741882. doi: 10.1016/j.aquaculture.2024.741882

104 Water Emerging Contaminants & Nanoplastics 4 2 (2025). doi: 10.20517/wecn.2024.80

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106 Nanotoxicology (2025): 1-14. doi: 10.1080/17435390.2025.2506586

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108 Microbial Ecology, 2025, 88(1),120. doi: 10.1007/s00248-025-02607-z

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110 Toxicology, 2025, 515, 154125. doi: 10.1016/j.tox.2025.154125

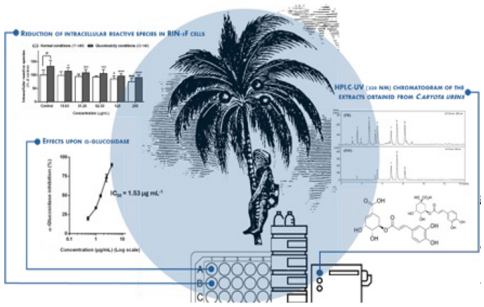
111 Nanotoxicology,2025, 9, 28-49. doi: 10.1080/17435390.2024.2446554

112 Nanotoxicology, 2025, 19, 141–155. doi: 10.1080/17435390.2025.2450372

HIGHLIGHTS

AN ETHNOPHARMACOLOGICAL APPROACH TO THE DISCOVERY AND CHARACTERIZATION OF A NEW FUNCTIONAL INGREDIENT

Kitul (Caryota urens L.) has long been valued as a traditional food and empirically labeled as having antidiabetic properties. These empirical claims have been confirmed with extracts obtained from the inflorescences, which were found to be nearly 70-fold more active than the reference drug acarbose towards -glucosidase. Higher inhibitory efficacy was also corroborated in human intestinal Caco-2 cells. The mode of action is now known to be pleiotropic, as the inflorescences also reduce the overproduction of intracellular reactive species in glucose-stimulated pancreatic RIN-F5 cells, being also able to inhibit a series of pro-inflammatory mediators in macrophages. Effects appear to be partially dependent on a series of antidiabetic and anti-inflammatory constituents, namely six hydroxycinnamic acid derivatives identified in the inflorescences extract.

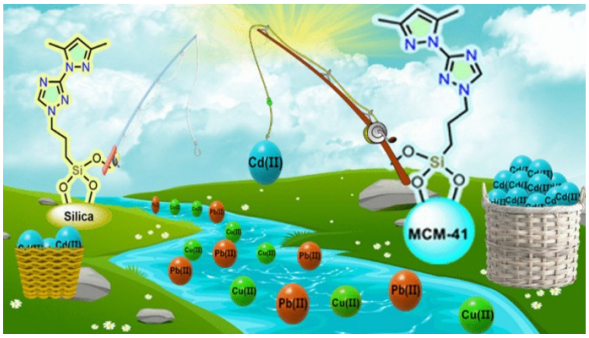


Kitul, a food plant with antidiabetic like effects: Reduction of intracellular reactive species in glucose-stimulated RIN-5F pancreatic -cells and mitigation of pro-inflammatory mediators in activated RAW 264.7 macrophages.

Food Research International, 2023, 167, 112615

DEVELOPING NEW HYBRID MATERIALS WITH HIGH EFFICIENCY TO REMOVE HEAVY METALS IN A REAL SCENARIO

Two novel silica-based hybrid materials (M1, M2), based on silica gel and MCM-41 with a ditopic triazole-pyrazole ligand grafted onto their surfaces, respectively, were synthesized and characterized. The adsorption capacity of these organic–inorganic hybrid materials was evaluated for copper(II), cadmium(II), and lead(II) ions. Adsorption isotherms and models were used to assess the behavior of the adsorbents. Notably, the synthesized materials had exceptional selectivity, ultra-rapid adsorption rates within the first minutes, and high removal towards Cd(II). Also, reusability assessments showed excellent consistency, with only marginal decreases in adsorption capacities over five consecutive cycles. Interestingly, the application of M1 and M2 for the extraction of transition metals from real contaminated river water showed their effectiveness in removing heavy metal ions even at low concentrations. This highlight demonstrates the potential of both materials as reliable systems for heavy metal removal in practical environmental remediation applications, with material M2 demonstrating superior performance over M1.



Tailoring selectivity and efficiency: pyrazolyl-1H-1,2,4-triazole MCM-41 and silica hybrid materials for efficient cadmium(II) removal from water

Environ Sci Pollut Res 32, 10984–11003 (2025)

HIGHLIGHTS

INNOVATIVE SCREENING APPROACHES TO IDENTIFY NEW TARGETING AGENTS OF TUMOR SUPPRESSOR PROTEINS

Innovative yeast-targeted screening approaches were developed to identify new targeting agents of relevant tumor suppressor proteins, e.g., BRCA1/2 and p53. Using human tumor cell lines, xenograft mouse models and patient-derived tumor cells, the antitumor activity of the compounds selected in yeast was validated. The identified compounds target major hallmarks of cancer through their antiproliferative, proapoptotic, antiangiogenic, anti- invasive and antimigratory properties. Also, they do not reveal toxic side effects in animal models. These preclinical results indicate that these compounds are promising drug candidates for anticancer therapy.

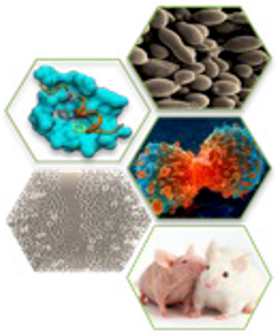
Another case study is the pancreatic cancer (PC) that often has defective p53 and BRCA pathways. p53 mutations are associated with PC aggressiveness and therapeutic resistance. BRCA-mediated DNA repair deficiency sensitizes tumours to chemotherapy.

We are studying the BRCA-mediated DNA repair deficiency sensitizes tumors to chemotherapy. In this context, a first-in-class inhibitor of homologous recombination DNA repair pathway was recently disclosed as an anticancer drug candidate for hard-to-treat cancers, including PC..

Small molecule regulators of p53 and BRCA1 pathways are the basis of two international patent applications.

"New pharmaceutical compounds, methods and uses thereof"

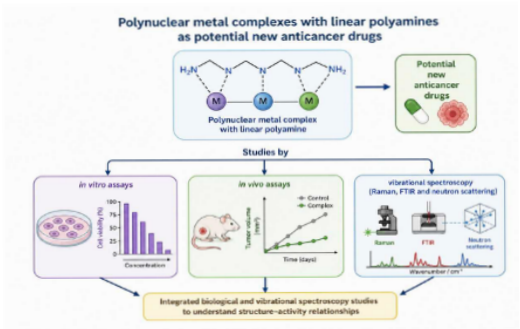
PCT/IB2021/058241, publication N° WO/2022/053998



ANTICANCER EFFICACY OF HOMO/HETEROMETALLIC COMPLEXES ASSOCIATED WITH BIOGENIC AMINES

New polynuclear metallodrugs (Pt-, Pd- and Ni-based) with biogenic polyamines are being designed and synthetised, with and without hydrolysable groups (such as Cl). Distinct modes of action and several pharmacological targets are envisaged (e.g. DNA, proteins, intracellular water), within a multitarget approach enabling circumvent therapy resistance.

Evaluation of the activity of the newly synthetised metal complexes as potential anticancer agents: (i) in vitro biological assays to assess cytotoxicity, anti-invasive and anti-angiogenic abilities; (ii) ex vivo and in vivo histopathological and haematological analysis in mouse models; (iii) pharmacodynamic and pharmacokinetic in mouse models iv) microRaman, synchrotron-FTIR, microFTIR (micrometer resolution), AFM-IR (nanometre resolution), as well as synchrotron-EXAFS (Extended X.ray Absorption Fine Structure) – to achieve sub-cellular information on the drug effect on cellular metabolism and identification of spectral biomarkers; (v) QENS experiments in human cells, to determine the drug impact on intracellular water – pioneer application of neutron scattering techniques to human cells. (vi) NMR metabolomic studies, to attain complementary information on the new drugs´ metabolic impact.



Pd_3Spd^2 on Mesenchymal TNBC-Sensitive and Resistant to Cisplatin: Vibrational Microspectroscopy to Evaluate Cellular Response

Anal. Chem. 2025, 97, 14709

Pd_2Spermine as an Alternative Therapeutics for Cisplatin-resistant Triple-negative Breast Cancer

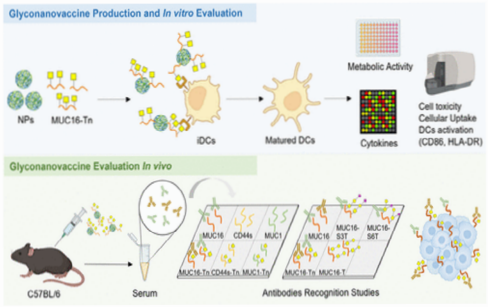
J.Med.Chem. 2024, 67, 6839.

HIGHLIGHTS

CANCER GLYCOVACCINES PROMOTING ANTIGEN RECOGNITION AND FOSTERING THE IMMUNE RESPONSE

Targeted and Self-Adjuvated Nanoglycovaccine Candidate for Cancer Immunotherapy.
ACS Nano 2024, 18(14):10088-10103

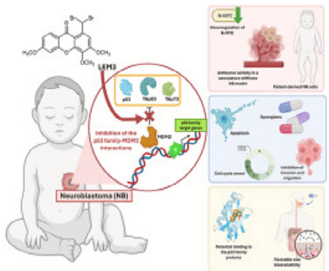
Advanced-stage solid primary tumors and metastases often express mucin 16 (MUC16), carrying immature glycans like the Tn antigen, resulting in specific glycoproteoforms not found in healthy human tissues. Targeted therapeutics like cancer glycovaccines may promote antigen recognition and foster immune responses.
We describe an adjuvant-free poly(lactic-co-glycolic acid) (PLGA)-based nanoglycoantigen delivery approach that outperforms conventional methods by eliminating the need for protein carriers, and has targeted and adjuvant properties. We synthesized a library of MUC16-Tn glycoepitopes through single-pot enzymatic glycosylation, which were stably engrafted onto the surface of PLGA nanoparticles, generating multivalent constructs that better represent cancer molecular heterogeneity. These glycoconstructs demonstrated affinity for Macrophage Galactose-type Lectin (MGL) receptor (highly expressed by immature antigen-presenting cells), enabling precise targeting of immune cells.
This nanovaccine candidate displayed minimal cytotoxicity and induced the activation of dendritic cells in vitro. In vivo, it was nontoxic and elicited the production of IgG specifically targeting MUC16 and MUC16-Tn glycoproteoforms in cancer cells and tumors, offering potential for precise cancer targeting



IMPROVING NEUROBLASTOMA THERAPY WITH A NEW P53 FAMILY-ACTIVATING AGENT

Improving neuroblastoma therapy with a new p53 family-activating agent.
European Journal of Pharmacology 2025, 1007, 178295

p53 family proteins play a critical role in protecting cells from genomic instability and malignant transformation. In Neuroblastome (NB), they are often inhibited by proteins like MDM2. We disclose 1-(dibromomethyl)-3,4,6-trimethoxy-9H-xanthen-9-one (LEM3) as a new p53 family-activating agent with potent NB anticancer activity. At 0.13–2.1 μM, LEM3 inhibited the growth of several NB cell lines. Its activity was evidenced in spheroids, patient-derived NB cells, and in a vasculature stiffness-based model of MYCN-amplified NB cells. This growth-inhibitory effect was associated with cell cycle arrest and apoptosis, without acquisition of resistance. LEM3 inhibited cell migration and invasion and reduced NB-related prognostic markers's expression, as MYCN mRNA and protein levels. LEM3 released p53, TAp63 and TAp73 from their interaction with MDM2 both in a yeast-based assay and NB cells; for p53, this led to increased protein stabilization, DNA-binding ability, and transcriptional activity. LEM3 also synergies with doxorubicin and cisplatin in NB cells. Given the central role of the p53 family-MDM2-MYCN axis in NB pathogenesis, our findings support LEM3 as a promising compound for advancing NB targeted therapy.



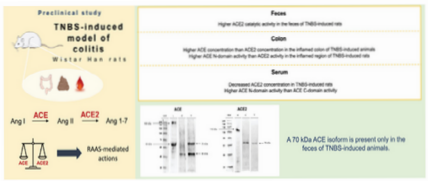
HIGHLIGHTS

ANGIOTENSIN-CONVERTING ENZYMES 1 AND 2 MAY PLAY A ROLE ON COLONIC LESIONS

Angiotensin-converting enzymes 1 and 2 in the feces: presence and catalytic activity in the rat 2,4,6-trinitrobenzene sulfonic acid-induced model of colitis.

Journal of Gastroenterology and Hepatology, 2024, 39: 1885–1894.

The renin–angiotensin-aldosterone system is implicated in intestinal inflammation. Angiotensin-converting enzyme (ACE) and angiotensin-converting enzyme 2 (ACE2) regulate its activity, but conflicting findings on these enzymes in colitis require further investigation.
Colitis was induced in male rats by rectal instillation. ACE and ACE2 presence in the feces was analyzed by western Blot, and colonic and serum enzymes' concentrations were quantified using ELISA kits. ACE activity was assessed. ACE2 activity was assessed using Mca-APK (Dnp). Results showed that an ACE isoform of ~70 kDa was found only in the feces of TNBS-induced rats. ACE concentration was higher than that of ACE2 in the serum and the inflamed colon. ACE N-domain activity was higher than that of the C-domain. ACE2 activity was higher in the feces of TNBS-induced animals compared to controls.
As conclusion, a 70 kDa ACE isoform only detected in the feces of TNBS-induced rats may have translational relevance. ACE N-domain seems to play a significant role in regulating colonic lesions. Further research using human samples is necessary to validate these findings

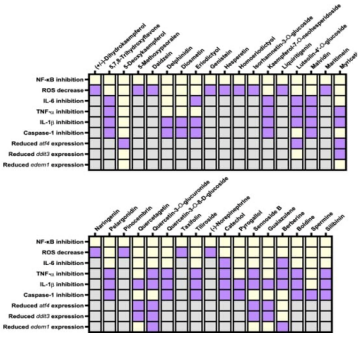


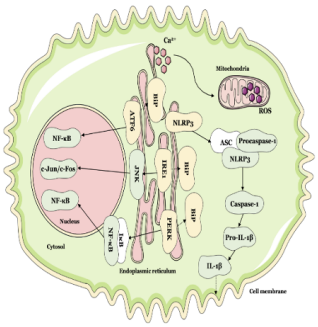
NATURAL SMALL MOLECULES WITH DUAL EFFECT UPON INFLAMMATORY SIGNALING PATHWAYS AND ER STRESS RESPONSE

Naturally occurring small molecules with dual effect upon inflammatory signaling pathways and endoplasmic reticulum stress response.

Journal of Physiology and Biochemistry 2024, 80(2):421-437

The endoplasmic reticulum (ER) is determinant to maintain cellular proteostasis. Upon unresolved ER stress, it activates the unfolded protein response (UPR). Sustained UPR activates occurs in inflammatory processes, deeming the ER a potential molecular target for the treatment of inflammation. We characterized the inflammatory/UPR-related machinery modulated by an in-house library of natural products, aiming to identify new selective drugs that act upon the ER to counter inflammation-related chronic diseases. Using a library of 134 natural compounds (eg., from medicinal plants) nontoxic molecules were screened for their inhibitory capacity against LPS-induced nuclear factor kappa B (NF-B) activation in a luciferase-based reporter gene assay.
We report the anti-inflammatory potential of guaiazulene and describe 5-deoxykaempferol as a novel inhibitor of inflammasome activation.
We also describe the dual potential of 5-deoxykaempferol, berberine, guaiazulene, luteolin-4'-O-glucoside, myricetin, quercetagetin and sennoside B to modulate inflammatory signaling ER stress. We show that some natural molecules are able to modulate the inflammatory response, as well as proteostasis and the UPR.

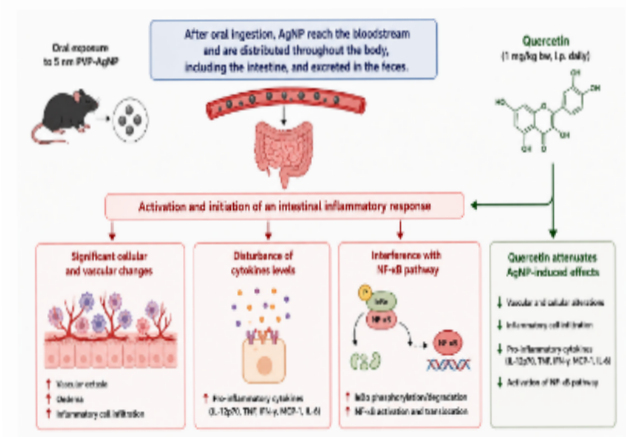




HIGHLIGHTS

MITIGATING NANOPARTICLE-INDUCED TOXICITY: QUERCETIN PROTECTS AGAINST AGNP-DRIVEN INFLAMMATION IN VIVO

The widespread use of silver nanoparticles (AgNP) as emerging environmental stressors has raised increasing concerns regarding their potential adverse effects on human health, particularly following oral exposure through food, including contamination resulting from the migration of nanoparticles from food contact materials..Therefore, the identification of effective strategies to mitigate AgNP-induced toxicity is of major importance. Quercetin, a dietary flavonoid with well-established anti-inflammatory and antioxidant properties, emerges as a promising candidate for this purpose. In an in vivo study, male C57BL/6J mice were orally exposed to 5 nm polyvinylpyrrolidone (PVP)-coated AgNP (1 or 10 mg/kg body weight) for 14 days using a novel administration technology (HaPILLness), with or without daily intraperitoneal administration of quercetin (1 mg/kg body weight). AgNP exposure induced a marked intestinal inflammatory response, characterized by vascular and cellular alterations, increased pro-inflammatory cytokine production, and activation of the NF-B signalling pathway. Quercetin significantly attenuated these effects, reducing histological damage and cytokine levels, and modulating NF-B activation through regulation of IB expression. Importantly, quercetin also exerted systemic protective effects, restoring inflammatory and redox homeostasis in the liver and lungs, as evidenced by normalization of CD4, superoxide dismutase 1 (SOD1), and catalase expression.
These findings demonstrate that quercetin effectively mitigates AgNP-induced intestinal and systemic inflammation, highlighting its potential as a dietary-based strategy to counteract nanoparticle-induced toxicity.



Exploring quercetin's protective potential against the pro-inflammatory effects of silver nanoparticles in C57BL/6J mice

Food and Chemical Toxicology, 195 (2025) 115081

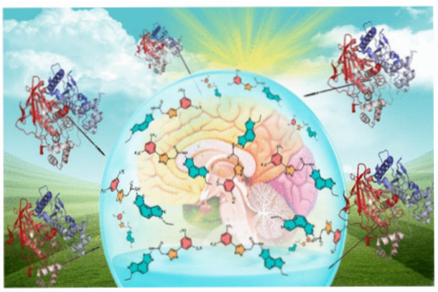
Quercetin protective potential against nanoparticle induced adverse effects

Nanotoxicology 19:1, 28-49

HIGHLIGHTS

ROLE OF NEW THIAZOLOINDAZOLE-BASED ACHE INHIBITORS TO THE TREATMENT OF NEUROLOGICAL DISORDERS: THE CASE STUDY OF ALZHEIMER'S DISEASE

The inhibition of acetylcholinesterase (AChE), responsible for breaking down the neurotransmitter acetylcholine, is relevant in the treatment of neurological disorders. Developing efficient AChE inhibitors capable of increasing acetylcholine levels, may ultimately lead to improved cholinergic neurotransmission. We showed that novel thiazoloindazole-based compounds are effective AChE inhibitors. Molecular docking studies revealed that certain of the evaluated nitroindazole-based compounds outperformed donepezil (an AChE inhibitor used in Alzheimer's treatment). Two series of compounds were synthesized. One series included a triazole moiety (Tl45a–c), the other incorporated a carbazole moiety (Tl58a–c). The Tl45b displays superior performance as an AChE inhibitor. Structure–activity relationship (SAR) analysis indicated that derivatives containing the bis(trifluoromethyl) phenyl-triazolyl group demonstrated the most promising activity against AChE. The combination of molecular docking and experimental synthesis provides a suitable and promising strategy for the development of new efficient thiazoloindazole-based AChE inhibitors.



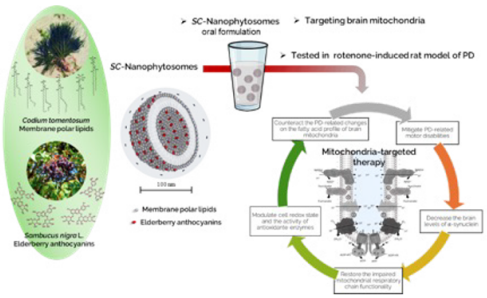
cells and tumors, offering potential for precise cancer targeting

Design of Promising Thiazoloindazole-Based Acetylcholinesterase Inhibitors Guided by Molecular Docking and Experimental Insights

ACS Chem. Neurosci. 2024, 15, 15, 2853–2869

NATURAL PRODUCT ENGINEERING: SC-NANOPHYTOSOMES TO FIGHT PARKINSON'S DISEASE BY TARGETING MITOCHONDRIA

The development of medicines to modulate the mitochondrial function is a great scientific challenge since mitochondrial dysfunction is a pathological hallmark of many degenerative brain pathologies, including Parkinson's and Alzheimer's diseases. To address this challenge, we propose SC-Nanophytosomes - innovative nanovesicles with soft architecture, built with anthocyanin-enriched extract (Sambucus nigra) and membrane polar lipid, from Codium tomentosum. In a rotenone-induced PD rat model, the oral administration of SC-Nanophytosomes demonstrated competence: (i) to alleviate motor disabilities; (ii) to mitigate mitochondrial dysfunction in brain and skeletal muscles tissues; (iii) to reduce brain -synuclein levels; (iv) to counteract PD-like changes in brain lipidome and skeletal muscle cells; (v) to improve cell redox state by modulating the activity of antioxidant enzymes. SC-Nanophytosomes emerge as new precision mitochondrial medicines to improve the quality of life of PD patients.



Mitochondrial Dysfunction in Skeletal Muscle of Rotenone-Induced Rat Model of Parkinson's Disease: SC-Nanophytosomes as Therapeutic Approach

International Journal of Molecular Sciences, 2023, 24, 16787

Brain Effects of SC-Nanophytosomes on a Rotenone-Induced Rat Model of Parkinson's Disease—A Proof of Concept for a Mitochondria-Targeted Therapyand pyrazoles

International Journal of Molecular Sciences, 2022, 23, 12699

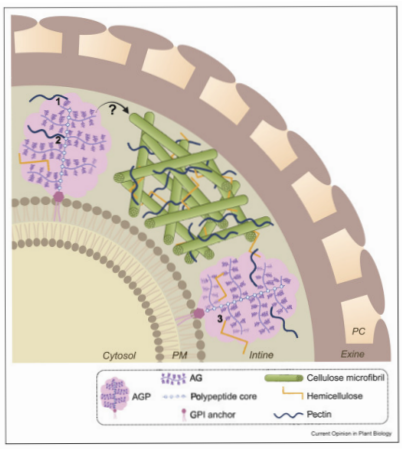
HIGHLIGHTS

ARABINOGALACTAN PROTEINS (AGPS) REGULATE PLANT SIGNALLING AND REPRODUCTION

Arabinogalactan proteins: Decoding the multifaceted roles in plant reproduction

Current Opinion in Plant Biology 88 (2025): 102800

Arabinogalactan proteins (AGPs) are highly glycosylated cell wall proteins essential for plant growth and reproduction. AGPs are extensively decorated with arabinogalactan polysaccharides. Their glycosylation patterns and glycosylphosphatidylinositol anchor enable interactions with receptors, modulating signal transduction pathways critical for reproduction. AGPs also associate with cell wall components like pectin and hemicellulose, impacting cellulose deposition and cell wall integrity. Recent research highlights AGPs' role as calcium (Ca^{2+}) capacitors, regulating Ca^{2+} storage and release during crucial reproductive stages.



We have developed extensive work on AGPs, exploiting the multifaceted roles of AGPs in plant reproduction, shedding light on the recent progress in their involvement in signalling pathways, cell wall interactions, and Ca^{2+} homeostasis, while highlighting the ongoing research needed to fully understand their mechanisms in reproductive success.

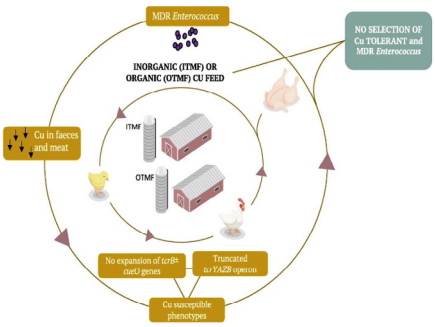
DOES CU PRESENT IN (IN)ORGANIC TRACE MINERAL FEEDS SELECT CU TOLERANT AND MULTIDRUG RESISTANCE IN ENTEROCOCCUS?

Uncovering the effects of copper feed supplementation on the selection of copper-tolerant and antibiotic-resistant Enterococcus in poultry production for sustainable environmental practices

Science of The Total Environment 900 (2023): 165769

The use of antibiotics in animal production is linked to the emergence and spread of antibiotic-resistant bacteria, a threat to animal, environmental and human health. Cu is essential in poultry diets and an alternative to antibiotics, supplementing inorganic or organic trace mineral feeds (ITMF/OTMF).

Cu contribution to select multidrug-resistant (MDR) and Cu tolerant Enterococcus (a bacteria with a human-animal-environment-food interface) remains uncertain. We evaluated whether feeding chickens with Cu-ITMF or Cu-OTMF contributes to the selection of Cu tolerant and MDR Enterococcus. Enterococcus were identified in 80 % of the samples, with >50 % carrying isolates resistant to tetracycline, quinupristin-dalfopristin, erythromycin, streptomycin, ampicillin or ciprofloxacin. Enterococcus with Cu tolerance genes, especially tcrB ± cueO, were mainly found in faeces. Similar occurrence and load of tcrB ± cueO Enterococcus in faeces was detected along the chickens' lifespan in ITMF/OTMF flocks, decreasing in meat. Most of the polyclonal MDR Enterococcus population carrying tcrB ± cueO or only cueO (67 %) showed a wild-type phenotype linked to absence of tcrYAZB or truncated variants.

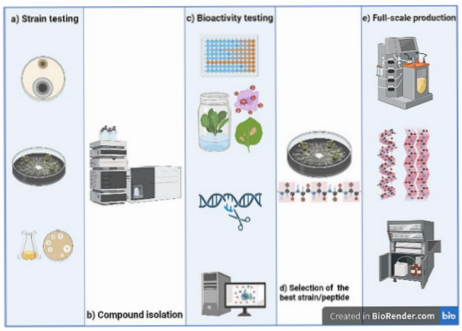


HIGHLIGHTS

PEPTAIBIOTICS: HARNESSING THE POTENTIAL OF MICROBIAL SECONDARY METABOLITES FOR MITIGATION OF PLANT PATHOGENS

Peptaibiotics have shown antibacterial, antifungal, and antiviral activity, also being potential inducers of plant resistance against a some phytopathogens. Peptaibiotics belong to the new generation of alternatives to agrochemicals, aligned with the UN SDG and the One Health approach, ensuring global food security and safety.

These fungi-derived, non-ribosomal peptides remain surprisingly understudied, especially in agriculture, where only a small number has been tested against a reduced number of phytopathogens. We provide an analysis of peptaibiotics' classification, biosynthesis, relevance to plant protection, and mode of action against phytopathogens, along with the techniques enabling researchers to extract, purify, and elucidate their structure, and the databases holding such valuable data. It is also discussed how chemical synthesis and ionic liquids could increase their solubility, how genetic engineering and epigenetics could boost in vitro production, and how omics can reduce screenings' workload through in silico selection of the best candidates. These strategies could turn peptaibiotics into effective, ultra-specific, biodegradable tools for phytopathogen control.

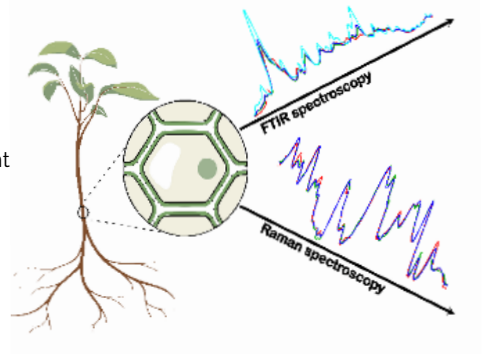


Peptaibiotics: Harnessing the potential of microbial secondary metabolites for mitigation of plant pathogens

Biotechnology Advances 2023, 68, 108223

PHYTOCHEMICALS AND PLANT STRUCTURAL BIOCHEMISTRY

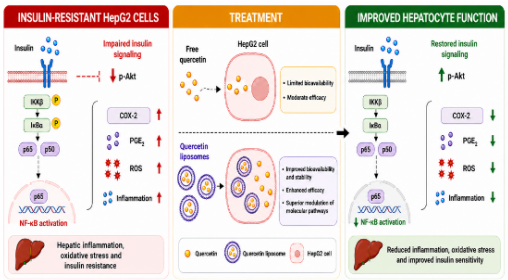
Study of plant cell wall-mediated mechanisms of disease progression and host resistance in species significant to the agroforestry sector, such as Pinus species. We aim at uncovering molecular mechanisms behind plant – pathogen interactions and how plant cell wall structure and composition influence plant responses to disease. This knowledge will facilitate the development of early disease mitigation strategies and the creation of improved, resistant plant cultivars. Focus on discovering and characterising natural products derived from plant biomass for human health, nutraceuticals, and sustainable agricultural applications. This involves extracting, processing, and purifying and/or characterising bioactive compounds from plants. Towards the optimisation of the use of these compounds and processes and to enhance the use of plants as reliable sources of useful molecules. Valorisation of lignocellulosic biomass resources and lead to the generation of value-added products from the Biorefinery. This research also includes the development of biomass pretreatments aimed at reducing the recalcitrance of plant cell wall to saccharification and fermentation. We mainly focus on improving our understanding of plant cell wall structures and composition, to optimise the conversion of lignocellulosic biomass for biorefinery applications and other biobased materials. Our techniques primarily involve vibrational spectroscopy (e.g., FTIR and Raman).



HIGHLIGHTS

QUERCETIN LIPOSSOMES SHOW EFFICIENT RESULTS IN MANAGING IS AN DIABETES

In type 2 diabetes mellitus, hepatic insulin resistance is intricately associated with oxidative stress and inflammation. Flavonoids have potential antidiabetic effects, but are associated with low bioavailability and high metabolization. Four flavonoids, kaempferol, quercetin, kaempferol-7-O-glucoside and quercetin-7-O-glucoside, were studied in a cellular model of hepatic insulin resistance using HepG2 cells. Quercetin was selected as the most promising flavonoid and incorporated into liposomes to enhance its therapeutic effect.



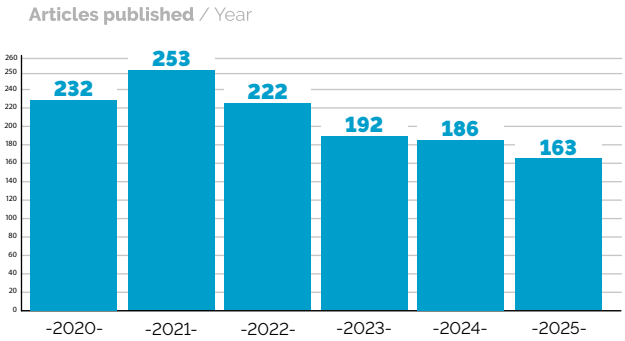
Quercetin liposomes (~ 0.12 µm, incorporation efficiency ~ 93 %) exhibited increased efficacy in modulating insulin resistance. This was achieved through the modulation of Akt expression and attenuation of inflammation, particularly via the NF-B pathway, and the regulation of PGE2 and COX-2 expression. Quercetin liposomes displayed a significant advantage over free quercetin in attenuating the production of reactive pro-oxidant species. These findings open new avenues for developing innovative therapeutic strategies to manage diabetes, emphasizing the potential of quercetin liposomes as a promising approach for targeting both hepatic insulin resistance and associated inflammation.

Liposomal quercetin: A promising strategy to combat hepatic insulin resistance and inflammation in type 2 diabetes mellitus

International Journal of Pharmaceutics, 2024, 661, 124441

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION



H-index: **75**

1248 articles*
67256 citations

***01/2020-12/2025**
From WOS core collection

FUNDED PROJECTS *(Representative projects)*

- **IBERPHENOL, Red cooperativa de investigación en el ámbito de polifenoles y sus aplicaciones industriales**
  INTERREG, 0377_IBERPHENOL_6_E, Paula Andrade (PI at FFUP),
  Total Funding: € 2,244,828.61
- **SHARP - Seaweeds for healthier traditional products**
  COMPETE 2020, POCI-01-0247-FEDER-003419, Susana M Cardoso (PI at UA).
  Total funding = € 633 721.67
- **HEPA-Healthier eating of pasta with algae**
  COMPETE 2020, CENTRO-01-0145-FEDER-023780, Susana M Cardoso (PI at UA).
  Total funding = € 125 696,92
- **AlgaPhlor: Brown algae phlorotannins: From bioavailability to development of new functional foods**
  FCT, POCI-01-0145-FEDER-031015, Susana M Cardoso (PI).
  Total funding = € 234 528.38
- **Interdisciplinary in silico, organic synthesis, in vitro, and in vivo studies towards new antidiabetic flavonoid scaffolds**
  FCT, PTDC/MED-QUI/29241/2017, Eduarda Fernandes (PI).
  Total Funding: € 239,996.98
- **Use of flavonoids in the prophylaxis of intestinal pro-inflammatory effects of silver nanoparticles.**
  FCT, PTDC/NAN-MAT/29248/2017, Marisa Freitas (PI).
  Total Funding: € 205,094.57
- **2-Styrylchromones in the treatment of rheumatoid arthritis: a promising therapeutic alternative?**
  FCT, PTDC/MED-QUI/29253/2017, Daniela Ribeiro (PI).
  Total Funding: € 236,207.66
- **Development of new inhibitors of invasive osteosarcoma based on fisetin derivatives**
  FCT, PTDC/MED-QUI/29243/2017, Miguel Oliveira (PI).
  Total Funding: € 233,069.57
- **Unravelling Data for Rapid Evidence-Based Response to COVID-19.**
  EU, H2020-SC1-PHE-CORONAVIRUS-2020-2, David Pereira (National PI).
  Total funding: €2,990,000.00
- **Milk Quality along the Dairy Chain for a Safe and Sustainable MILK"**
  EU/PRIMA Foundation, PRIMA/0007/2018, David Pereira (National PI).
  Total funding: €1,648,120.00
- **Biopesticides and Food Preservatives from Nanoencapsulated Plant Extracts: Biological Evaluation, Molecular Modelling and Synthesis"**
  FCT, PTDC/ASP-AGR/30154/2017, David Pereira (LAQV PI)Total funding: €239,758.00
- **Self-assembled minimalist peptide hydrogels inspired by mussel adhesive proteins for biomedical applications**
  FCT, PTDC/QUI-QOR/29015/2017, David Pereira (LAQV PI)
  Total funding: €225,445.00
- **ChemiTumorTher -Marine chemiluminescence as a broad-spectrum anticancer therapy with enhanced tumor-selectivity and activity**
  FCT, PTDC/QUI-QFI/2870/2020, David Pereira (LAQV PI)
  Total funding: €257.794
- **Screening and pharmacological characterization of flavonoids as lead compounds for obesity treatment**
  FCT, EXPL/MED-QUI/0815/2021, Carina Proença (PI).
  Total Funding: € 49,908.98
- **Exploring salt tolerant plants as sources of innovative food additives**
  FCT, PTDC/BAA-AGR/1391/2020, Paula Andrade (PI at LAQV)
  Total funding: €249.581,45
- **Novos IngreDiEntes IDEAS4life—Alimentares de Plantas MarítimaS**
  FCT, PTDC/BAA-AGR/29305/2017, Carmen Diniz (Co-PI)
  Total funding: €239.355,55
- **BioCosMAp- BioCosMAp-Estratégia de valorização de produtos apícolas do Parque Natural de Montesinho através do desenvolvimento de cosméticos biológicos**
  COMPETE2030-FEDER- 02162400

GROUP IN NUMBERS

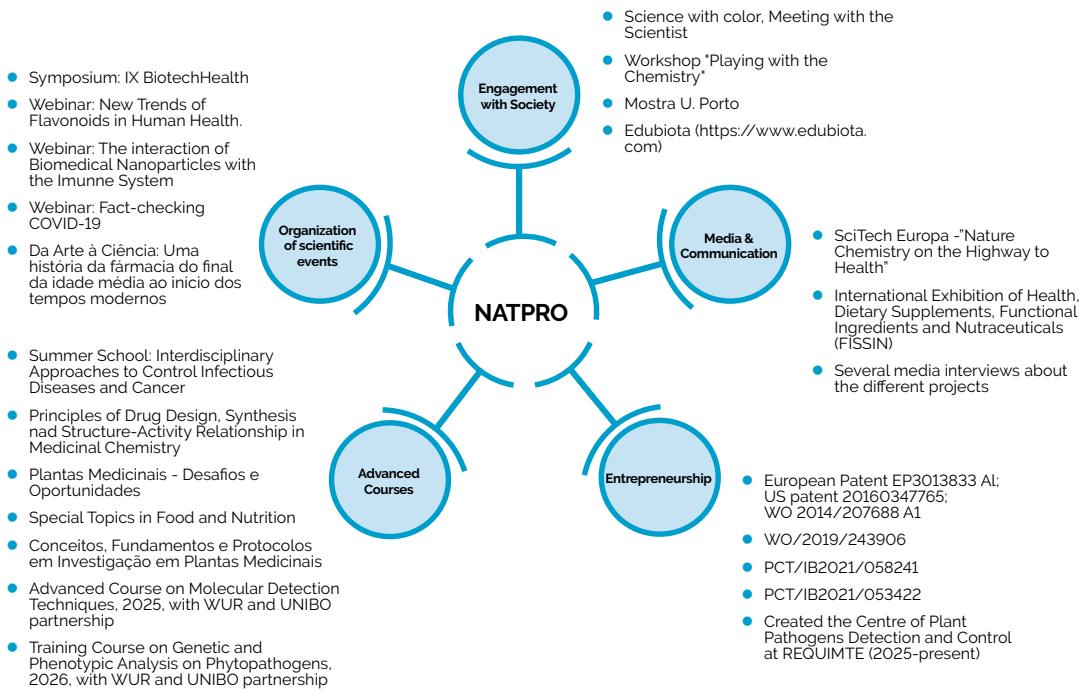
FUNDED PROJECTS *(Representative projects)*

- **BIOMEHEALTH-Boosting the detection and control of plant pathogens in Portugal, Twinning EU Grant agreement ID: 101159978, 10.3030/101159978 (1 july 2024-30 june 2027)**
  Principal Researcher: Conceição Santos,
  Funding: 1499851,31 €,
- **SHARP - Seaweeds for healthier traditional products**
  COMPETE 2020, POCI-01-0247-FEDER-003419, Susana M Cardoso (PI at UA).
  Total funding = € 633 721.67
- **Desvendando as vias causadoras de diabesidade induzida pelos desreguladores endócrinos, COMPETE2030-FEDER-00834300, operação 17050, from 1/10/2025 to31/01/ 29/09/2029**
  Principal Researcher: Eduarda Fernandes.
- **Síntese verde de nanomateriais para aplicação em sensores eletroquímicos 403757/2024-0, from 07/01/2025 to 31/01/2027**
  Researcher: Eduarda Fernandes
- **RE-SHRIMP - Upcycling shrimp waste into food-grade astaxanthin: a zero-waste approach towards a circular economy**
  2024.17544.PEX, from 01/07/2025 to 31/12/2026
  Principal investigator: Edgar Pinto
- **SALIVA+ - Novel tools for exposure assessment of food contaminants by saliva multiple biomarker monitoring.**
  2022.08978.PTDC, from 01/01/2021 to 31/12/2024.
  Principal investigator: Edgar Pinto
- **Explore the impact of DIETary-eXPOSOME on chronic inflammation assessed through in vitro assays and mathematical modelling**
  PTDC/SAU-NUT/6061/2020, from 01/01/2023 to 31/12/2025 .
  Investigator: Edgar Pinto
- **Valorization of the protein fraction from Moringa oleifera**
  PTDC/OCE-ETA/32567/2017, 01/10/2018 to 30/09/2022.
  Investigator: Edgar Pinto
- **Institute for Health and Bioeconomy.**
  LA/P/0140/2020, 10.54499/LA/P/0140/2020, from 01/01/2021 to 12/31/2025.
  Researcher: Andreia Gonçalves
- **RESOLVE: Rational Design of Multivalent Glycocode-Inspired Nanovaccines for Gastric Cancer**
  PTDC/MED-OUT/2512/2021, from 01/02/2022 to 12/31/2024
- **Keep fertility at advanced maternal age: on the track of uterine senescent cells**
  2022.04368.PTDC, from 03/01/2023 to 08/31/2024
  Investigator André Silva
- **eQuaNTI: An enzymatic assay for the determination of blood serum non-transferrin-bound iron.**
  2023/01/02 - 2024/06/30 , 2022.06328.PTDC,
  Investigador responsável André Silva
- **NUTRIBRAIN - Coastal Flora for Mental Well-being Promotion: Development of food supplements based on dune plant compounds with impact on BDNF-TrkB signalling**
  COMPETE2030-FEDER-00686600 (operação 15759) 2025/09/01 - 2028/08/31,
  Researcher: Ana Isabel Oliveira

INTERNATIONAL COOPERATION AND NETWORKING

- COST Action ca20121: Bench to bedside transition for pharmacological regulation of NRF2 in noncommunicable diseases (BenBedPhar), 2021 - 2025Consortium for Mitochondrial Research, University College London, UK
- COST ACTION 19105: Pan-European Network in Lipidomics and EpiLipidomics (EpiLipidNET), 2020 - 2024
- COST Action CA16119: In vitro 3D-total cell guidance and fitness (CellFit), 2017 - 2021
- COST Action CA22158: coordinated by C Santos, a REQUIMTE researcher, with networking with researchers from 29 countries on the topic of microbiomes, molecular signaling in agrifood systems
- Collaboration with Wagningen and Univ. Bologne to study microbiomes in crops, and develop techniques to analyse aerobiomes, using molecular tools (within the scope of the Twinning Project Biomehealth), 2024-2027
- Collaboration with the International Microbiology Literacy Initiative (IMiLI) to widen the pedagogical tools on microorganisms and microbiomes, together with the Edubiota site, 2025-2027
- Collaborations with Universities from several countries, namely Italy, Guinea-Bissau, Croatia, Ivory Coast, Morocco, Thailand, Brazil, Germany, UK, Spain, Argentina, Mexico, Australia, India, USA, Czech Republic, Serbia, and Mozambique, Turkey

DISSEMINATION & OUTREACH



LABORATÓRIO ASSOCIADO
PARA A QUÍMICA VERDE

OAD

OMICS & ANALYTICAL DEVELOPMENT

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

Group Coordinator:

José Luis Capelo-Martínez

The OMICS and Analytical Development group is a multidisciplinary international research group that integrates analytical and inorganic chemists, biochemists, biologist, biochemist, veterinaries, materials science, and biotechnological researchers. Their common goal is to gain insight into complex biological systems, real-life problems concerning quantification of small molecules in a plethora of matrixes and environmental problems using multidisciplinary approaches. They combine expertise in Instrumental Methods of Analysis, Organic Chemistry, Chemometrics, and Chemical Engineering to develop new analytical solutions using preferably sustainable methods. The Group focuses on modernization of analytical methods, developing innovative approaches towards reduction of reagents consumption, protection of work/lab environment, deployment of point-of-care/in situ analysis, and exploitation of technological developments from other areas, namely from mechanical and electronic engineering.
Our research labs work in an integrative and cooperative approach, with a strong relationship with several International and National universities, hospitals, research centers, and industries. The research group comprises an extensive experience in i) synthesis of organic dyes, inorganic complexes, multifunctional materials, emissive liquid crystals, nanoparticles, and nanomaterials; ii) innovative approaches for large- scale quantification of biomolecules; iii) characterization and quantification of small molecules; iv) characterization of metalloenzymes and proteins (structural and function); v) Nano proteomics | Proteomics and Oncoproteomics for the identification on tumor specific antigens; vi) quantitative characterization post-translational modification in complex biological systems and in the analysis of bacteriology, mycology and viruses samples, vii) the miniaturization of devices and methods, viii) the advanced data analysis through chemometrics, and ix) the development of high-throughput methods mainly through intervention on sample preparation.

RESEARCH OBJECTIVES [2025-2029]

The OMICS & Analytical Develpment group will continue to work aiming the identification, characterization, and quantitation of a wide array of biomolecules to gain new insights into underling molecular mechanisms in complex biological systems. This will be achieved by integrating nanotechnology and multiplex-probing systems, biophysical techniques, a wide range of spectroscopies, and high-resolution mass spectrometry. In particular, we intend to strengthen:

- The design of new nanotechnology-based multiplex- probing systems with application in the fields of environment, sustainable health, well-being, and point-of-care. Specifically, we will work on the innovation of new synthetic protocols using environmentally friendly reagents applied for nanomaterials and new smart functionalized nanoparticles and smart materials (UNL).
- The development of innovative methods to unravel the biochemical mechanisms of antibiotics resistance (UTAD and UNL).
- Proteomics approaches to discover new biomarkers in Cancer, Aging, and Degenerative diseases (UNL and UA).
- The identification and characterization of CO2 reductases with biotechnological interest for the utilization of the abundant atmospheric CO2 in the synthesis of added value compounds (UNL).
- The characterization of a N2O reductase aiming to develop a new biotechnological system to efficiently reduce the green-house effect gas N2O concentration (UNL).
- The design of new oxidative enzymatic systems for the conversion of lignocellulose into valuable products, as well as, artificial metal-substituted proteins for the development of novel catalysts.
- Human biomarkers detection for sensing devices development (UNL) Development of environmentally friendly strategies for sample treatment prior to analysis;
- Application of chemometrics and reagentless methods towards in situ analysis;
- Use of mobile devices as instrument of analysis;
- Automation of analytical methods;
- Development of comprehensive analytical strategies using 2D and hyphenated techniques.

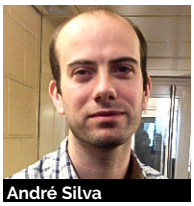
RESEARCH TEAM

SENIOR RESEARCHERS

Agostinho Almeida

Alberto Araújo

Ana Martins


André Silva

Artur Figueirinha

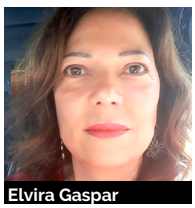
Carlos Lodeiro

Célia Amorim

Cristina Costa

David Pereira

Elisabete Oliveira


Elvira Gaspar

Francisco Amado

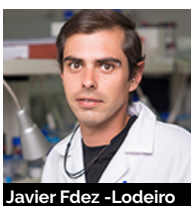
Gilberto Igrejas

Helena Soares

Hugo Miguel Santos

Isabel Moura

Iola Duarte


Javier Fdez -Lodeiro

João Paulo Noronha

João Prior

J. António Rodrigues

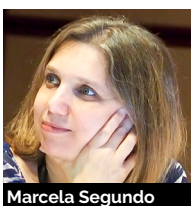
José Luís Capelo

José Moura

Júlia Magalhães

Luisa Barreiros

Mafalda Sarraguça


Marcela Segundo

Marco G. Silva

M. Beatriz Quinaz

M. Conceição Branco

Marta Carepo

Nádia Silva

Paulo Almeida

RESEARCH TEAM

SENIOR RESEARCHERS

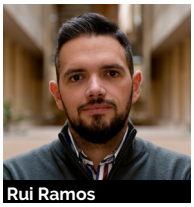
Pedro Domingues

Pedro F. Oliveira

Ricardo Páscoa

Rita Ferreira

Rui Lapa


Rui Ramos

Sara Marques

Tânia Melo

OTHER DOCTORATE RESEARCHERS

Adrian F. Lodeiro
Agostinho Santos
Ana Martins
Ana Marta Pereira
Ana Figueiredo
António Amorim
Bruno Neves
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Cristian Cuerva
Cristina Barros
Cristina Couto
Eduarda Silva
Elisabete Costa
Fernando Ricardo
João Monteiro
Leandro Dias
Laura Cainé
Luis Carvalho
M. Gabriela Ribeiro
Maria Maciel
Mary Duro
Rita Duarte
Susana Jorge
João Pinto
Luis Intriago
Luís M. Fernandes
Luís Pinto
Marcelo Queiroz
Márcia Silva
Margarida Sousa
Maria Ferreira
Mariano Costa
Mohammad Ahmad
Muath Mousa
Patrícia Matos
Pedro Varandas
Raquel Fonseca
Rebeca André
Ricardo Santos
Ricardo Teixo
Sandia Machado
Sara Fernandes
Sara Pinheiro
Sara Pinto
Sara Sario
Sandra Copeto
Telma Sousa
Teresa Lapa
Vanessa Silva

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Ana Luisa Silva
André Figueiredo
Bruno Gregório
Carina Vieira
Carolina Sabença
Catarina Martins
Catarina Mendes
Catarina Nunes
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Davide Mendes
Cláudia Covas
Diana Cunha
Diana Moreira
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Flávia Freitas
Frederico Duarte
Gabriel Valério
Gonçalo Pedro
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Isabel Carvalho
Jaime Mendoza
Javier Bullón
Jennifer Fadoni
Jessy Silva
Joana Galhano
João Montes

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Luz Fernandes
João Luís Santos
Patrícia Silva das Neves
Paula Melo
Pedro Costa
Ricardo Belinha

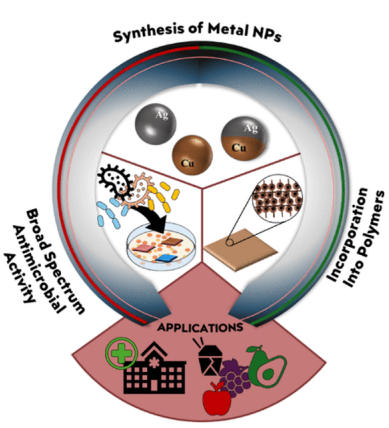
RESEARCH GRANTEES

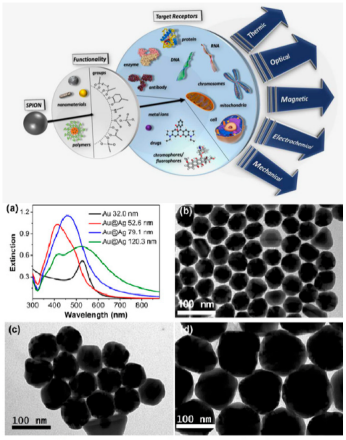
Beatriz Teixeira
Hugo Andrade
Mariana Pereira
Rui Azevedo

RESEARCH THEMES/
SYNTHESIS OF NANOMATERIALS, EMISSIVE PROBES, AND SMART MATERIALS

We have focused our work on the Synthesis of new Fluorescent and Colorimetric dyes, emissive liquid crystals, developing novel functionalized anisotropic nanoparticles and composites (Au, Ag, Pt, Pd, SiO2,Fe2O3), doped polymers, mesoporous materials for drug cargo delivery, and nanoprobes for applications in environmental detection of Pollutants, Drug delivery, Drug sensing and Biomedical and Proteomics Studies. Substantial efforts have been dedicated to developing new green synthetic methodologies applied in the synthesis of Nanoparticles and Composites.[1-11]

NEW EMISSIVE LIQUID CRYSTALS AND SMART MATERIALS; NANOMATERIALS FOR CATALYSIS, OPTOELECTRONIC APPLICATIONS AND DRUG DELIVERY; CHEMOSENSORS AS SCAVENGERS AND IMAGING SYSTEMS; BIOMEDICAL AND ANTIBACTERIAL APPLICATIONS





SELECTED PUBLICATIONS

1 C. Cuerva et al. Nanoresearch 2021, 245-254.
doi: 10.1007/s12274-020-3078-0

2 C. Cuerva et al., Chemical Reviews 2021, 20, 12966-13010.
doi: 10.1021/acs.chemrev.1c00011

3 S. Nuti et al., Materials J. Coll. Inf. Science, 2022, 611, 695-705.
doi: 10.1016/j.msec.2019.110104

4 A. Fernández-Lodeiro, et al., Nanoscale Adv, 2023, 5(17):4415-4423.
doi: 10.1039/d3na00158j

5 F. Duarte et al., Dyes and Pigments, 2023, 218, 111428.
doi: 10.1016/j.dyepig.2023.111428

6 C. Fernández-Lodeiro et al., J. Mat Chem C, 2023, 11(37), 12626 -12636.
doi: 10.1039/d3tc01567j

7 J. Hernández-Contreras et al, Microchimica Acta, 2025, 192:275.
doi: 10.1007/s00604-025-07134-9

8 F. Duarte et al. Dyes and Pigments, 2025, 243, 113088.
doi: 10.1016/j.dyepig.2025.113088

9 I. Ortiz-Gómez et al. Green Anal. Chem., 2025, 15, 100305.
doi: 10.1016/j.greeac.2025.100305

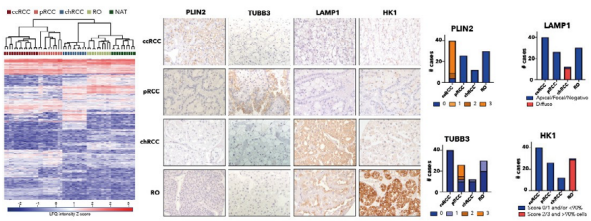
10 J. Galhano et al. ACS Nano, 2025, 19, 31301-31330.
doi: 10.1021/acsnano.5c08822

11 G. Pedro et al. Inorg. Chem. Commun., 2025, 101, 115290.
doi: 101016/j.inoche.2025.115290

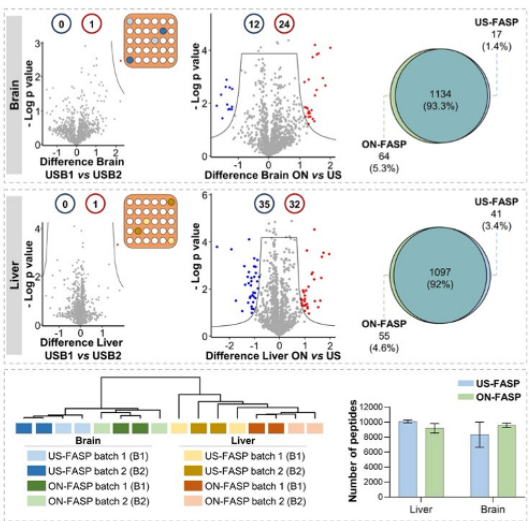
RESEARCH THEMES/
FUNCTIONAL ASSOCIATIONS OF POST-TRANSLATIONAL MODIFICATIONS & PRECISION HEALTH

We are on the brink of an amazing transformation in how we approach health. Instead of a frantic race to cure disease after the fact, we can increasingly prevent disease before it strikes. With this aim, we are using state-of-the-art technology to uncover tumor-specific antigens and post-translational modifications, which can be targeted for personalized therapy. We are using the multiplexing capabilities of mass spectrometry to build permanent digital quantitative maps of proteins to follow disease progression, response to therapy, and microbial resistance.[12-16]

https://www.youtube.com/watch?v=8DAZq40wmMo



We are also interested in developing innovative approaches for large- scale identification, characterization, and quantification of proteins. We use mass spectrometry and bioinformatics to identify the molecules involved in complex biological processes, characterize their structure, and monitor how their abundance or structure may change during these processes to gain new insight into the underlying molecular mechanisms.[17-21]



SELECTED PUBLICATIONS

12 S. Jorge, et al., BCM Medicine. 2021, 19, 1, 196. **doi: 10.1186/s12916-021-02071-9**

13 J. L. Capelo, et al., J. Integrative OMICS. 2022, 12, 1. **doi: 10.5584/jiomics.v12i1.211**

14 L. Carvalho, et al., Communications Medicine, 2023; 3:8. **doi: 10.1038/s43856-023-00238-4**

15 L. Carvalho, et al., Clinical Proteomics 2023, 20(1);54. **doi: 10.3390/microorganisms10010147**

16 L. Mercolini, et al., J. Integrated OMICS, 2023, 13, 1. **doi: 10.5584/jiomics.v13i1.221**

17 I. Domingos et al. Talanta, 2024, 279, 126589. **doi: 10.1016/j.talanta.2024.126589**

18 H. M. Santos et al., Microchemical Journal. 2023. 186:108323. **doi: 10.1016/j.microc.2022.108323**

19 L. Carvalho, et al., J. Proteomics 2023, 278, 104865. **doi: 10.1016/j.jprot.2021.104381**

20 H. M. Santos., Advances in Experimental Medicine and Biology, 2021, 1306 v-vi. **doi: 10.1002/9781118886953.fmatter**

21 M. Proti et al., Bioanalysis 2025, 13:2, 1-5. **doi: 10.1080/17576180.2025.2546782**

RESEARCH THEMES/
BIOLOGICAL CHEMISTRY AND DISEASE-RELATED MECHANISMS

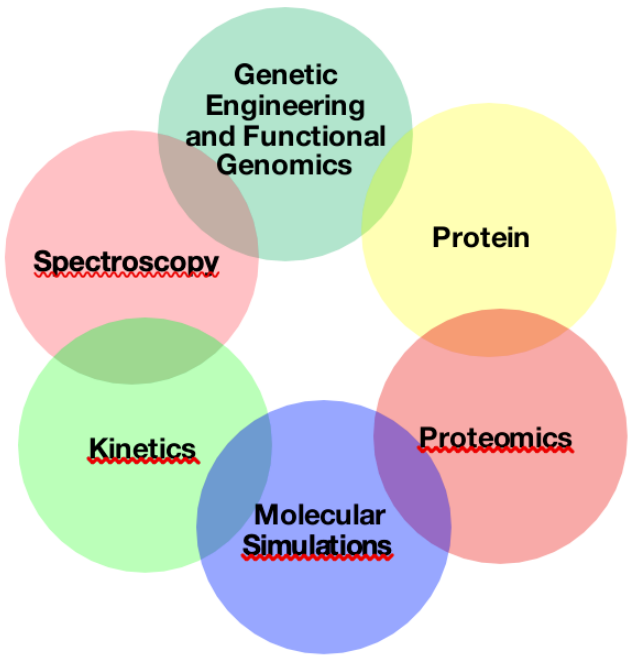
We aim to solve complex biological problems using the know-how gathered from Chemistry and Biology.[22-31]

NITROGEN BIOGEOCHEMICAL CYCLE – DENITRIFICATION

Denitrification is a key anaerobic process in the N- biocycle, converting nitrate to dinitrogen in sequential redox reactions catalyzed by metalloenzymes. Biophysical and structural studies of electron-transfer complexes highlight the role of transient protein–protein interactions and molecular recognition in ensuring relevant pathways with implications on environmental, agriculture, and global warming. Mechanistic and structural characterization of nitric and nitrous oxide reductases has revealed how metal centers (Cu and Fe), enable efficient electron and proton transfer.

Molybdenum (and Tungsten) Enzymes in N - C Biocycles

Mo- and W-dependent enzymes play central roles in nitrogen and carbon cycling in key transformation of nitrate, nitrite, and carbon dioxide, coupling redox chemistry to metal cofactors, fine-tuning catalytic activity and substrate specificity, particularly in nitrate reduction, nitrite reduction, and nitrite oxidation. Structural and spectroscopic relate active-site architecture and electron-transfer pathways. Novel Mo-dependent nitrite reductases have been studied, and formate dehydrogenases have been discovered that reversibly catalyze formate and carbon dioxide interconversion, with important implications for CO_2 scavenging. Artificial model Mo-enzymes have been developed.



SELECTED PUBLICATIONS

22 J. J. G. Moura, et al., Eds.; Springer: Cham, Switzerland, 2021.
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RESEARCH THEMES/ BIOLOGICAL CHEMISTRY AND DISEASE-RELATED MECHANISMS

METABOLOMICS, LIPIDOMICS, AND PROTEOMICS PROFILING OF METABOLIC SIGNATURES

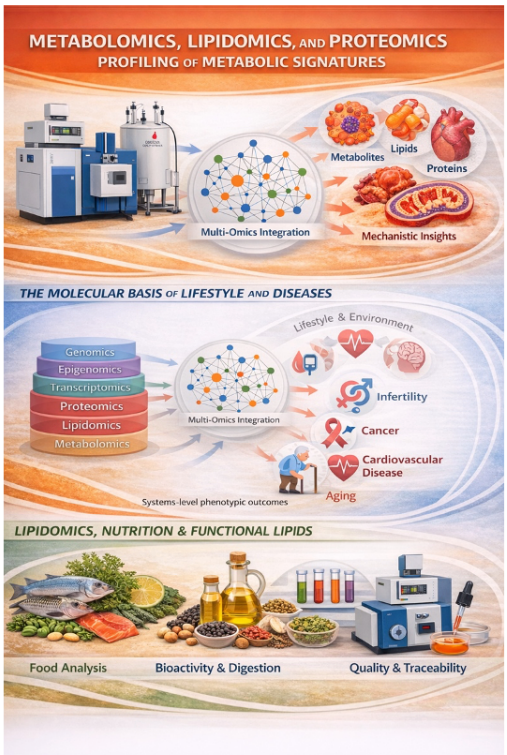
We use mass spectrometry–based metabolomics, lipidomics, and proteomics, and NMR when useful, to map metabolic signatures and pathway reprogramming under defined elicitors. By integrating multi-omics, we connect metabolites, lipids, and proteins to regulation and functional readouts, moving from descriptive profiles to mechanisms that explain adaptation to disease and environmental stress.

THE MOLECULAR BASIS OF LIFESTYLE AND DISEASES

We study noncommunicable diseases using immunohistochemistry and omics across in vitro, ex vivo, and in vivo models plus human fluids and biopsies. We focus on wasting syndromes, biomarker discovery/validation, lifestyle-driven biochemical effects, and mitochondrial bioenergetics and plasticity in pathophysiological states, aiming for measurable endpoints for stratification and intervention monitoring.

THE BRIDGE BETWEEN LIPIDOMICS, NUTRITIONAL VALUE AND FUNCTIONAL PROPERTIES OF LIPIDS

We apply MS-lipidomics to foods, by-products, plants, marine organisms, and algae to identify and characterize value-added lipids. We link composition to bioactivity, digestibility, and bioavailability; quantify lipid plasticity in response to environment and processing; and develop lipid markers for authentication, adulteration detection, and traceability, supporting quality control and biotechnological applications.



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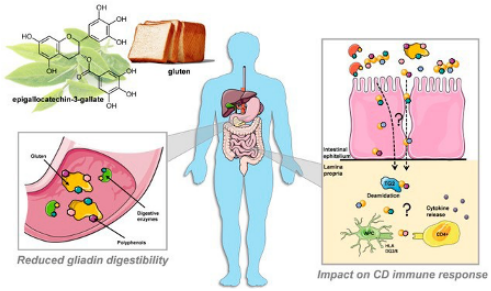
RESEARCH THEMES/
FUNCTIONAL GENOMICS AND PROTEOMICS

This unit develops research work focused on the use of omics tools, particularly genomics, transcriptomics, and proteomics, at the molecular genetics and biotechnology level of various microbial, plant, and animal species. Research carried out is focused on i) storage proteins characterization of populations/landraces of vegetables, cereals, grain legumes, fruit trees, medicinal and aromatic species and industrial crops; ii) recovery and breeding of Portuguese landraces of vegetables and cereals; iii) identification of genes responsible for important economic fruit traits and antibiotic resistance in bacterial strains; and iv) evaluation through genomic-transcriptomic-proteomic platform linked to agriculture and natural ecosystems.



Genomic, transcriptomic, and proteomic characterization of genetic resources of Gramineae;

Proteomic of new genes controlling grain functionality and allergenicity applied to wheat, rye, and triticale;

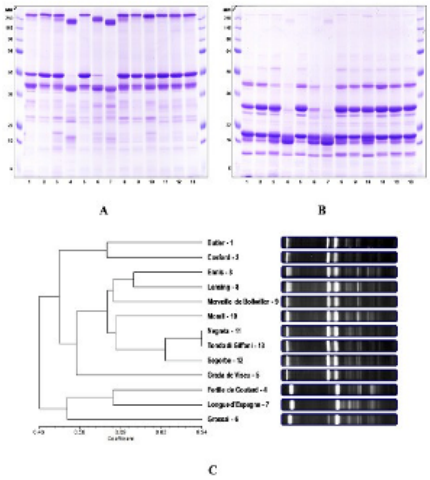
Nutrigenomics, nutriproteomics applied to proteaginous species; Proteomics applied to the detection of genes responsible for the of wheat grain;

Phenotyping through nutrigenomics and proteomics applied to the evaluation of species:

Yield nutritional, quality, functionality and allergenicity

Probiotics in biotechnology health and the hydrogenome role;

BACT_ONE_OMICS: Genomic and proteomic evaluation of antibiotic resistance in bacterial strains of wild and domestic animals and humans.



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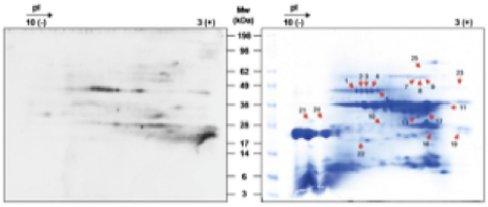
RESEARCH THEMES/
ANTIMICROBIAL RESISTANCE SURVEILLANCE IN PORTUGAL

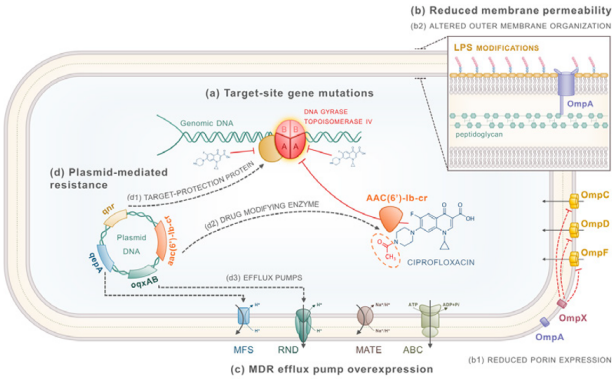
Antimicrobial resistance has become one of the most serious public health concerns of the 21st century, with modern medicine now facing increasing numbers of severe multidrug-resistant infections alongside a dwindling pipeline of new antimicrobials. Improved detection of the multiple, overlapping, and compensatory mechanisms typically involved in the acquisition of resistance has been achieved through the coordinated use of high-throughput proteomics and bioinformatics techniques, complemented by various genomics, transcriptomics, and metabolomics approaches.



MECHANISMS OF MULTIDRUG RESISTANCE

The group develops part of its research activities on the detection of foodborne pathogens and specific spoilage organisms in foods of animal origin across different food production chains. Within this scope, major microbiological hazards involved in foodborne outbreaks—such as Salmonella spp., Escherichia coli, and methicillin-resistant Staphylococcus aureus (MRSA)—are investigated. The team is also developing novel approaches to analyze and interpret complex and emerging microbial pathogens using molecular techniques, serotyping, and phylogenetic analyses. Furthermore, efforts are directed toward improving knowledge on pathogen prevalence, identifying sources of contamination, assessing risks to public health, and developing strategies to enhance food safety and quality.

Antibiotic resistance is addressed within a One Health framework, integrating human, animal, and environmental perspectives..



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RESEARCH THEMES/
EMERGING CHALLENGES ON AGRIFOOD MODELS

Aligned with the EU Green Deal Pillars, our research is focused on using biochemistry, omics and biology tools to understand how emerging environmental challenges impact agrifood production and quality. From the molecule to the field, we are focused on understanding cell-cell relations and finding sustainable solutions towards a Greener world.

BIOTECHNOLOGY FOR AGRIFOOD SECURITY AND SAFETY[61-63]

Antimicrobial peptides (AMPs), nanoformulations, and essential oils are developed to control plant diseases or improve resistance to climate change, using in vitro/ in vivo crop models, and physiological, molecular, transcriptomic, and metabolomic data are integrated for defining functional models.

PLANT-MICROBIOME SOCIAL RELATIONS AND SYNTHETIC COMMUNITIES[64, 65]

The structural composition of microbiomes/phytobiomes and their social networks are characterized by cytometry, metagenomics, transcriptomics, in in vitro/in vivo models. Pathogens (Xanthomonadales, Pseudomonadales), and new BCAs and PGPs, are characterized, through SynComs, and using wild and mutant strains.

MOLECULAR PLAYERS INVOLVED IN SEED PRODUCTION[66-69]

We unveil how plants' plasticity to environment influence their reproductive performance. We use transcriptomics, proteomics, histological and imaging techniques to exploit gene regulatory networks controlling cell communication and wall composition from ovule to seed dehiscence.

BIOCHEMISTRY OF GLYCOSYLATED PROTEINS[70]

Sugars are key signaling molecules for the plant's life, and can be released from glycosylphosphatidylinositol (GPI)-anchored proteins present in cell walls. To understand aspects of the proteins' glycosylation we perform structural carbohydrate biochemistry, enzymology, biophysics of cell walls, and proteins' subcellular localization and function.

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RESEARCH THEMES/
INNOVATIVE SAMPLE TREATMENT

Sample treatment is the bottleneck of analytical procedures as it takes about 70% of total analysis time and is labor intensive. Almost all advanced instrumental methods of analysis require samples to be as much as possible free from interfering molecules, namely biomolecules and dissolved salts. Further, societies' pressure for knowledge about trace levels demands for extraction and concentration of target analytes.

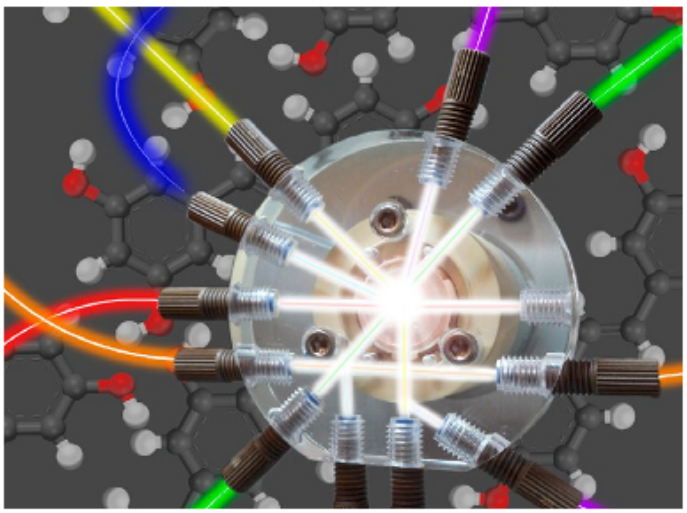
Therefore, research efforts will be focused on innovative strategies for sample treatment, aiming the reduction of time, cost, and reagents spent in this analytical step. Three main vectors will be exploited: (i) automation; (ii) new devices based on 3D printing; (iii) miniaturization.

Automation will be sought through flow-based schemes, fostering online hyphenation to other instrumentation for integrated, streamlined methods with minimal intervention from operators, including solid-phase extraction using tubular capillaries and new sorbent phases.

3-D printing is revolutionizing many areas and analytical development is included. Microfabricated devices are now designed and prepared within hours, providing fit-for-purpose solutions. This enticing area for sample treatment will be implemented through the design of microdevices for membrane-based separation of analytes, aiming desalting of complex samples or extraction of organic compounds through membrane assisted liquid extraction.

Miniaturization is the third vector to be pursued for innovative sample treatment as it will have a direct impact on the amount of sample needed and on method sustainability. This will be implemented through 3-D printing of low scale devices, with extraction/

reaction chambers with volumetric capacity within the microliter range. Miniaturized, renewable solid-phase schemes will be also implemented through the Lab-on-Valve platform using the bead injection concept.



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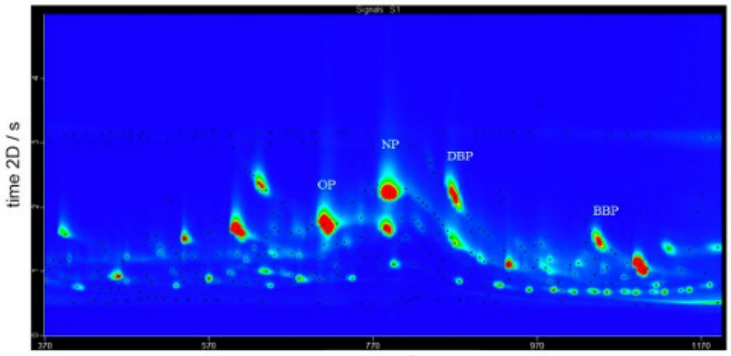
RESEARCH THEMES/
MULTIDIMENSIONAL METHODS FOR TOTAL ANALYSIS

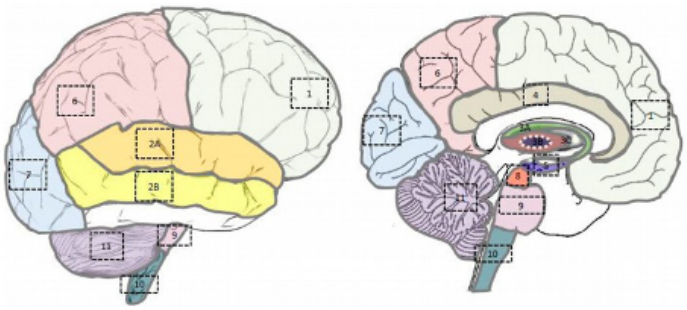
One of the trends in analytical sciences is the implementation of comprehensive methods, able to extract the maximum amount of information from a given sample within a single analytical run. This is possible using multidimensional setups, consisting of several detectors in series, orthogonal separative methods, and/or multidimensional mass spectrometry.

Research efforts in this area will address bidimensional gas chromatography coupled to mass spectrometry for evaluation of traditional products and food commodities, aiming to collect science-based evidence for the promotion of economic value added. Orthogonal separative methods (e.g. size exclusion × hydrophobic interaction or immunoaffinity × hydrophilic interaction) will be developed to provide complete profiles and characterization of samples.

Concerning multidimensional mass spectrometry, research will be focused on inductively coupled plasma mass spectrometry for multi-elemental analysis, and on tandem mass spectrometry methods for screening and quantification of emerging contaminants in environmental and food samples.

For biological applications, namely differentiation of bacterial species and strains, matrix-assisted laser desorption/ionization (MALDI) coupled to time-of-flight mass spectrometry (ToF-MS) developments will provide comprehensive information to be untangled by chemometric tools.





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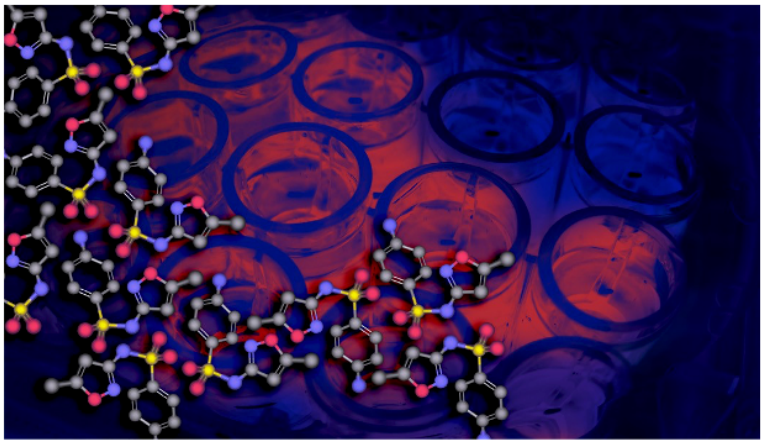
RESEARCH THEMES/
GREENER ANALYTICAL METHODS

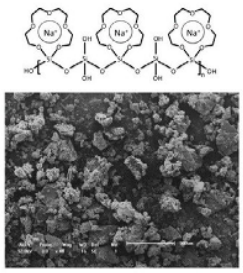
Sustainability is the key word in modern Chemistry. Analytical developments must embrace this paradigm and research within this topic will focus on providing analytical solutions with low environmental impact.

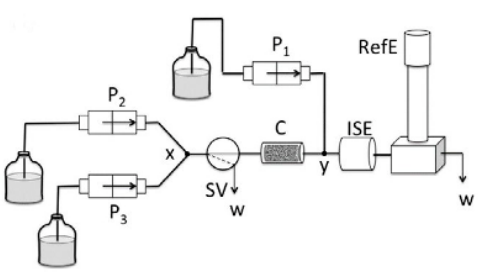
For this, methods based on the physical-chemical properties of target analytes will be sought, namely using electrochemical-based detectors and infrared/Raman spectroscopy associated to data fusion chemometrics.

Innovative sensor construction, using 3-D printing for the fabrication of supports and sensor layer deposition, will be pursued. Further, advanced chemometrics for sample classification (random forests, Tucker 3 and PARAFAC), and for concentration estimation (group-wise, and support vector machine partial-least squares) will be tested to design robust, portable, in situ methods for evaluation of food and environmental contaminants, with low cost and reagentless features.

Methods based on image analysis, using reagent volumes in the microliter range, will be developed. Through the design of dedicated apps, mobile devices, namely smart-phones and tablets, will be used to gather images and analytical information from photos upon reaction development, providing low-cost and accessible analytical platforms.







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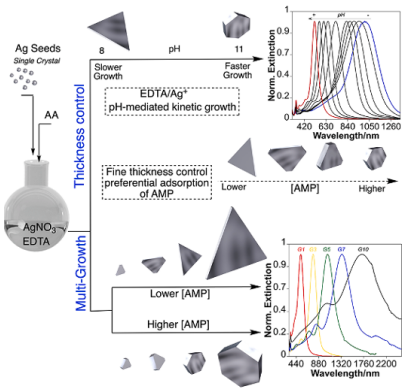
HIGHLIGHTS

PRECISE CONTROL OF SILVER NANOPLATE DIMENSIONS AND OPTICAL PROPERTIES VIA PH, EDTA AND AMP MEDIATED SYNTHESIS

We studied a seed-mediated synthesis method for producing silver nanoplates (AgNPTs) with customizable size and thickness, ensuring high yield and precise optical properties. This approach leverages ethylenediaminetetraacetic acid (EDTA) as a key component in the synthesis process, utilizing small single-crystal silver seeds. The interaction between Ag+ ions and EDTA at varying pH levels dynamically regulates silver complexation and reduction kinetics during seed overgrowth, leading to the formation of truncated nanoplates with superior optical responses. By adjusting the pH within the range of 8–10.5, we can manipulate the growth of the nanoplates, enabling a flexible optical response ranging from 519 to 1006 nm due to changes in their size and thickness

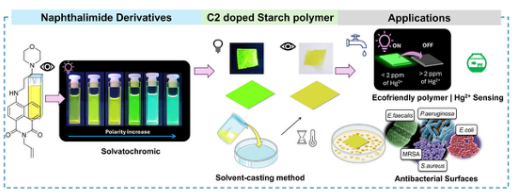


Precise control of silver nanoplate dimensions and optical properties via pH, EDTA and AMP mediated synthesis .

J. Col. Intf. Science, 2025, 680, 286-2979

FLUORESCENT POLYMERS FOR ENVIRONMENTAL MONITORING: TARGETING PATHOGENS AND METAL CONTAMINANTS WITH NAPHTALIMIDE DERIVATIVES

Monitoring Hg2+ levels in aqueous environments is crucial to assess the potential methylmercury contamination via bacterial conversion, however, existing methods often require extensive sample treatment and expensive equipment. To mitigate this issue, this study examines the synthesis and application of three naphthalimide-based compounds, with significant fluorescent and solvatochromic behavior. Two Compounds demonstrated a strong affinity for Hg2+ metal ions, with the other showing selectivity and a strong antibacterial profile, particularly against S. aureus (MIC50 (C2) = 0.01 µg/mL). Moreover, these compounds were incorporated into three polymeric matrices, namely polyvinyl chloride (PVC), poly (methyl methacrylate-co-methacrylic acid) (PMMMA), and Starch, allowing for the development of solid-support sensors/surfaces with a strong antibacterial profile, highlighting the inherent dual-functionality of the compounds. Interestingly, the C2-doped Starch biopolymer detected low concentrations of Hg2+ ions, such as 23 nM in tap water (value within the WHO standards for drinking water), through a rapid spectroscopic evaluation without sample treatment. green-chemistry-oriented, temperature-dependent water/Starch. synthetic route, without the addition of plasticizers and any associated ecotoxicity.



The study used sustainable methods for environmental monitoring and antibacterial applications, advancing material science to offer effective, accessible, and eco-friendly solutions for detecting and mitigating mercury pollution and bacterial contaminations, enhancing environmental and health safety.

Fluorescent Polymers for Environmental monitoring: Targeting pathogens and metal contaminants with naphatalimide derivatives.

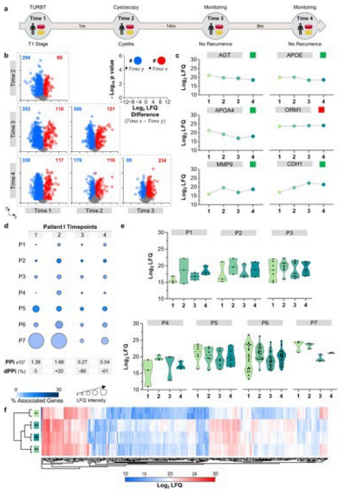
J. Haz. Mat, 2024, 480, 136107

HIGHLIGHTS

PATHWAY-GUIDED MONITORING OF THE DISEASE COURSE IN BLADDER CANCER WITH LONGITUDINAL URINE PROTEOMICS

Monitoring bladder cancer over time requires invasive and costly procedures. Less invasive approaches are required using readily available biological samples such as urine. In this study, we demonstrate a method for longitudinal analysis of the urine proteome to monitor the disease course in patients with bladder cancer.

We compared the urine proteomes of patients who experienced recurrence and/or progression (n = 13) with those who did not (n = 17). We identified differentially expressed proteins within various pathways related to the hallmarks of cancer. The variation of such pathways during the disease course were determined using our differential personal pathway index (dPPi) calculation, which could indicate disease progression and the need for medical intervention. Seven hallmark pathways are used to develop the dPPi. We demonstrate that we can successfully longitudinally monitor the disease course in bladder cancer patients through a combination of urine proteomic analysis and the dPPi calculation, over a period of 62 months. Using the information contained in the patient's urinary proteome, the dPPi reflects the individual's course of bladder cancer, and helps to optimise the use of more invasive procedures such as cystoscopy.

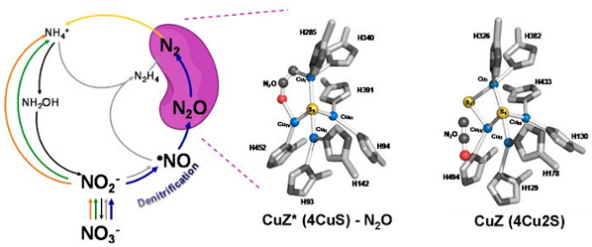


Pathway-guided monitoring of the disease course in bladder cancer with longitudinal urine proteomics

Communications Medicine (Nature), 2023, 3-8

UNVEILING THE DENITRIFICATION SECRETS: UNDERSTANDING THE REDUCTION OF N_2O

In denitrification, bacteria reduce NO3- to N2 gas through 4 steps catalyzed by metalloenzymes to derive energy. In the last step, N2O, a powerful greenhouse gas is reduced to N2 by N2O reductase a copper-containing enzyme harboring a unique tetranuclear catalytic center, that can exist as a [4Cu2S] center, named CuZ, or as a [4CuS] center, named CuZ*. We have characterized kinetically and spectroscopically the CuZ center and accessed the effect of pH in in the denitrification pathway of M. hydrocarbonoclasticus and on N2O reductase. We also estimated the reduction potential of CuA and CuZ(4Cu2S) by potentiometry to be +275 ± 5mV and +65 ± 5mV vs SHE, respectively, at pH 7.6. Understanding this enzyme that can transform N2O in an inert gas, is a crucial step to the design of N2O mitigation strategies..



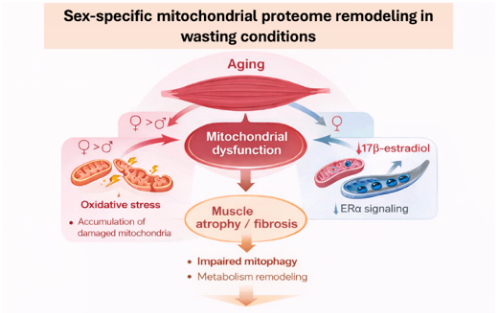
Spectroscopic definition of the CuZ* intermediate in turnover of nitrous oxide reductase and molecular insight into the catalytic mechanism.

Coordination Chemistry Reviews, 2019, 387, 436-449

HIGHLIGHTS

SEX-SPECIFIC MITOCHONDRIAL PROTEOME REMODELING IN WASTING CONDITIONS

Sex-specific mitochondrial remodeling represents a shared mechanism linking aging, cancer, and therapeutic wasting, potentially driving sex differences in disease progression and treatment response. This study presents the first sex-specific mitochondrial proteomic analysis of aging skeletal muscle, revealing more severe age-related mitochondrial dysfunction in females, marked by altered fatty acid oxidation, respiratory chain loss, oxidative damage, and impaired mitophagy, highlighting sex-dependent vulnerabilities relevant to sarcopenia interventions.

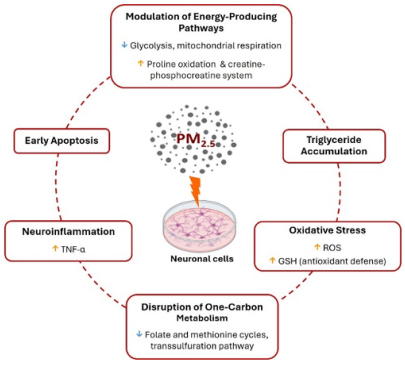


Mitochondrial remodeling underlying age-induced skeletal muscle wasting: let's talk about sex.

Free Radic Biol Med. 2024; 218:68-81

CYTOTOXIC AND METABOLIC EFFECTS OF ORGANIC EXTRACTS FROM AIRBORNE FINE PARTICULATE MATER (PM2.5) IN NEURONAL CELLS

Fine particulate matter (PM2.5) is associated with neurological diseases, but its cellular effects are poorly understood. This study examined PM2.5 from São Paulo, Brazil, on SH-SY5Y neuroblastoma cells. At low toxicity levels, PM2.5 organic extracts induced apoptosis, increased TNF- release, and triggered oxidative stress. Metabolomics revealed reduced glycolysis and TCA activity, lower ATP, and compensatory proline oxidation and lipid accumulation. Disruption of one-carbon metabolism and elevated glutathione suggested disturbed energy and redox homeostasis underlying PM2.5 neurotoxicity.



Cytotoxic and metabolic effects of organic extracts from airborne fine particulate matter (PM2.5) in neuronal cells.

Environ Toxicol Pharmacol. 2025; 116:104707

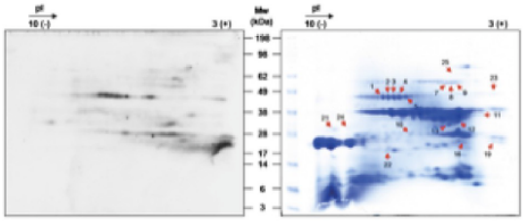
HIGHLIGHTS

ANTIMICROBIAL RESISTANCE SURVEILLANCE IN PORTUGAL

Antimicrobial resistance has become one of the most serious public health concerns of the 21st century, being modern medicine presently challenged with increasing numbers of severe multiresistant infections in face of a drying pipeline for new antimicrobials. An improved detection of the multiple, superposing, and compensatory mechanisms usually involved in resistance acquisition was achieved through the coordinated use of high-throughput proteomics and bioinformatics techniques complemented with different genomics, transcriptomics, and metabolomics methods.

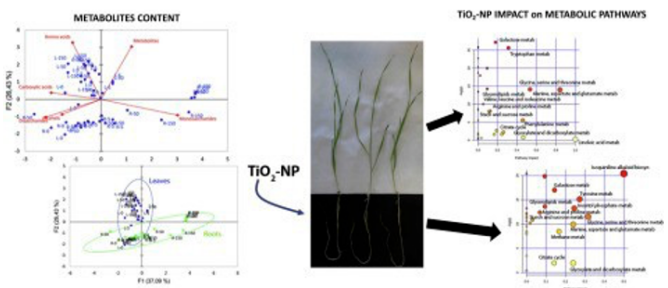
Multiomics Substrates of Resistance to Emerging Pathogens? Transcriptome and Proteome Profile of a Vancomycin-Resistant Enterococcus faecalis Clinical Strain.

OMICS A Journal of Integrative Biology, 24(2):81-95



BIOACTIVITY OF ENGINEERED NANOPARTICLES COVERING DIFFERENT BIOLOGICAL MODELS

Nanomaterials have multiple sources of origin, characteristics, composition, form, bioactivity and function. They present unique properties opening wide technological possibilities, but also their bioactivity must be followed as their toxicity is highly complex and dependent on multiple variables. We have addressed the bioactivity of metal nanoparticles (eg AgNPs, TiNPs) on multiple models, from plant crops to human cells. The screen for bioactivity in human cells involves transcriptomics and metabolomics and cell biology tools to
search for functional pathways, in eg intestinal, lung and epidermal cells in response to concentration, size, coating and composition of several metal NPs. Besides energetic shifts also oxidative stress and necrosis/ apoptosis related pathways are surveyed. The screen for their toxicity/ bioactivity on plants was assessed on multiple crop models, unveiling disruption at photosynthetic and redox status levels in a way dependent on the dose, type, formulation, coating, species, organ, etc. The potential of some NPs on agrifood systems and in remediation is under study.



TiO2 nanoparticles induced sugar impairments and metabolic pathway shift towards amino acid metabolism in wheat.

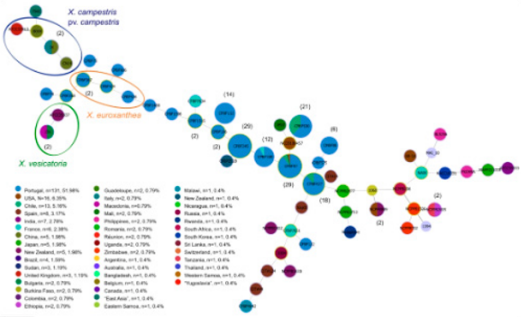
J. of Hazardous Materials 2020, 399, 122982

HIGHLIGHTS

TARGETED ENGINEERING OF MICROBIOMES AS A NEW GENERATION IN AGRIFOOD BIOCONTROL

Along with the Farm-2-Fork EU strategy, biotechnology, omics, and bioinformatics gather efforts to develop new biocontrol strategies aligned with precision agriculture, reducing food waste in pre- and post-harvest, and valorizing local genetic resources.

The microbiomes contribute to the plants' performance, signaling, and resistance to diseases. We have characterized by metagenomics the microbiomes of multiple crops (e.g., Actinidia, Vitis vinifera, Vaccinum spp.), and pests (e.g., D. suzukii), and isolated several BCAs against pathogens (e.g., from Pseudomonadales), and PGPs (e.g., Trichoderma spp, Bacillus spp.). Candidate strains compatibility is in sillico characterized, and they are combined as SynCOMs to optimize targeted functions of the plant. This approach of studying the microbial diversity and their mode of interaction (microbiome shifts, antibiosis, etc) allows identifying antagonisms and synergisms, that combined in SynCOMs, are being used for identifying new pathogenic species in Portugal (e.g., Erwinia rhapontici), new BCAs and PGPs.



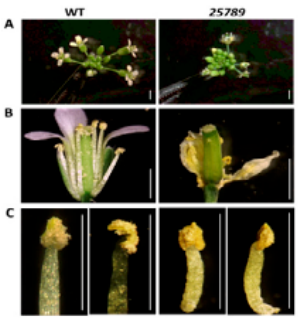
Comprehensive diversity assessment of walnut associated xanthomonads reveal the occurrence of distinct Xanthomonas arboricola lineages and of a new species (Xanthomonas euroxanthea) within the same tree.

Plant Pathology, 2021, 70(4): 943-958

JAGGER LOCALIZATION AND FUNCTION ARE DEPENDENT ON GPI ANCHOR ADDITION

Successful double fertilization in flowering plants relies on precise delivery of two sperm cells to the female gametophyte within the ovule. Arabidopsis ovules prevent polyspermy by limiting attraction of multiple pollen tubes. However, Arabidopsis jagger mutants exhibit impaired synergid degeneration, resulting in multiple pollen tubes attracted to a single ovule. JAGGER encodes a putative arabinogalactan protein which is predicted to be anchored to the plasma membrane by a glycosylphosphatidylinositol (GPI) anchor.

Here, we show that JAGGER fused to citrine yellow fluorescent protein (JAGGER-cYFP) is functional and localizes mostly to the periphery of ovule integuments and transmitting tract cells. We further investigated the importance of GPI-anchor addition domains for JAGGER localization and function. Different JAGGER proteins with deletions in predicted-site regions and GPI attachment signal domain, expected to compromise the addition of the GPI anchor, led to disruption of JAGGER localization in the cell periphery. All JAGGER proteins with disrupted localization were also not able to rescue the polytubey phenotype, pointing to the importance of GPI-anchor addition to in vivo function of the JAGGER protein.



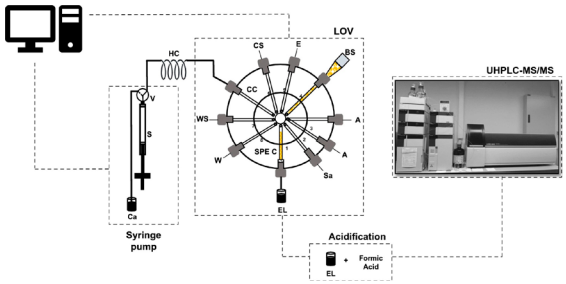
JAGGER localization and function are dependent on GPI anchor addition.

Plant Reproduction, 2024, 37(3): 341-353

HIGHLIGHTS

AUTOMATION OF SAMPLE TREATMENT FOR NON-INVASIVE SAMPLING

Tranexamic acid (TXA) is a synthetic analogue of the amino acid lysine and an important antifibrinolytic agent used in the prevention of bleeding in several haemorrhagic scenarios. An automatic micro-solid-phase extraction (μSPE) method using on-line renewable sorbent beads followed by liquid chromatography–tandem mass spectrometry was established for the determination of TXA in urine. The μSPE method was based on the bead injection (BI) concept combined with the mesofluidic lab-on-valve (LOV) platform. All steps of the μSPE–BI–LOV were implemented by computer programming, rendering enhanced precision on time and flow events. The sample treatment was implemented using a hydrophilic-lipophilic balanced mixed-mode sorbent, decorated with sulfonic acid groups, while chromatographic separation was performed using a BEH amide column coupled to MS/MS detection in positive ionization mode. The method was successfully applied to urine samples collected during scoliosis surgery of paediatric patients treated with TXA using non-invasive sampling, and the information obtained enabled a better understanding of the drug elimination profile of TXA.

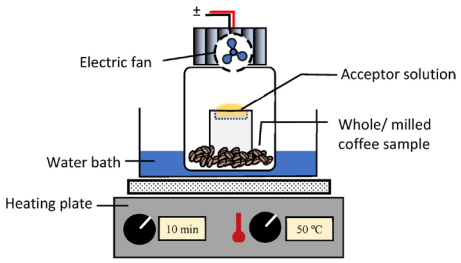


Automatic and renewable micro-solid-phase extraction based on bead injection lab-on-valve system for determination of tranexamic acid in urine by UHPLC coupled with tandem mass spectrometry.

Anal. Bioanal. Chem., 2022, 414, 649-659

FAN-ASSISTED EXTRACTION OF COFFEE VOLATILES

Defective coffee beans may represent up to 20% of the coffee production and the removal of defective coffee beans is needed to increase the market value of this good and/or to fulfil the commercialization quality criteria. Therefore, analytical methodologies to evaluate roasted coffee quality are needed to identify the volatile compounds which are the most predominant in defective and healthy beans. An innovative and simple approach for volatile compounds extraction based on fan-assisted extraction system was established for enhanced sample treatment. The extraction system comprised a closable flask inside which the solid sample and the reservoir containing the acceptor solution (with a derivatizing reagent) are previously placed. The flask features an internal electric fan that increases the mass transport in the gaseous phase. Due to the derivatization reaction involved, the equilibrium state of the volatile compounds between the headspace and the solid sample is not reached and the extraction process is continuous, providing a fast and high extraction yield. The further characterization of the volatile carbonyl compounds of roasted healthy and defective coffee beans by HPLC-DAD-MS/MS showed differences among the distinct bean typologies assayed, including the presence of 2-methyloxolan-3-one and furfural as the most important indicators of healthy beans.



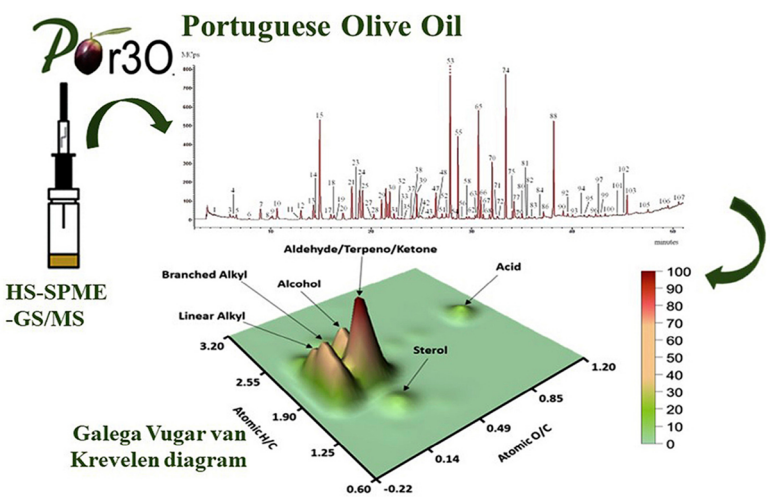
Fan assisted extraction and HPLC-DAD-MS/MS identification of volatile carbonyl compounds as chemical descriptors of healthy and defective roasted coffee beans.

Food Control, 2022, 138, 109014

HIGHLIGHTS

COMPREHENSIVE GAS CHROMATOGRAPHY FOR ADVANCED SAMPLE PROFILING

A method based on head-space solid phase micro- extraction hyphenated to gas chromatography-mass spectrometry (GC-MS) provided the identification and semi-quantification of a total of 107 compounds belonging essentially to the chemical classes of esters, alcohols, aldehydes, acids, ketones, linear and branched alkyl sulphur compounds and terpenoids, present in olive oil. Total abundances were plotted in modified 3D van Krevelen diagrams. Discriminant analysis confirmed that the pattern of volatile compounds included enough information to group sample variety amongst discrete monovarietal extra-virgin olive oil. The combination of statistical analysis (t-Student) and graphical-tools (van Krevelen diagram) was demonstrated to be a powerful approach to determine which molecular families were characteristic of each olive oil variety, contributing to the valorization of monovarietal Portuguese olive oil. Comprehensive GC-MS has also been instrumental to unveil olfactory responses of wasps and to assess the impact of storage conditions on the chemical profile of beers, contributing to establish enhanced, discriminatory profiles of complex samples.



Revisiting 3D van Krevelen diagrams as a tool for the visualization of volatile profile of varietal olive oils from Alentejo region, Portugal.

Talanta, 2020, 207, 120276

Olfactory responses of Anaphes nitens (Hymenoptera, Mymaridae) to host and habitat cues.

J. Appl. Entomol., 2021, 145, 675-687

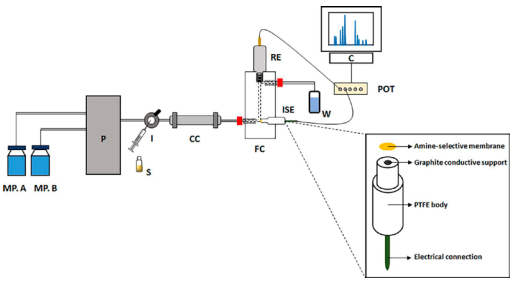
Impact of temperature during beer storage on beer chemical profile.

LWT, 2022, 154, 112688

HIGHLIGHTS

COUPLING POTENTIOMETRIC SENSORS TO LIQUID CHROMATOGRAPHY FOR GREENER ANALYTICAL METHODS

Potentiometric sensors have an underexploited potential for detection of families of compounds, with improved selectivity when associated to separative techniques such as liquid chromatography. Potentiometric sensors based on cucurbit[n]uril as ionophore have been proposed for molecular recognition of positively charged guests, including biogenic amines and tetracyclines after separation by HPLC. A wall-jet flow-cell was used to hold an amine-selective electrode, based on cucurbit[6]uril as an ionophore, and the target biogenic amines present in tomatoes were separated in < 20 min using a C18 column as the stationary phase and gradient elution with a mobile phase containing lithium formate buffer, acetonitrile, and butane-sulfonic acid sodium salt as an ion-pair agent. For analysis of biogenic amines in alcoholic beverages, the incorporation of multi-walled carbon nanotubes in the sensing membrane and the replacement of the acidifying agent in the mobile phase, from lithium formate buffer to acetic acid, were the most relevant factors for lowering the detection limits and achieving a high separation efficiency in < 25 min. For determination of tetracyclines, a new tetracycline-selective electrode, based on a polymeric membrane incorporating cucurbit[8]uril as a macrocyclic host, potassium tetrakis(p-chlorophenyl) borate as an ionic additive, 2-fluorophenyl 2-nitrophenyl ether as a plasticizer, and multi-walled carbon nanotubes as nanostructured materials, was proposed and coupled to chromatographic separation by a C8 column using a gradient mobile phase of sulfuric acid and acetonitrile.



Determination of biogenic amines in tomato by ion-pair chromatography coupled to an amine-selective potentiometric detector.

Electrochim. Acta, 2021, 378, 138134

HPLC-potentiometric method for determination of biogenic amines in alcoholic beverages: A reliable approach for food quality control.

Food Chem., 2022, 372, 131288

Cucurbit[8]uril-based potentiometric sensor coupled to HPLC for determination of tetracycline residues in milk samples.

Chemosensors, 2022, 10, 98

MOBILE DEVICES FOR ANTIBIOTICS SCREENING

The presence of antibiotics in the environment, particularly in water resources, can stimulate the emergence of resistant microorganisms, requiring affordable methods for screening and monitoring. A chemosensor for screening of sulfonamides in environmental waters was developed, based on the retention of sulfamethoxazole (as model sulfonamide) in disks containing polystyrene divinylbenzene sulfonated sorbent particles and on the colorimetric detection using a computer vision algorithm, after reaction with p-dimethylaminocinnamaldehyde. Images were acquired using a mobile device and several color spaces (RGB, HSV, CIELAB) were tested, with the coordinate a_star, from the CIELAB color space, providing the highest sensitivity. In order to avoid bias from illumination conditions, a correction using the a_star value from one of the color patches present in a color palette disposed in the same picture as the analytical disk was also implemented. The method was applied to field experiments with insitu sampling, allowing the quantitative determination of sulfonamides at microgram per litre level using only 10 mL of sample, rendering a cost-effective approach where positive samples were directed to laboratory-based comprehensive reanalysis.

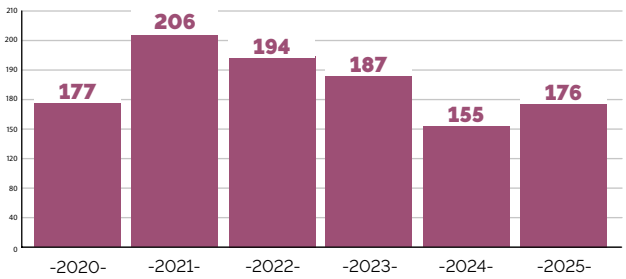
Development of a screening method for sulfamethoxazole in environmental water by digital colorimetry using a mobile device.

Chemosensors, 2022, 10, 25

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION

Articles published / Year



H-index: **52**

1095 articles*
16846 citations

*01/2020-12/2025
From WOS core collection

FUNDED PROJECTS

(Representative projects)

- **Optimized oxidative enzyme systems for efficient conversion of lignocellulose to valuable products - OXYMOD,**
  ES583910 / Forskerprosjekt - BIOTEK2021, José Moura (co-PI). Total funding: € 55,000.00
- **Optimizing natural low toxicity of wheat for celiac patients through a nano/microparticles detoxifying approach.**
  PTDC/BAA-AGR/29068/2017, Gilberto Igrejas (PI). Total funding: € 233,673.90
- **Bio-HhOST next generation 3D tissue models: Bio-hybrid hierarchical organoid-synthetic tissues (Bio-HhOST) comprised of live and artificial cells.**
  Funded by European Union's Horizon Europe EIC 2023 Pathfinder Open programme under grant agreement No 101129734; 466 020.00 €; Local PI: Iola Duarte
- **BIOmimetic selective extraction MEMbranes (BIOMEM).**
  Horizon Europe EIC 2023 Pathfinder Open programme, UA: 449 360.00€ PI UA: Tânia Melo
- **Exploring gut microbiota-metabolome interactions in breast cancer neoadjuvant therapy: searching for new response predictors.**
  Funded by Fundação para a Ciência e a Tecnologia, Ref. 2023.14914.PEX; 49 991.00 €; PI: Iola Duarte
- **Development of adjustable Silver@Silica nanocarriers and their stabilization in solid materials against drug resistant and non-resistant pathogenic bacteria.**
  PTDC/QUI-COL/1517/2020. (PI: J. Fernández-Lodeiro, CoPI: C. Lodeiro). Total funding: € 233,038.50
- **Pinpointing absolute phosphorylation stoichiometry in human cells using new polystyrene nanoparticle-based immobilized lanthanide ion affinity chromatography and motif-targeting quantitative proteomics.**
  Hugo Santos (PI). Total funding: € 50,000.00
- **MET4Cat - synthetic methodologies for metal nanocatalyst based in Gold, Palladium and Platinum and the study of their catalytic performance in key reactions.**
  EXPL/QUI_COL/0263/2021 (P.I: A. Fernández-Lodeiro. CoPI: J. Fernández-Lodeiro). Total Funding: € 50,000.00
- **Reducing the Water misuse in a Nano@Dyes Synthesis Lab.**
  The Royal Society of Chemistry (Registered No. RC000524) and a Registered Charity No. 207890, March 2024. – (P.I: C. Lodeiro, CoPI: Hugo M Santos). € 11398.84
- **Development of Rare Earth based light converters: Luminescent Markers, Optical Sensors and Amplifiers.**
  Tematico FAPESP (Brazil) . (P.I.: Hermi Felinto de Brito (USP) – Member C. Lodeiro) 2022-2027 667.310,43,00 $

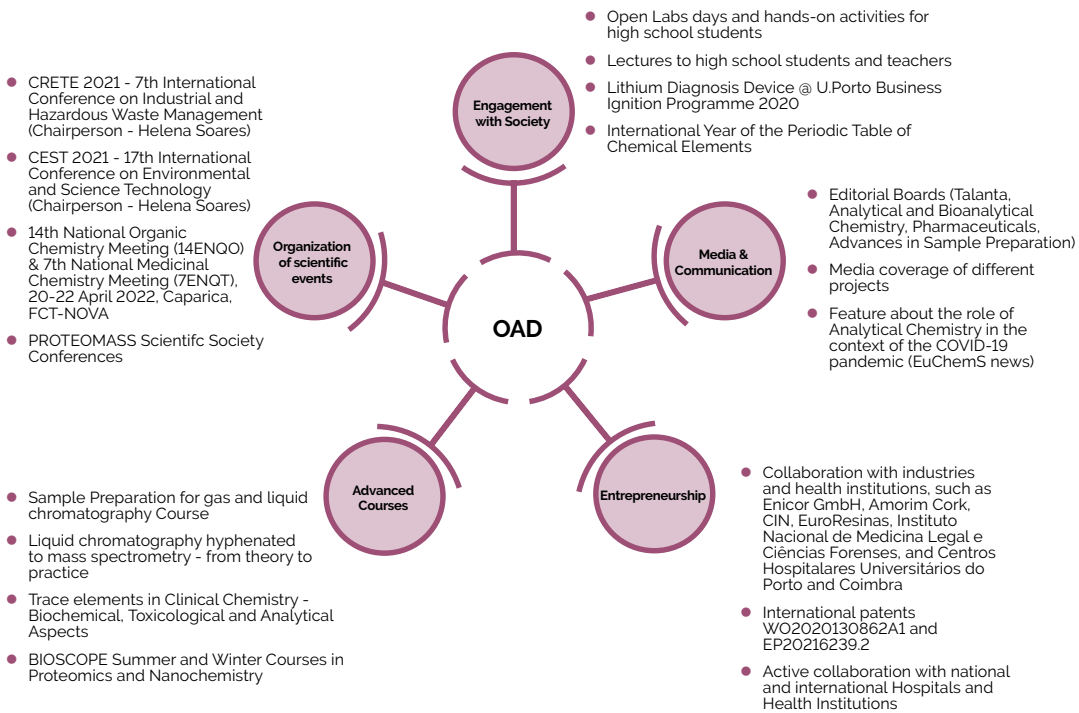
- **Unique Cu cluster in the mitigation of green house gas.**
  PTDC/QUI-BIOQ/01152 /2022 (PI I. Moura). 249 999,99 €
- **Electrochemical systems for CO2 Mittigation.**
  PTDC/BTA-BTA/0935/2020 (PI José J. G. Moura). 249.752,16 €
- **Applicability of new redox enzyme systems for the efficient biocatalytic conversion of lignocellulose - OXYMOD.**
  Project Code nº 269408/O70 - Norway / Portugal. 51 078,42 €
- **Screening of antibiotic contamination by mobile devices.**
  FCT, PTDC/CTA-AMB/31756/2017, Marcela Segundo (PI). Total Funding: € 239,106.00 (2018-2021)
- **Dialysis membranes by design: targeting neutrophil elastase to reduce inflammation/ oxidative stress in end-stage renal disease**
  PTDC/MEC-CAR/31322/2017; Conceição Branco (PI). Total Funding: € 232,938.00 (2018-2021)
- **Sensitization of urologic tumors therapy driven by nanotechnology.**
  FCT, PTDC/MED-QUI/29800/2017, João Prior (co-PI). Total Funding: € 239,937.55 (2018-2022)
- **ALGA4FOOD - Algas na Gastronomia - Desenvolvimento de técnicas inovadoras de conservação e utilização.**
  European Maritime and Fisheries Fund – Operational Program MAR2020, MAR-01-03-01-FEAMP-0016, João Paulo Noronha (PI). Total Funding: € 571,086.00 (2017-2020)
- **VolWood - Volatile profile characterization of wood-based panels leading to new production strategies using forest and agricultural surpluses.**
  FCT, PTDC/CTM-PAM/1348/2021, Rui Ramos (PI). Total Funding: €216,621.66 (2021-2024)
- **Analytics2H – Advanced analytical strategies based on 3D printing to unveil the health-to disease transition,**
  FCT, EXPL/QUI-QAN/0360/2021, Sara Marques (PI), Total Funding: € 49 997,11 (2021-2023)
- **ACT4Nano - Development of analytical methodologies to accelerate the translation of nanoparticles into clinical practice,**
  FCT, EXPL/QUI-QAN/0360/2021, Sara Marques (PI), Total Funding: € 49 997,11 (2021-2023)
- **TRANSFORM – Digital transformation of the forest sector for a resilient and low-carbon economy – "Study and characterization of semiochemical compounds with an effect on the tritrophic interactions of Coroebus undatus.**
  PRR FCT Financing, Marco Gomes da Silva (PI), Total Funding: € 345,789 (2022-2026)
- **Monitoring of plant protection compounds in rigid plastic packaging, Private funding with Valorfito - Sigeru Lda,**
  Marco Gomes da Silva (PI), Total Funding: € 15 000 (2022)
- **Study and characterization of semiochemical compounds with effect on the tritrophic interactions of Coroebus undatus,**
  Private funding with Amorim Cork Research Funding, Marco Gomes da Silva (PI), Total Funding: € 30 000 (2022-2023)
- **Determination of emamectin benzoate in 96 samples of cork and cork leaves,**
  Private funding with Amorim Cork Research Funding, Marco Gomes da Silva (PI), Total Funding: € 6000 (2022-2023)
- **e.THROUGH - Thinking rough towards sustainability,**
  Period: 2018-2021; PI: Alexandra Ribeiro, (local PI Marco Gomes da Silva); Financial support: H2020-MSCA-RISE- Research and Innovation Staff Exchange; Total funding: 733,500€
- **MedOOmics - Mediterranean Extra Virgin Olive Oil Omics: profiling and fingerprinting,**
  Period: 2016-2019; PI: M. João Cabrita, (local PI Marco Gomes da Silva); Financial support: ERA-NET ARIMNET2 - research coordination in mediterranean agriculture; Total PT funding: 112,366€
- **Portuguese Olive Oil Omics for traceability and authenticity,**
  Project P2020-PTDC/AGR-PRO/2003/2014; Period: 2016-2019; PI: Maria João Cabrita (local PI Marco Gomes da Silva); Total funding: 198,655€
- **From molecularly imprinted polymers to MIP-based optical sensors: a "light-up" tool for the analysis of pesticide residues in olive oil,**
  Project PTDC/ASP-AGR/30097/2017; Period: 2019-2022; PI: Raquel Garcia (local PI Marco Gomes da Silva); Total funding: 236,373€
- **Integrated approach to study the movement dynamics of the meagre Argyrosomus regius**
  Project PTDC/BIA-BMA/30517/2017; Period: 2019-2022; PI: Bernardo Quintella (local PI Marco Gomes da Silva); Total funding: 237,073€.

- **INOVA4AQUA - Uma abordagem inovadora rumo à sustentabilidade ambiental da aquicultura**
  Project MAR-02-01-01-FEAMP -0042; PI: Luis Branco (FCT-UNL), (local PI João Paulo Noronha); Total funding: 549,533€
- **Integrated management of biotic agents associated to the loss of pine seed production,**
  Project PDR2020-101-FEDER-031186; Period: 2019-2022; PI: Eduardo Mateus (local PI Marco Gomes da Silva); Total funding: 70,000€
- **Prevention, management and control of Gonipterus platensis, the eucalyptus weevil,**
  Project PDR2020-101-FEDER-031159; Period: 2019-2022; PI: Eduardo Mateus (local PI Marco Gomes da Silva); Total funding: 99,000€
- **DEPCAT - Demonstration of new EquiPment involving integrated CATalytic processes for the treatment of organic pollutants and disinfection of water,**
  NORTE-01-0247-FEDER-033330; Period: 2018-2020; PI: Sérgio Silva (Adventech), (local PI Marcela Segundo); Total funding: 695,996€
- **Identificação precoce de marcadores moleculares de defeito em azeites virgem extra – estudo de rácios entre compostos responsáveis por atributos positivos e o ácido acético,**
  Coordenação: M.D.R. Gomes da Silva, Financiamento privado com Victor Guedes: Financiamento NOVA.ID.FCT 61500 € (2019-2020)
- **Estudo da perigosidade das embalagens de plástico rígido de produtos fitofarmacêutico,**
  Coordenação: M.D.R. Gomes da Silva, Financiamento privado com Valorfito - Sigeru Lda., Financiamento NOVA.ID.FCT 64268 € (2017- 2020)
- **Determinação de compostos orgânicos voláteis em rolhas de cortiça para indústria de champagne e espumantes),**
  M.D.R. Gomes da Silva, Financiamento privado com Valorfito - Sigeru Lda., Financiamento NOVA.ID.FCT 15000 € (2020)
- **Goat farming systems characterization and novel strategies to sustain production in the changing climate scenario in the Mediterranean regions,**
  PRIMA/EU/FCT, David Pereira (WP/National Leader), Total Funding: €1 286 901 (2023-2026)
- **MedAIVeritas - Inovação e Validação de IA em Medicina,**
  COMPETE 2030 MPr-2023-7, David Pereira, Total Funding: €1 088 942 (2025-2028)
- **Development of naturally inspired insecticides and/or fungicides: synthesis, bioactivities and nanoformulations,**
  COMPETE2030-FEDER-00755600, operação 16390, Period: 2025-2028, David Pereira (WP Leader) Total funding: €249 955 (2025-2028)
- **The endoplasmic reticulum as a pharmacological target for proteinopathies,**
  COMPETE2030-FEDER-0067960, operação 15697, David Pereira (PI) Total funding: €248 812 (2025-2028)
- **Marine chemiluminescence as a broad-spectrum anticancer therapy with enhanced tumor-selectivity and activity,**
  PTDC/QUI-QFI/2870/2020, David Pereira (WP Leader) Total funding: €257 496 (2021-2023)
- **InBioXplorAir - Inhalation bioaccessibility and bioavailability approaches to explore the risks of per- and polyfluoroalkyl substances in airborne particulate matter,**
  FCT, 2023.11715.PEX, Joel Sanchéz-Piñero (PI), Total Funding: € 49 999,80 (2025-2026)
- **SEC-MODE - Detection of emerging contaminants through mobile devices,**
  COMPETE e FCT, COMPETE2030-FEDER-00864800, Operação 017171, Marcela Segundo (PI), Total Funding: € 245 851 (2025-2028)
- **Sens4FireBlight - Development of a field-portable biosensor as a specific and reliable device for the early detection of fire blight disease,**
  COMPETE, COMPETE2030-FEDER-00713400, Operação 015995, Total Funding: € 249 220 (2025-2028)

INTERNATIONAL COOPERATION AND NETWORKING

- COST Actions CA16215, CA 18224, CA 18112,
- Portuguese member of the Expert Working Group (EWG): Improving wheat quality for processing and health of the Wheat Initiative.
- National delegate in the European Proteomics Association (EuPA)
- Vineprotect Networking with Italy, France, Turkey, Morocco, Universities
- Microbiome networking with Valencia, Turim, Bologna and Universities
- International Cooperation with several research centres, hospitals, and universities from: Argentina, Australia, Belgium, Brazil, Canada, Cyprus, Denmark, France, Finland, Germany, The Netherlands, Italy, Israel, India, Poland, Romania, Spain, Sweden, Tunisia, United Kingdom, United States of America
- European representative and Member of the Board of the International Association of sexual plant reproduction
- Main strategic partner of STARSS
- Main strategic partner in project "Analysis of the influence of glycans and microelements, as potential new biomarkers, in assessing the severity of the clinical picture of COVID-19 patients"

DISSEMINATION & OUTREACH



LABORATÓRIO ASSOCIADO
PARA A **QUÍMICA VERDE**

EnvChem

ENVIRONMENTAL CHEMISTRY

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

Group Coordinator:

Cristina Delerue Matos

Nowadays, the quality of the environment and its effects on citizens' welfare is one of the world's major issues of the utmost importance. Environmental Science is a multidisciplinary field that integrates physical, chemical, and biological sciences to study the natural environment. It focuses on how the environment may affect human life and proposes solutions to current environmental challenges.

The major topics of investigation of the Environmental Chemistry group include, but are not limited to, mineral and organic pollutants and xenobiotics in water, soil, sediment, air, organisms and food, and their impact on environmental quality, human health, and food safety; their origin, fate, biodegradation and transport in the environment; modelling of environmental chemical processes; environmental toxicology, microbiology, chemistry, engineering and hazard/risk assessment; environmental technologies, soil control and remediation; monitoring and treatment of water and wastewater, municipal and industrial solid wastes, as well as toxic and hazardous substances. Emerging concerns such as microplastics, PFAS, circular economy and climate-related impacts are also addressed.

In addition, the field of Environmental Science relies heavily on analytical chemistry. Therefore, the group develops screening methods and improves confirmatory methods for the analysis of the above-mentioned contaminants, based on the principles of Green Chemistry and environmental and economic sustainability. These methods comply with current or proposed legislative requirements and are mainly based on chromatography, spectrophotometry, and biosensing tools.

The group combines research, advanced training, and knowledge transfer through national and international collaborations, competitive projects, and support to public and private stakeholders in environmental monitoring, risk assessment, and sustainable solutions.

RESEARCH OBJECTIVES [2025-2029]

The major research objectives of the Environmental Chemistry group are:

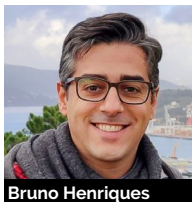
- to develop new analytical methods with higher performances, lower costs and environmental impacts for the quantification and monitoring of pollutants (pesticides, brominated flame retardants, pharmaceuticals, polycyclic aromatic hydrocarbons, PFAS, metals,…) and contaminants in food (fresh and processed); in the environment (in surface, ground, and drinking waters, wastewaters, soils, sediments, sludge, air); and in biological samples, such as tissues, urine, and blood;
- to establish environmental monitoring programs;
- to develop miniaturized and portable sensors (such as electrochemical and luminescent devices) for food and environmental control and for the detection and follow-up of several diseases;
- to develop technologies and new products for pollution prevention and/or environmental remediation (water, wastewaters, solid wastes, soils, air);
- to evaluate ecotoxicological effects of compounds and products for remediation technologies;
- to valorize industrial and agro-food wastes and natural products for industrial, environmental, health, and cosmetic applications through their nutritional characterization (minerals, antioxidants, vitamins, amino acids, fatty acids);
- to improve the sustainability of solutions and to provide decision-makers effective information by using tools to be applied in the initial phase of a project life cycle;
- to perform/include life cycle assessment and risk analysis during the development of analytical, pollution prevention or remediation technologies and new products;
- to promote advanced training, scientific dissemination, knowledge transfer, and citizen involvement through collaboration with academia, industry, and public authorities.
- To develop scalable and sustainable processes for recovering critical metals from e-waste and acid mine waters to support energy systems and emerging technologies.

RESEARCH TEAM

SENIOR RESEARCHERS

Álvaro Torrinha

Ana Grosso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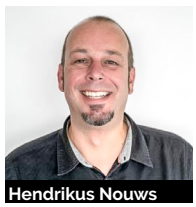
Cristina Soares

Cristina Delerue-Matos

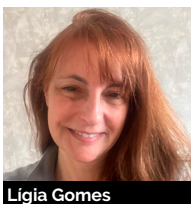
Diana Rede

Elsa Vieira


Hendrikus Nouws

Henrique Vicente

João Pacheco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M. Aurora Silva

M. Cristina Freitas

M. Conceição Manso

M. Fátima Barroso

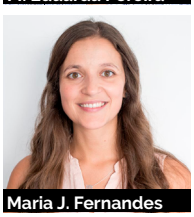
M. Eduarda Pereira

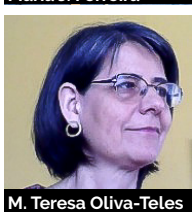
Maria J. Ferreira

M. Luísa Correia Sá

M. Manuela Correia

M. Manuela Carvalho


Maria J. Fernandes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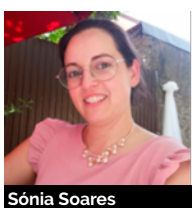
Salomé Teixeira

Sara Sousa

Simone Morais

Sónia Figueiredo


Sónia Soares

Valentina Domingues

RESEARCH TEAM

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Azadeh Abdolvasei
Bruno Santos
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Mónica Silva
Paula Paiga

RESEARCH THEMES/
MONITORING OF CONTAMINANTS AND TREATMENT

MONITORING OF CONTAMINANTS IN ENVIRONMENTAL SAMPLES

In the last century, modern societies have benefited from the introduction of thousands of synthetic chemicals. However, the importance of their environmental fate has only been recognized in the last few decades, particularly in the case of micropollutants. The assessment of their presence in different environmental compartments, at very low levels, has been possible due to significant developments in analytical determination, such as the use of chromatographic techniques coupled to mass spectrometry.

The introduction of these xenobiotics into the environment may affect water, soil and air quality and potentially impact ecosystems and human health. The research group has been actively engaged in the development of analytical methodologies for the quantification and monitoring of pollutants (pesticides, pharmaceuticals, polycyclic aromatic hydrocarbons, brominated and phosphorus flame retardants, polychlorinated biphenyls, metals, particulate matter, and microplastics) in environmental samples (surface, ground, and drinking waters, wastewaters, soils, sediments, sludge, air). Different sample preparation methods, focusing on those following the principles of green chemistry, such as solid-phase extraction, solid-phase micro-extraction, QuEChERS, microwave-assisted extraction, supercritical fluid extraction or subcritical water extraction, are privileged. The development of miniaturized and portable (bio)sensors for environmental control is another area of expertise.

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4 M. Conde-Cid, et al., Environ. Res. 2021, 198, 110451. **doi: 10.1016/j.envpol.2020.114711**

5 J. Vera, et al., Separations 2021, 8, 81. **doi: 10.3390/separations8060081**

6 A. Maia, et al., Molecules. 2021, 26, 5774. **doi: 10.3390/molecules26195774**

7 S. D. Martinho, et al., Polymers 2022, 14, 3645. **doi: 10.3390/polym14173645**

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RESEARCH THEMES/
MONITORING OF CONTAMINANTS AND TREATMENT

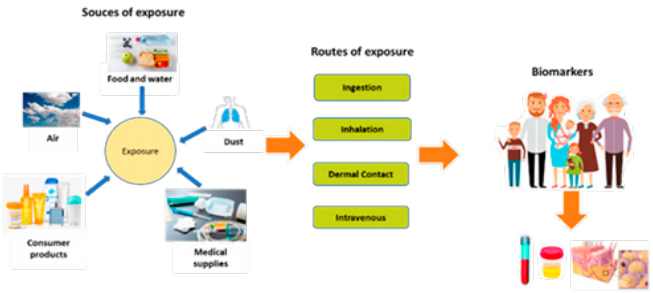
BIOMONITORING: SOURCES AND EXPOSURE ASSESSMENT

The chemical pollution crisis is an undeniable worldwide reality that severely impacts human health. Human biomonitoring assesses the total internal dose of environmental pollutants, regardless the route of exposure (inhalation, ingestion, dermal absorption) in multiple biological fluids and tissues (e.g., blood, urine, breast milk, saliva, skin samples, adipose tissue, etc.). This methodological approach has been widely used to characterize human exposures – by measuring these chemicals or their main metabolites known as biomarkers of exposure – to health-relevant pollutants, including those in the international priority list of substances, some already classified as possible/probable/known carcinogens to humans, as well as their interaction with environmental media and during regular working activities. Potential health risks to human health are dependent on the route and duration of exposure as well as on the composition, concentration, and toxicity of the mixture of targeted pollutants.

Human biomonitoring assays focused on the assessment of biomarkers of effect, including Clara cell 16, 8-iso prostaglandin F2, and 8- hydroxy-2-deoxyguanosine, key biomarkers of lung injury, lipid peroxidation (oxidative stress), DNA oxidative damage, and micronucleus frequency respectively, characterize early inflammatory, oxidative stress, and early cancer risks in humans, allowing its association with environmental and occupational causal factors. The characterisation of early biological effects in humans exposed to a specific environment and/or involved in a specific activity, and their association with internal exposure biomarkers, is essential to generate evidence that can inform and support the development of preventive and protective measures to mitigate health outcomes and promote human health.

The research group is engaged in biomonitoring:

- to determine which part of the population has levels above those associated with adverse health effects for chemicals with a known toxicity level;
- to assess occupational exposure of firefighting forces and associated health risks;
- to establish reference values to determine whether a person or group has an unusually high exposure;
- to assess the effectiveness of public health efforts to reduce exposures;
- to determine whether exposure levels are higher among minorities, such as children and obese people;
- to determine which chemicals get into the bodies of a population and at what concentrations and related health risks.



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42 F. Esteves, et al., Int. J. Hyg. Env. Health 2025, 266, 114576. doi: 10.1016/j.ijheh.2025.114576

RESEARCH THEMES/
MONITORING OF CONTAMINANTS AND TREATMENT

ADVANCED SUSTAINABLE WATER TREATMENT PROCESSES

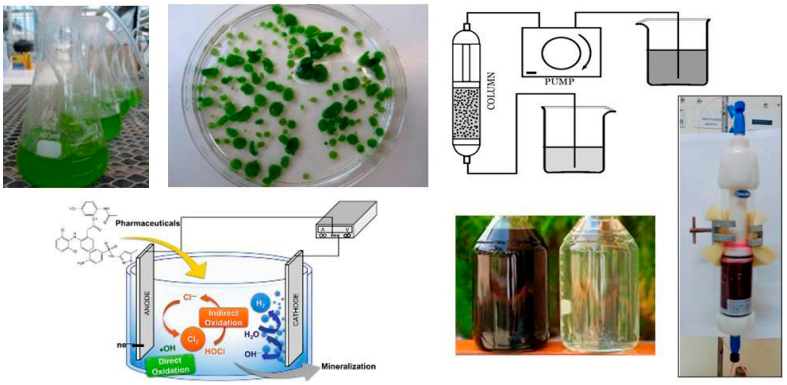
Water resources are under increasing pressure due to rapid population growth and industrial expansion. The contamination by emerging pollutants, particularly pharmaceutical compounds, which are frequently detected in treated wastewaters and receiving water bodies due to their low removal efficiency in conventional wastewater treatment plants, represents a growing environmental and public health concern.

The recently adopted Urban Wastewater Treatment Directive (EU) 2024/3019 marks a turning point in European wastewater policy, by supporting circular economy strategies, climate-neutrality targets, and improved environmental and public health protection. It introduces more stringent removal targets for nutrients (nitrogen and phosphorus) through tertiary treatment and for organic micropollutants (pharmaceutical compounds) through quaternary treatment, while establishing monitoring requirements for emerging contaminants (e.g. microplastics and PFAS) and health parameters.

This research group has been actively developing and applying advanced treatment processes (particularly quaternary treatments) based on adsorption and advanced oxidation processes, aiming at integrated solutions that can contribute for improving water quality and enhancing the possibility of reusing treated wastewater.

Adsorption studies have been focused on the use of low-cost raw materials such as microalgae, industrial and agroforestry wastes, and clays, used in original or modified forms (by physical, physico-chemical, or chemical treatments) to develop environmental and economically sustainable solutions. Three-dimensional electrochemical processes have also been investigated for the removal of refractory contaminants, combining electrochemical and adsorption mechanisms to enhance performance.

The sustainability of the proposed technologies has been evaluated using SWOT analysis and Life Cycle Assessment (LCA), minimising environmental impacts and supporting sustainable water management practices.



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RESEARCH THEMES/
LIFE CYCLE THINKING

VALORIZATION OF AGRO-FOOD AND INDUSTRIAL WASTES

Valorization of agro-food and industrial by-products has emerged a central strategy in sustainable bioeconomy, driven by the urgent need to reduce environmental burdens and recover high-value compounds from underutilized residues. Significant research has focused on transforming a wide range of residues - including fruit and vegetable by-products (pomace, peels, seeds), cereal and brewing wastes (spent grain, yeast), dairy streams, marine biomass (microalgae and seaweeds), and crop side-streams from rice, maize, chayote, kiwano, apples and chestnut production - into high-value resources. These residues are rich in bioactive compounds, dietary fibers, proteins, polysaccharides, pigments, and other functional molecules, which offer opportunities for multiple industrial applications across food, nutraceutical, cosmetic, bio-based materials and pharmaceutical sectors. Current research focuses on the development of efficient, low-impact extraction and fractionation methods to recover these compounds, followed by detailed characterization of their functional and biological properties. Considerable attention has been directed toward green extraction, enzymatic hydrolysis, and advanced separation processes to recover ingredients suitable for food fortification, with the aim of enhancing nutritional value, health-promoting properties, and sensory quality. Beyond food applications, recovered compounds are used in cosmetic and personal care formulations due to their bioactivity and stability, and as feedstocks for biodegradable bioplastics and bio-based materials (e.g., polysaccharides, proteins, nanocellulose). They are also applied in the enrichment of dairy- and cereal-based products, improving nutritional and functional properties while reducing environmental impact. Overall, integrated valorization pathways position agro-industrial residues as sustainable feedstocks, contributing to resource efficiency, waste minimization, and the establishment of circular and resilient value chains.

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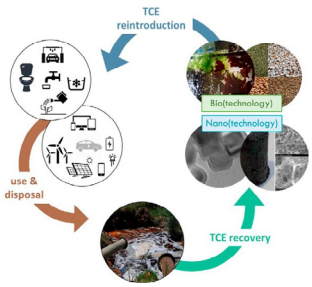
RESEARCH THEMES / LIFE CYCLE THINKING

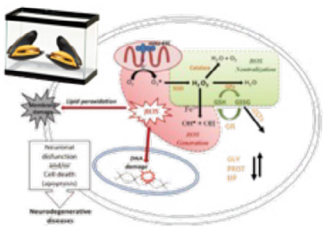
TECHNOLOGY-CRITICAL ELEMENTS: SUSTAINABLE RECOVERY FROM SECONDARY SOURCES & ENVIRONMENTAL TOXICOLOGY

Technology-Critical Elements (TCE) (e.g. rare earth elements, platinum group) comprise a group of chemical elements that are vital to emerging technologies (e.g. clean energy, LEDs) and daily high-tech products (e.g. smartphones), whose supply is scarce relative to demand, having a high economic value. The primary production of TCE is achieved, mostly, by the extraction from ores, which requires a large volume of chemicals, water, and generates complex waste, making it a polluting and expensive method. Due to technology proliferation, the rejection of TCE together with classical contaminants (e.g. Pb, Hg) through sewage is increasing but information on their occurrence and potential toxicity to aquatic organisms is very scarce. Also, waste electrical & electronic equipment (e-waste) is one of the fastest growing waste streams worldwide (3-5% year), representing a hazard if appropriate management strategies are not implemented.

One of the group's areas of research is the development of environmentally sustainable and economically viable processes for TCEs recovery from secondary sources (wastewaters and e-waste), with a view to their reintroduction into industrial processes. One of the most successful approaches emerged from the co-promotion I&D project N9ve.REE (funded with 1.1 million euros), which proposes macroalgae-based technologies for use in industrial processes for the recovery of REEs. This project won the "Born from Knowledge" award (ANI) in 2022, the Everis Awards Portugal (NTT DATA Foundation) in 2021 and was among the top 3 finalists of the Altice International Innovation Award in 2020. International Patent WO 2021/040551 A1 and more than 16 papers were other important outputs of the N9ve.REE project. Biosorbents (valorization of food/agro-industrial waste) and nanomaterials have been also studied for REEs recovery.

To fill the gap in the literature regarding TCE toxicity in marine ecosystems, the research team has been studying the impacts of this group of elements in oyster's embryo development, bivalve's and macroalgae's biochemical performance (biomarkers analysis) align with foreseen climate changes such as water salinity shifts, ocean acidification and temperature rise.





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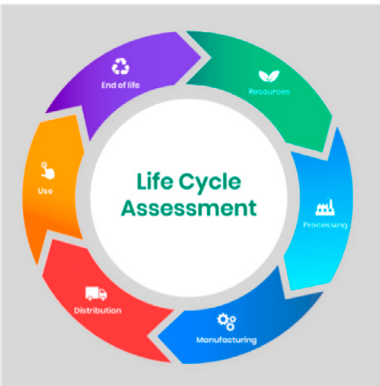
RESEARCH THEMES/
LIFE CYCLE THINKING

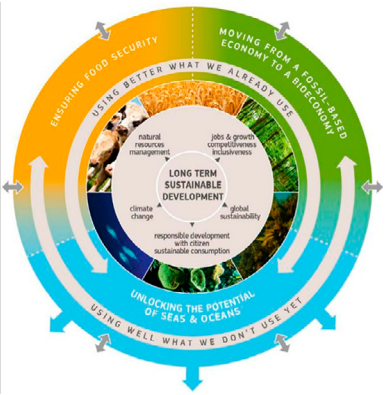
SUSTAINABILITY STUDIES AND LIFE CYCLE THINKING

Nowadays there are several challenges that should be overcome, namely scarcity of raw materials, pollution, sustainable production and consumption, and issues concerning globalization and markets' stability. Sustainability studies considering the three pillars of sustainable development, especially with a life cycle perspective can help the different stakeholders to adopt and implement sustainable practices and behaviours. These studies can also be very helpful in the decision-making process for several levels and sectors. In this context, indicators based on several criteria are a very comprehensive tool. Research efforts will be focused on various domains and sectors, in products, processes or services, since sustainability and life cycle tools, such as material flow, material design guidelines, LCA (Life Cycle Assessment), LCC (Life Cycle Costing), and SLCA (Social Life Cycle Assessment) can be widely applied. The main objective is to maximize positive impacts and minimize negative impacts by looking at all phases of a product life cycle, trying to involve the different players, such as designers, industry, retailers, and consumers and creating windows of opportunity to improve social, economic, and environmental performance.

This is a horizontal research line inside the research group that covers all the R&D topics developed by the team. The main aim is to ensure that the new methods, technologies, and products developed within the research group have effective environmental, economic and social benefits when compared to the traditional solutions.

Moreover, this research line also aims to identify new opportunities of research for the development of new products and technologies. It points-out critical points in the traditional production systems, or even in by-products with no-economic value that are produced in the current European linear economy, trying to contribute for a more circular-shape economy and for the EU sustainability goals defined in the Agenda 2030.





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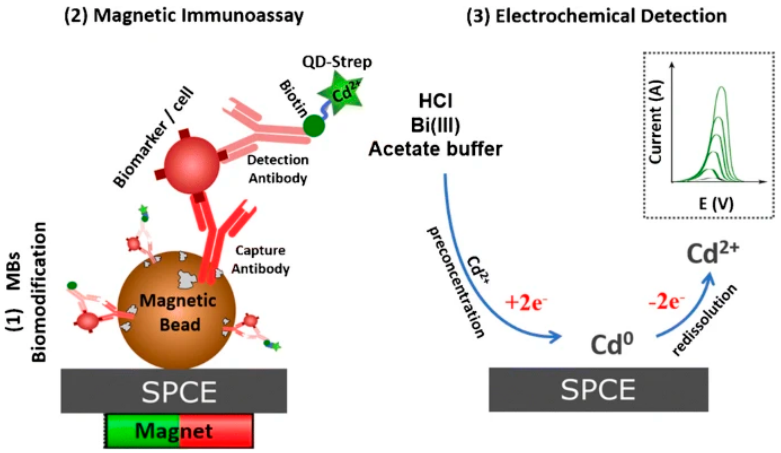
RESEARCH THEMES / ELECTROCHEMICAL (BIO)SENSING TOOLS

The advances in engineering have contributed decisively to the innovation of analytical (bio)sensing tools. Electronic devices have become smaller, allowing their use as portable instruments to monitor concentrations in real-time and in situ. The accomplishments in nanotechnology assure that ultrahigh sensitivity, selectivity, and low detection limits can be reached with (bio)sensors. Research efforts are focused on various domains for which novel sensors, using chemical, biological, or bio- inspired molecular recognition elements, and paper-based platforms, are developed, including, but not limited to:

• environmental control (e.g. micropollutants and their corresponding metabolites and/or degradation products, namely pharmaceuticals and pesticides in natural and wastewaters);
• assessment of food quality and safety (e.g. allergens, emerging contaminants, biogenic amines, pathogenic microorganisms, and toxins)
• disease diagnostics and follow-up (e.g. cancer, Alzheimer's and Parkinson's disease, chronic kidney disease, and single-nucleotide polymorphisms).

These challenges are the aim of several ongoing national and international projects.



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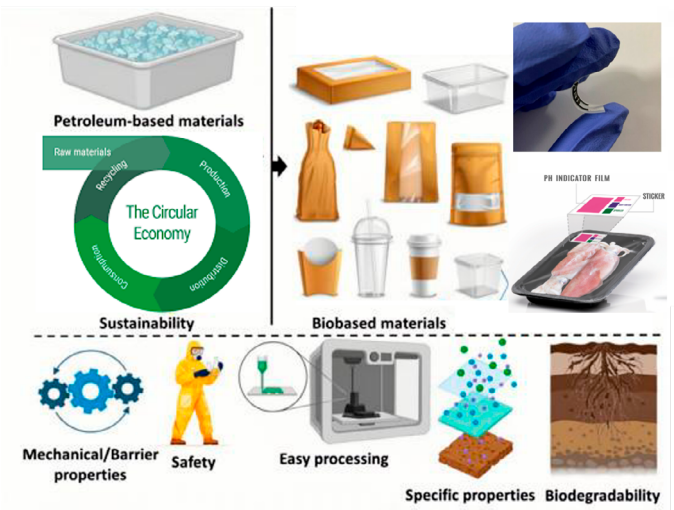
RESEARCH THEMES /
GREEN ENGINEERING OF BIO-BASED FILMS AND BIOCOMPOSITES FROM AGRO-INDUSTRIAL WASTE

The development of biodegradable films and biocomposites from agro-food waste constitutes a strategic research line within the circular economy, addressing the need to replace persistent, fossil-based plastics. This research line focuses on the valorization of agricultural and industrial residues as renewable feedstocks for bio-based materials, including starch-, protein-, and nanocellulose-based systems. Emphasis is placed on green processing approaches and the design of functional materials through the incorporation of bioactive compounds and nanostructures to enhance mechanical performance, barrier properties, and active functionalities (e.g., antioxidant and antimicrobial activity).

These materials are developed for multi-sectoral applications, including sustainable food packaging, smart sensing platforms, pharmaceutical delivery systems, and water quality monitoring and treatment. In food systems, they enable active and intelligent packaging solutions; in sensing, they support biodegradable and low-impact analytical devices; in pharmaceutical contexts, they offer biocompatible matrices for controlled release; and in water applications, they contribute to pollutant detection and remediation.

This research line is aligned with the EU legislative framework, requiring compliance with the Waste Framework Directive, the Packaging and Packaging Waste Regulation (EU) 2025/40, and food contact legislation (Regulation (EC) No 1935/2004), particularly for applications involving direct human exposure. Materials are therefore designed not only for bio-based origin but for clearly defined and legally supported end-of-life pathways, such as recyclability or, where appropriate, industrial compostability, while ensuring safety and functional performance.

Overall, this research line contributes to reducing dependence on fossil-based plastics, promoting waste valorization, and enabling the development of circular, resource-efficient material systems across multiple sectors. It is aligned with the objectives of the United Nations Agenda 2030, particularly Sustainable Development Goals 12 (responsible consumption and production), 13 (climate action), and 14 (life below water).



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HIGHLIGHTS

ENVIRONMENTAL AND WASTEWATER MONITORING

Environmental pollution is increasing daily and has become a global transboundary challenge that is difficult to control or eliminate. Among emerging contaminants, pharmaceuticals are of particular concern due to their potential risks to human, animal, and environmental health. Studies worldwide consistently report their presence in different environmental compartments, even at low concentrations (ng/L to µg/L), yet advancements in analytical methods have enabled the detection of a growing number of these compounds. Environmental monitoring, improving treatment processes, and enhancing regulation and public awareness are critical steps to address this growing issue.

BioReset - Biodiversity restoration and conservation of inland water ecosystems for environmental and human well-being.

BiodivRestore-406 / DivRestore/0002/2020

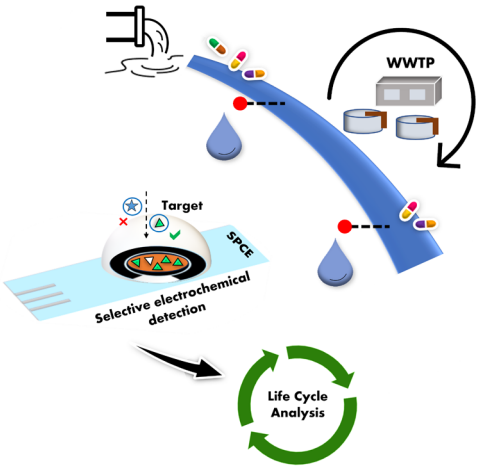
https://www2.isep.pp.pt/bioreset

In recent years, microplastic pollution has garnered significant attention owing to its ability to permeate various ecosystems. These particles can infiltrate the environment, either directly or through the degradation of larger plastic items. The analysis protocols for microplastics typically follow a common structure involving pre-treatment to reduce organic matter, extraction methods, and identification techniques.

ANALYSIS OF ATORVASTATIN IN WATER SAMPLES

Atorvastatin (ATV) is a widely consumed statin and its occurrence in environmental waters has become a reality, highlighting the need for rapid and sensitive analytical monitoring devices.

An electrochemical molecularly imprinted polymer (MIP) sensor for the detection of ATV in water samples was developed. The MIP was prepared by electropolymerisation of 4-aminobenzoic acid and ATV on a screen printed carbon electrode. Quantitative measurements were carried out with differential pulse voltammetry. After optimisation, a limit of detection of 0.049 µM was achieved. The performance of the developed MIP sensor was evaluated for the selective detection of ATV in wastewater treatment plant effluents and surface water samples, and results were compared with those obtained by ultra-high performance liquid chromatography coupled to tandem mass spectrometry. A life cycle assessment (LCA) was conducted to compare the environmental impact of both methodologies. The results showed that the MIP sensor provides reliable ATV quantification, comparable to UHPLC-MS/MS, while offering a significantly lower environmental impact.



A simple electrochemical detection of atorvastatin based on disposable screen-printed carbon electrodes modified by molecularly imprinted polymer: Experiment and simulation

Analytica Chimica Acta, 2022, 1194, 339410

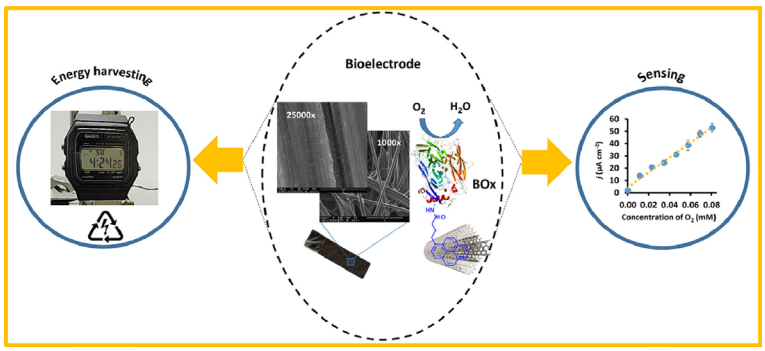
Analysis of atorvastatin in environmental waters: Validation of an electrochemical molecularly imprinted polymer sensor with application of life cycle assessment

Science of The Total Environment, 2024, 921, 171169

HIGHLIGHTS

SIMPLE BIOELECTROCHEMICAL SYSTEM FOR BOTH MICROENERGY GENERATION AND DIOXYGEN SENSING

In this work, bilirubin oxidase (BOx) was conjugated with the exceptional properties of a carbon paper transducer to efficiently convert the reduction of oxygen into water. This bioelectrochemical process can either be used for sensing applications or to harvest energy. When applied as a biocathode and connected to a zinc anode, this biobattery generated 40 µW, enabling the powering of a digital watch, using only oxygen as "fuel". When applied as a dioxygen biosensor, the biocathode revealed high sensitivity and a limit of detection of 1.3 ± 0.2 µM. Therefore, bioelectrochemical systems can be envisaged as self-powered biosensors or as energy suppliers for small electronic devices.

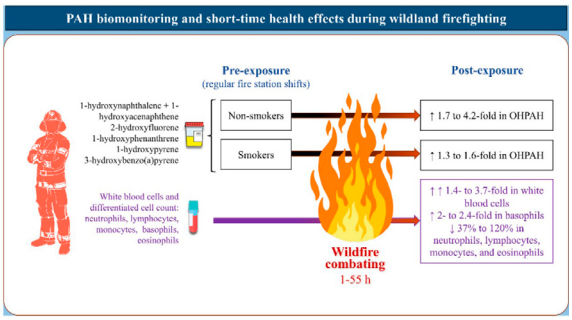


Microenergy generation and dioxygen sensing by bilirubin oxidase immobilized on a nanostructured carbon paper transducer.

Electrochimica Acta, 2023, 445, 142061

BIOMONITORING OF POLYCYCLIC AROMATIC HYDROCARBONS EXPOSURE AND SHORT-TIME HEALTH EFFECTS IN WILDLAND FIREFIGHTERS DURING REAL-LIFE FIRE EVENTS

Human biomonitoring data retrieved from real-life wildland firefighting in Europe and, also, worldwide are scarce. This study biomonitored firefighters (non-smoker vs smokers; non-exposed vs exposed) pre- and post- unsimulated wildfire combating to evaluate the impact on the levels of urinary polycyclic aromatic hydrocarbons hydroxylated metabolites (OHPAH) and the associated short-term health effects. The exposure to wildfire emissions significantly elevated the levels of each individual and total OHPAH compounds, with more pronounced effect in non-smoking (1.7–4.2 times; p≤0.006) than in smoking firefighters (1.3–1.6 times; p≤0.03). The greatest discriminant of exposure was 1OHNaph + 1OHAce (increase of 4.2 times), while for tobacco smoke it was 2OHFlu (increase of 10 times). Post-exposure, white blood cells count significantly increased ranging from 1.4 (smokers, p=0.025) to 3.7-fold (non-smokers, p<0.001), which was accompanied by stronger significant correlations (0.480<r<0.882; p<0.04) between individual and total OHPAH and total white blood cells (and lymphocytes>monocytes>neutrophils in non-smokers), evidencing the impact of PAH released from wildfire on immune cells.



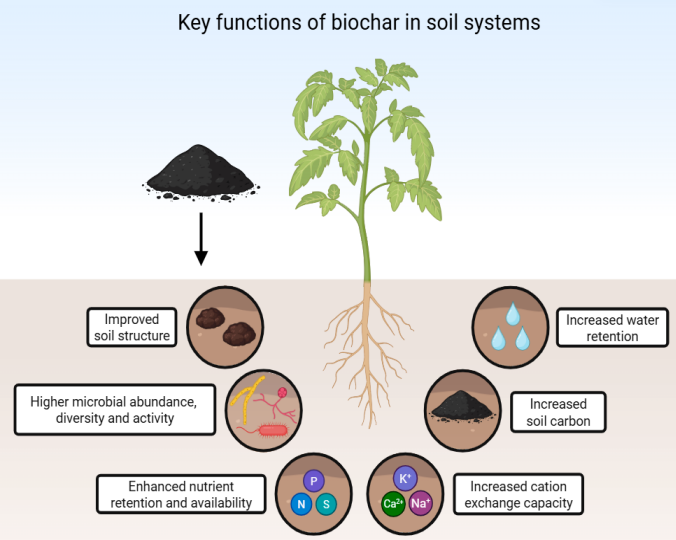
Biomonitoring of polycyclic aromatic hydrocarbons exposure and short-time health effects in wildland firefighters during real-life fire events

Science of the Total Environment, 2024, 926, 171801

HIGHLIGHTS

BIOCHAR FOR SOIL RESTORATION AND NUTRIENT USE EFFICIENCY: FROM POST-WILDFIRE REMEDIATION TO SUSTAINABLE FERTILIZATION

Biochar has emerged as a key tool in addressing soil degradation and promoting sustainable nutrient management, particularly in the context of climate change, wildfires, and agricultural intensification.
In Mediterranean ecosystems, increasingly affected by moderate to high-severity wildfires, soil quality decline poses a major challenge for ecosystem recovery. This work highlights the potential of biochar as a sustainable solution for soil restoration and nutrient management.
A review of post-wildfire Mediterranean ecosystems identifies biochar as a promising strategy to improve soil structure, enhance water retention, and restore nutrient balance in moderate to high-severity burned areas.
Complementing this perspective, an experimental study explores the production of four vineyard pruning-derived biochars optimized for nutrient adsorption, specifically targeting phosphorus, potassium, and nitrogen. Results demonstrate that tailored biochars can effectively capture and retain essential nutrients, supporting their reuse as slow-release fertilizers.
Together, these studies emphasize the dual role of biochar in mitigating wildfire-induced soil degradation and promoting circular, sustainable agricultural practices through nutrient recovery and soil amendment.



Moderate to high-severity wildfires: Main restoration strategies applied in Mediterranean ecosystemst.
Journal of Environmental Management, 2025, 380, 125149

Optimizing Vineyard Pruning Biochars for Nutrient Adsorption: Toward Sustainable Fertilizer Applications.
Environments, 2025, 12, 491

HIGHLIGHTS

ALPROSOS - IBERO-AMERICAN NETWORK OF REGIONALLY SOURCED, SUSTAINABLE HIGH-PROTEIN FOODS

The AlProSos project aims to establish an Ibero-American network dedicated to the production, selection, purification, and functionalization of alternative proteins derived from regional sources, with the goal of developing sustainable, high–nutritional-quality food prototypes. The AlProSos working group coordinates activities related to the identification, characterization, extraction, purification, functionalization, allergenicity, safety, and application of these proteins in novel food products.

The specific objectives are:
- to select, characterize, and implement alternative proteins from regional sources
- to evaluate emerging technologies for their extraction, purification, and enhancement
- to develop and commercialize food products incorporating these proteins
- to assess consumer acceptance in Ibero-American contexts
- to evaluate nutritional quality and address antinutritional, allergenic, and safety aspects
- to conduct life cycle and socio-economic assessments
- to prepare joint research proposals and develop collaborative activities in research, training, dissemination, and technology transfer
- to strengthen technical capacity through academia–industry exchange.

The network responds to the growing global demand for protein by promoting the identification and valorization of new, sustainable sources, while considering economic, health, and environmental factors. It will generate context-specific innovative solutions and foster sustained, multidisciplinary collaboration among Ibero-American research groups, with active involvement of the productive sector. This approach is expected to support the local food industry, generate positive societal impact, and ensure the long-term viability of the network.

AlProSos - Red de Alimentos ricos en Proteínas regionales Sostenibles.

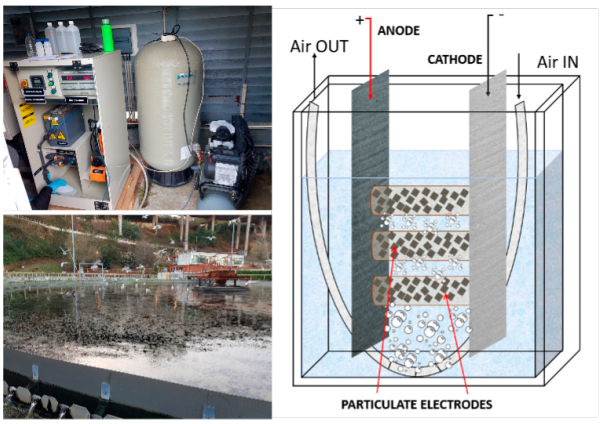
CYTED – Programa Iberoamericano de Ciencia y Tecnología para el Desarrollo - 125RT0165

https://www.cyted.org/web_redes.php?id_rede=537

HIGHLIGHTS

A THREE-DIMENSIONAL ELECTROCHEMICAL PROCESS FOR THE REMOVAL OF PHARMACEUTICAL COMPOUNDS

Electrochemical and adsorption processes were combined in a three-dimensional electrochemical system to remove pharmaceutical compounds, persistent pollutants frequently detected in treated wastewaters and surface waters due to their insufficient removal in conventional wastewater treatment plants.
A mixed metal oxide anode (titanium coated with RuO_2-IrO_2-TiO_2), a stainless-steel cathode, and several biochars produced from agroforestry residues were used as particulate electrodes. Different reactor configurations were tested. The results demonstrated that the introduction of particulate electrodes significantly improved removal efficiency compared to the conventional two-dimensional process, as they act as microelectrodes. This enhancement can also be attributed to the simultaneous occurrence of multiple phenomena, such as adsorption/electrosorption, electrocoagulation, oxidation, and catalytic degradation. This cost-effective, and sustainable quaternary treatment shows strong potential for implementation in urban wastewater treatment plants, to achieve at least 80% removal of selected pharmaceutical compounds, as required by the Urban Wastewater Treatment Directive (EU) 2024/3019.



A Three Dimensional Electrochemical Process for the Removal of Carbamazepine

Applied Sciences, 2021, 11, 6432

Electro-Fenton degradation of a ternary pharmaceutical mixture and its application in the regeneration of spent biochar

Journal of Electroanalytical Chemistry, 2021, 886, 115135

Removal of diclofenac and sulfamethoxazole from aqueous solutions and wastewaters using a three-dimensional electrochemical process

Journal of Environmental Chemical Engineering, 2022, 10, 108419

Efficient carbamazepine removal from wastewater using a continuous three-dimensional electro-Fenton system at natural pH

Journal of Water Process Engineering, 2024, 64, 105690

Novel 3D electro-Fenton reactor based on a catalytic packed bed reactor of perovskite/carbon microelectrodes for the removal of carbamazepine in wastewater

Journal of Environmental Chemical Engineering, 2024, 12, 113154

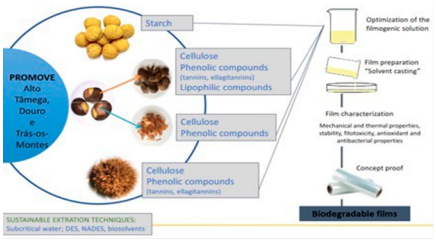
3D electrochemical cork granule process for the removal of pharmaceuticals from urban wastewater:

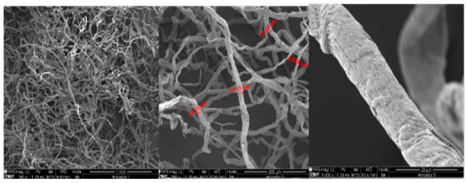
Journal of Environmental Management, 2025, 396, 128096

HIGHLIGHTS

VALORIZATION OF SOLID WASTE FROM CHESTNUT PROCESSING: EXTRACTION OF BIOACTIVE MOLECULES AND PREPARATION OF BIODEGRADABLE FILMS AND BIOCOMPOSITES

Bioplastics are derived from natural sources capable of bacterial digestion and environmental reabsorption. These represent innovative products of the 21st century and hold significant importance, particularly due to their ability to decompose naturally. It is estimated that around 40 to 50% of the chestnuts are lost along the production chain, between harvesting and marketing. This loss could represent around 12,000 tons (around 24 M€). This high percentage of waste generated is almost exclusively used as biofuel to heat the boilers of the processing companies.





The CHESTFILM project aims to valorize the chestnut processing waste, an important agri-food waste in the regions of Alto Tâmega, Douro and Trás-os-Montes. It is a consortium between REQUIMTE/LAQV, University of Aveiro and Sortegel and is financial supported by "La Caixa" Foundation and Fundação para a Ciência e a Tecnologia through the 4th edition of Promove program "O Futuro do Interior".

The operation consists of the differential fractionation of chestnut processing waste (nuts with worms, rot, small caliber, pericarp, tegument, and hedgehogs) applying ecological extraction techniques. The isolated compounds (starch, cellulose, phenolic and fibers) were characterized. These films and composites underwent thorough characterization including mechanical, thermal, and stability tests, as well as assessments for phytotoxicity, antioxidant properties, and antibacterial performance. Furthermore, the environmental and economic viability of the produced biocomposites and films was evaluated. Finally, proof of concept is carried out by scaling up film production for use as packaging material.

Hydrophobicity Strategies of Starch-Based Films: Recent Advances and Perspectives.
Polymers, 2026, 18, 490

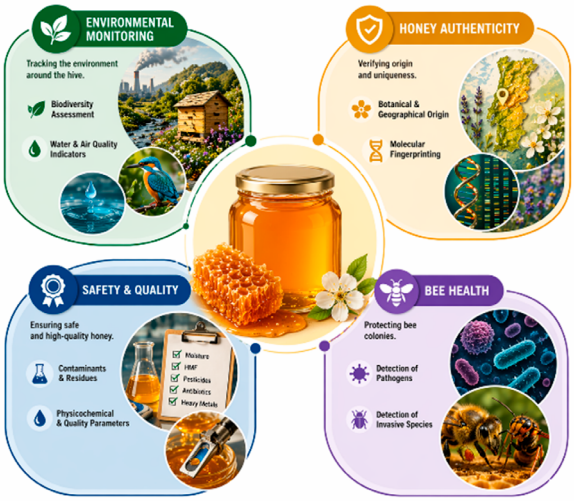
Eco-Friendly Biocomposites from Chestnut Waste: Production, Optimization, Characterization, and Application.
Polymers, 2025, 17, 616

Reinforcement of starch film with Castanea sativa shells polysaccharides: Optimized formulation and characterization.
Food Chemistry 2022, 396, 133609

HIGHLIGHTS

HONEY AS A TOOL FOR ENVIRONMENTAL MONITORING, AUTHENTICITY AND BEE HEALTH

The unique composition of honey positions it as a promising tool for environmental monitoring, traceability, and food authenticity assessment. Current research focuses on developing innovative approaches to explore honey as a source of environmental DNA (eDNA) and DNA-based signatures, enabling the characterization of its botanical and geographical origin. Ongoing work aims to establish molecular fingerprints of honey by combining DNA-based and analytical methods to improve the reliability of geographic authentication frameworks. Complementary research addresses bee health and sanitary status through the development of molecular tools for the detection of pathogens, parasites, and invasive species in honey and other beehive products. The integration of genetic and chemical data aims to enable the identification of risk indicators and early warning signals for colony health, contributing to more sustainable apiculture systems.



Overall, this research contributes to the development of integrated, DNA-based and multi-analytical frameworks for honey authentication, environmental monitoring, and apicultural sustainability, while also addressing challenges related to food fraud, biodiversity loss, bee health, and product quality.

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Exploring the Nutritional Value and Health Benefits of Honey from the Portuguese Protected Area of Montesinho Natural Park.

Foods, 2025, 14, 963

Exploring Geographical Influences on Physicochemical Characteristics of Honey: The Montesinho Natural Park scenario.

Food Quality and Safety, 2024, 8, fyae015

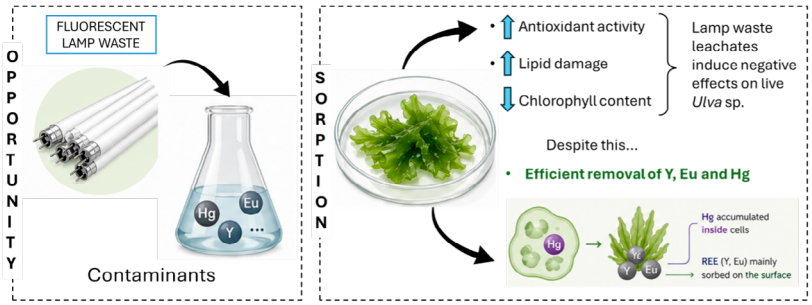
Contaminant Cocktails of High Concern in Honey: Challenges, QuEChERS Extraction and Levels.

Separations, 2023, 10, 142

HIGHLIGHTS

TURNING LAMP WASTE INTO OPPORTUNITY: ECOTOXICOLOGICAL AND BIOSORPTION INSIGHTS WITH ULVA SP

Despite regulations promoting their phase-out, fluorescent lamps remain widely used and generate improperly disposed waste that poses environmental risks due to Hg, while representing a potential source of critical rare earth elements (REEs). Recovery of REEs from FL waste commonly relies on acid extraction, generating concentrated leachates. Although algal-based sorbents show promise, the influence of leachate toxicity on sorption performance remains largely overlooked, and the limited ecotoxicological data on FL wastewater hinders informed management decisions. Therefore, this study investigated the ecotoxicological effects of real FL waste leachates on the macroalga Ulva sp. Macroalgae were exposed for 3 days to different dilutions of FL waste leachate, and mortality, relative growth rate, chlorophyll content, and biochemical alterations were assessed. Positive correlations were observed between Hg, Y, and Eu concentrations in the macroalgae and their initial concentrations in solution. All treatments reduced chlorophyll content and growth rates compared with the control. Exposure to FL leachates activated antioxidant and biotransformation enzymes. Nevertheless, lipid peroxidation was detected, although cellular defence mechanisms appeared sufficient to prevent discoloration and mortality. Importantly, the efficiency of REE accumulation did not seem to be compromised. Since Hg was predominantly accumulated intracellularly, whereas REEs were mainly sorbed onto the algal surface, the use of macroalgae for REE recovery from FL leachates may also provide a simultaneous purification step within the recovery process. The development of bio-based technologies capable of treating these leachates could therefore represent a sustainable source of REEs while mitigating the environmental impacts associated with conventional extraction.



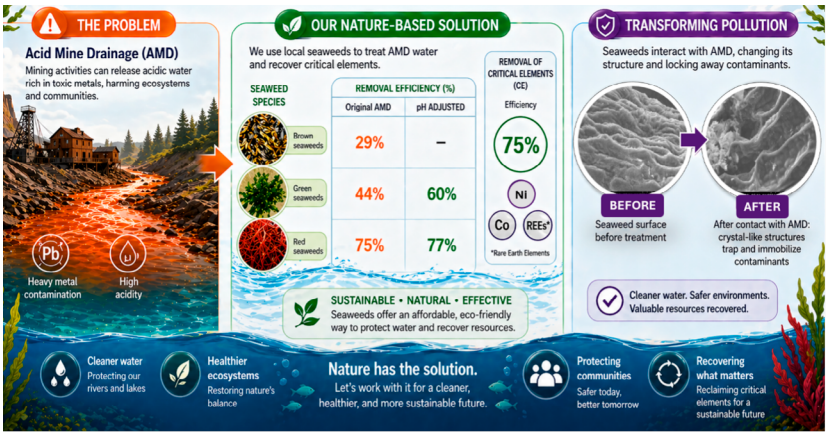
Ecotoxicological impacts associated with fluorescent lamp waste leachates on the marine macroalga Ulva sp.

Science of the Total Environment 2021, 786, 147176

HIGHLIGHTS

FROM POLLUTION TO PROTECTION: SEAWEEDS CLEAN ACID MINE DRAINAGE

Acid mine drainage (AMD) is a persistent environmental challenge characterized by high acidity and elevated concentrations of toxic elements, leading to severe ecological degradation. Conventional passive treatment systems primarily target AMD neutralization and the removal of common metal(loid)s, often overlooking the recovery of economically valuable elements such as rare earth elements (REEs). This study presents, for the first time, the use of marine macroalgae as a dual-function, nature-based solution for AMD treatment and REE recovery. The performance of three seaweed species—Gracilaria sp., Ulva sp., and Fucus sp.—was evaluated in both dried (biosorption) and living (bioaccumulation) forms. Results demonstrate that bioaccumulation is the more efficient mechanism, with Gracilaria sp. and Ulva sp. achieving REE removal efficiencies of up to 75% and 44%, respectively, alongside substantial iron removal (>60%). Chemical pre-treatment through pH adjustment (NaOH) enabled the selective removal of competing elements with minimal loss of REEs, although it did not significantly enhance overall REE uptake, except in the case of dysprosium (Dy). Seaweed dosage was identified as a critical operational parameter, with Gracilaria sp. exhibiting a high bioconcentration factor (up to 1470). Spectroscopic and microscopic analyses (FTIR and SEM-EDS) revealed that functional groups such as sulphonate, carboxyl, and alkyne moieties play a key role in metal binding. Overall, this work highlights the potential of seaweed-based biotechnologies as an effective, sustainable, and easily integrable approach for AMD remediation and the recovery of critical raw materials.



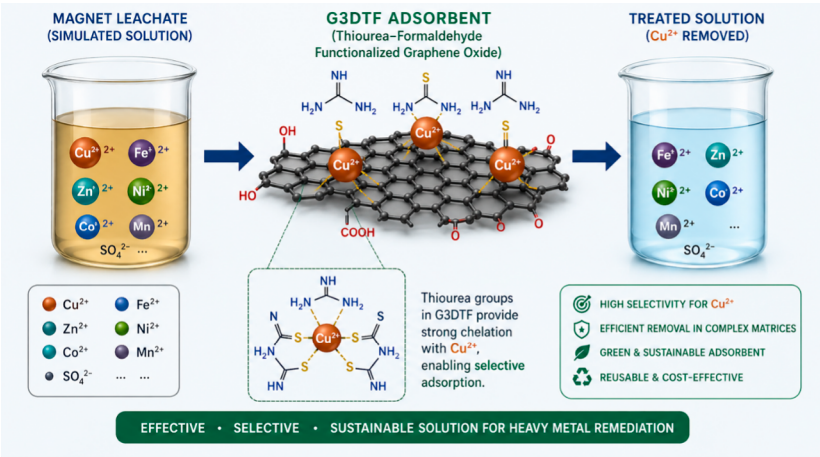
Valorisation of acid mine drainage: Studying biosorption and bioaccumulation of rare earth elements by seaweeds.

Science of The Total Environment, 2024, 957, 177761

HIGHLIGHTS

SELECTIVE RECOVERY OF CU2+ FROM MAGNET LEACHATE USING GRAPHENE OXIDE FUNCTIONALIZED WITH THIOUREA FORMALDEHYDE

Copper (Cu), a critical raw material for renewable energy technologies, requires efficient and sustainable recovery strategies. However, its separation from complex matrices such as wind turbine leachates is hindered by the presence of competing base metals and rare earth elements. In this work, a thiourea–formaldehyde functionalized graphene oxide (G3DTF) is developed as a sulfur- and nitrogen-rich sorbent for highly selective Cu removal. The incorporation of tailored S/N donor sites creates preferential coordination environments, enhancing Cu affinity over other metals. G3DTF demonstrates outstanding performance, achieving up to ~99 % Cu removal in multielement systems while showing negligible uptake of competing ions. The material exhibits a maximum adsorption capacity of 23.4 mg g-1 and maintains high efficiency under optimised conditions (pH 5.2, 1.1 g L-1). Mechanistic analysis confirms that selective Cu binding is governed by Cu–S interactions. The material's effectiveness in leachate-mimicking systems highlights its potential as a sustainable solution for recovering Cu from CRM-rich waste streams..

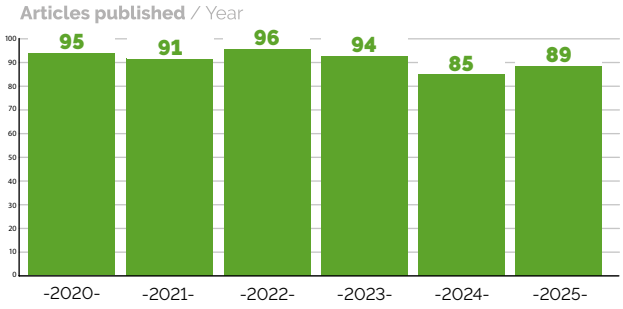


Thiourea-formaldehyde-Functionalized Graphene Oxide for the Selective Removal of Copper from Multielement Solution.

ACS Omega ,2026, 11, 14, 22158−22170

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION



H-index: **45**

550 articles*
36607 citations

***01/2020-12/2025**
From WOS core collection

FUNDED PROJECTS *(Representative projects)*

- **BioFirEx – A panel of (bio)markers for the surveillance of firefighter's health and safety**
  Funded by the Portuguese Foundation for Science and Technology - FCT (PCIF/SSO/0017/2018), Simone Morais (PI)
  Funding: € 99,325, Total Funding: € 299,625
- **Honey+ - New reasons to care honey from the Natural Park of Montesinho: A bioindicator of environmental quality & its therapeutic potential**
  (MTS/SAS/0077/2020). 01/08/2021 – 31/01/2025. Fundação para a Ciência e a Tecnologia (FCT). Cristina Delerue-Matos (PI), Francisca Rodrigues (co-PI).
  Funding: € 189,845. Total Funding: € 249.827.
- **4FirHealth - Firefighting occupational exposure and early effects on the health of operational forces**
  (PCIF/SSO/0090/2019). 01/03/2021 – 28/02/2025. Fundação para a Ciência e a Tecnologia (FCT). Marta Oliveira (PI). Funding: € 182.269. Total Funding: € 276,135.
- **PaperSenseMIP - Paper-based molecularly imprinted polymer devices for the analysis of pharmaceuticals**
  (PTDC/QUI-QAN/3899/2021). 01/01/2022 – 30/06/2025. Fundação para a Ciência e a Tecnologia (FCT). João Pacheco (PI). Hendrikus Nouws (co-PI). Funding: € 243,076.
- **Chestfilm - Valorization of solid residues from the processing of chestnuts: extraction of biopolymers and preparation of biodegradable films**
  (PD21-00024). 01/07/2022 – 31/12/2025. Fundação "la Caixa", BPI & Fundação para a Ciência e a Tecnologia (FCT) - 4ª Edição do Programa Promove - Concurso 2022 - o Futuro do Interior. Funding: € 77,578. Total Funding: € 242,530.
- **BioReset - Biodiversity restoration and conservation of inland water ecosystems for environmental and human well-being**
  (BiodivRestore-406 / DivRestore/0002/2020). Fundação para a Ciência e a Tecnologia (FCT) - BiodivRestore Joint Call 2020-2021 - European Union's Horizon 2020 research and innovation programme. 01/04/2022 – 31/12/2025. Cristina Delerue-Matos (PI), Hendrikus Nouws (co-PI). Funding: € 61,593. Total Funding: € 898,338
- **NATURIST - Carbon paper and carbon cloth-based sensors for pharmaceutical pollutants: Novel green tools to guarantee fish safety and surveil ecosystems**
  (2022.07089.PTDC). 01/02/2023 – 31/07/2026. Fundação para a Ciência e a Tecnologia (FCT). Simone Morais (PI). Funding: € 140,172. Total Funding: € 249,918
- **AGRIMA - Agri-food Waste Management for Sustainable bio-economy through Higher Education curricula and upskilling**
  (2024-1-PT01-KA220-HED-000243242). 01/10/2024 – 30/09/2026. European Union – Erasmus+. Hendrikus Nouws (PI). Funding: € 74,245. Total Funding: € 400,000.
- **Sens2BiteSafe - Allergen Analysis Breakthroughs: Enhancing Food Safety with Electrochemical Paper-based Analytical Devices**
  (COMPETE2030-FEDER-00713900 (nº 16000)). 01/07/2025 – 30/06/2028. FEDER (COMPETE 2030) and Fundação para a Ciência e a Tecnologia (FCT) / Ministério da Educação, Ciência e Inovação (MECI). Hendrikus Nouws (PI). Funding: € 230,299.
- **WISE - Water Improvement for a Safer Environment**
  (COMPETE2030-FEDER-00841800 (nº 17091)). 01/07/2025 – 30/06/2028. FEDER (COMPETE 2030) and Fundação para a Ciência e a Tecnologia (FCT) / Ministério da Educação, Ciência e Inovação (MECI). Sónia Figueiredo (PI). Funding: € 234,749
- **NeuroDevice - Challenging the Analytical Diagnosis of Neurodevelopmental Disorders: Pioneering Neurochemical Devices**
  (COMPETE2030-FEDER-00699000 (nº 15875)). 01/07/2025 – 30/06/2028. FEDER (COMPETE 2030) and FCT) / MECI. Fátima Barroso (PI). Funding: € 175,694. Total Funding: € 237,470

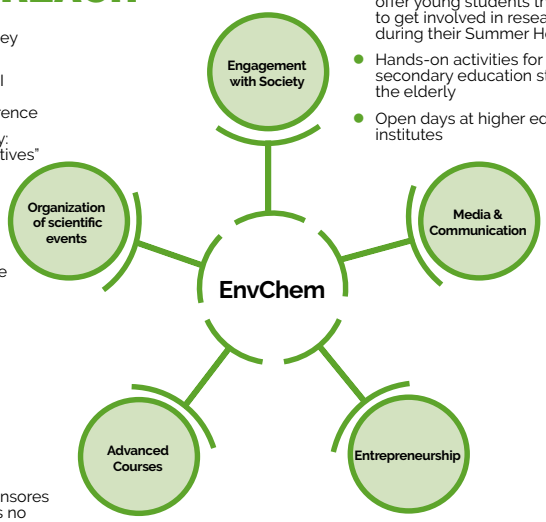
FUNDED PROJECTS *(Representative projects)*

- **NUTRIBRAIN - Coastal Flora for Mental Well-being Promotion: Development of food supplements based on dune plant compounds with impact on BDNF-TrkB signalling**
  (COMPETE2030-FEDER-00686600 (nº 15759)). 01/09/2025 – 31/08/2028. FEDER (COMPETE 2030) and Fundação para a Ciência e a Tecnologia (FCT) / Ministério da Educação, Ciência e Inovação (MECI). Clara Grosso (PI). Funding: € 215,266. Total Funding: € 249,480
- **SUSTAIN - Sustainable Development in agri-food sector: by-products, Emergent Ingredients and Transparent Labeling**
  (COMPETE2030-FEDER-01459400). 01/10/2025 – 30/09/2027. Portugal 2030 – European Regional Development Fund (ERDF) COMPETE 2030. Cristina Delerue-Matos (PI). Funding: € 488,543. Total Funding: € 667,252.
- **Blue Bioeconomy Pact**
  (C644915664-00000026). 01/10/2022 – 31/12/2026. Portuguese Republic - Recovery and Resilience Plan European Union – NextGenerationEU. Cristina Delerue-Matos (PI). Funding: € 730,691. Total Funding: € 133,084,958.
- **REValue- Tecnologias Sustentáveis para a Recuperação de Matérias-primas Críticas de Resíduos Industriais**
  Funded by the Portuguese Foundation for Science and Technology, COMPETE2030-FEDER-00847800, Eduarda Pereira (PI), Funding: 249 264,00€.

INTERNATIONAL COOPERATION AND NETWORKING

- Coordination of the Portugal-Serbia Bilateral Cooperation project "Development of functional foods incorporating a chestnut shells extract obtained by subcritical water" (5537 DRI, Sérvia 2020/21) (2020-2022).
- Coordination of the European project "BioReset - Biodiversity restoration and conservation of inland water ecosystems for environmental and human well-being" (BiodivRestore-406 / DivRestore/0002/2020).
- Coordination of the Portugal-France Bilateral Cooperation project "PLASTOXIC - Microplastics-Toxic Chemicals Occurrence: From the Aquatic Environment Toward Food" (2022.15094.CBM) (2023-2025).
- Coordination of the Erasmus+ project "AGRIMA - Agri-food Waste Management for Sustainable bio-economy through Higher Education curricula and upskilling" (2024-1-PT01-KA220-HED-000243242) (2024-2026).
- Coordination of the Portugal-France Bilateral Cooperation project "FIRESKIN – Firefighters' dermal exposure to fire toxic chemicals: contamination of turnout gear, skin levels, and in vitro health risk assessment" (2024.07134.CBM) (2025-2027)
- Collaboration with several international research institutions and universities from Argentina, Belgium, Brazil, Czech Republic, Denmark, France, Germany, India, Italy, Paraguay, Poland, Romania, Serbia, Slovenia, Spain, Sweden, Netherlands
- Supervision of PhD students in cotutelle (Argelia, Czech Republic, Brazil, Italy, Morrocco, Poland, Spain, and Tunisia)
- Cooperation with several research entities and networks, namely British Antarctic Survey (BAS); International Union of Pure and Applied Chemistry (IUPAC); Natural Environment Research Council (NERC); Network for Industrially Co-ordinated sustainable Land management in Europe (NICOLE); and International Waste Working Group (IWWG).
- Participation in the Special Interest Group "Food" of CARPE, the European Consortium of Applied Research and Professional Education.

DISSEMINATION & OUTREACH



- Conference "BeeCarefull: Honey and Related products value"
- International conference "XXVI Meeting of the Portuguese Electrochemical Society onference
- Conference "Circular Economy: Science and Industry Perspectives"
- Workshop "Exposição ocupacional no combate a incêndios e riscos associados para a saúde dos bombeiros"
- International conference "Water Reuse for a Sustainable World"
- International conference "Occupational Exposure as a Firefighter – Health Risks and Mitigation Strategies.
- Seminar "A importância da qualidade nas instituições"
- Seminar "Quality Concepts in Laboratories"
- I Workshop GEnoPsySEn - Desenvolvimento de genossensores para alvos farmacogenómicos no sistema nervoso central"
- Short course "Mastering Microplastics and Related Chemicals: 2-Day Training in Extraction and Analysis Techniques for Water, Soil and Human Samples"
- Lecture series on Agri-food Waste Management

- "Verão com Ciência" projects, which offer young students the opportunity to get involved in research teams during their Summer Holidays
- Hands-on activities for primarey and secondary education students, and the elderly
- Open days at higher education institutes

- Dissemination of projects in several media, such as TVI 24, RTP, Diário de Notícias, TSF, and Porto Canal
- University of Aveiro Open campus exhibition dedicated to "Materiais para promover a recuperação e reutilização de água contaminada"
- TECHDAYS exhibitions at "Centro de Exposições de Aveiro" dedicated to "Estratégias sustentáveis para o reaproveitamento de águas residuais e industriais" and "Remoção sustentável de contaminantes de água"

- Co-Development TR&D project Blue Bioeconomy Pact
- Active collaborations with several industries.

LABORATÓRIO ASSOCIADO
PARA A **QUÍMICA VERDE**

BCPE

(BIO)CHEMICAL PROCESS ENGINEERING

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

Group Coordinator:

Ana Rita Duarte

The Bio(Chemical) Process Engineering (BCPE) research line integrates 8 research laboratories from Universidade Nova de Lisboa and Universidade de Évora committed to the collaborative development of sustainable (bio)chemical processes and supporting technologies. The group activity is aligned with the National and International R&D agenda, as a response to global challenges and the recognised need for a sustainable economy that protects Citizens, Society, and the Planet. The BCPE research laboratories cover the key scientific disciplines for the integrative development of sustainable chemical and biochemical processes, (bio) reaction engineering, solvents and reaction media, materials and thermophysics, separation/purification, synthesis/ processing, data science and process systems engineering. The key research themes are the following:

- Alternative greener solvents
- Functional materials for process intensification
- (Bio)catalysis and (Bio)refinery
- Sustainable energy, climate change mitigation and pollution control
- Digitalization

RESEARCH OBJECTIVES [2025-2029]

- Functionalized ionic liquids and eutectic systems for delivery of biomolecules, protein crystallization, microfluidics, electrochemical devices, and gas separation.
- Extraction and fractionation of high added-value compounds present in by-product streams, using ionic liquids, eutectic solvents, enzymatic pre-treatment, near- critical water, supercritical carbon dioxide and membrane processing;
- Carbon dioxide capture with ionic liquids, eutectic solvents, membranes and novel adsorption processes, and its (electro-/ bio-)chemical reduction to fuels or use as a green solvent in extraction or (bio) reaction processes;
- Development of functional materials (membranes and adsorbents) with the ability to establish specific molecular interactions and to support the development of cell tissues by dynamic regulation of specific cell biochemical pathways;
- Development of integrated processes for water/wastewater treatment, valorisation and reuse;
- Optimisation of biogas/biomethane and biohydrogen production from biowastes;
- Sustainability assessment of new products and processes through LCA, LCC and sLCA;
- Development of new approaches and membrane sensors for process monitoring, at molecular/ nanoscale, online, real-time or non-invasively, allowing for improved process control;
- In situ transformation of target solutes and their fractionation and purification using sustainable processes;
- Data science and process digitalization by machine learning and hybrid physical/ machine learning techniques for improved process design, optimisation and control.

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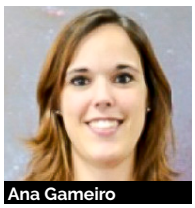
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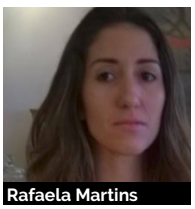
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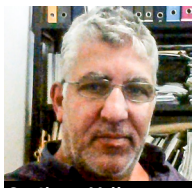
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RESEARCH THEMES/
ALTERNATIVE GREENER SOLVENTS

BCPE has a very strong research activity on the development of alternative green solvents for (bio)chemical processes, covering all critical development stages, from the fundamental chemistry, physicochemical characterization, to tailored design for particular applications.

IONIC LIQUIDS (IL'S)

Playing with ionic liquids structure to discover unusual properties and applications.
Magnetic ILs (Charge-inverted IL pairs) and their applications on the development of high-performance materials.
Cholinium-based ILs for extraction of pharmaceutical compounds using benign Aqueous Biphasic Systems and also for the removal of CO2 from gaseous streams. Amino acid-based ILs to improve enzymatic activity
Pharmaceutically active ionic liquids (API-ILs) to upgrade the chemical, physical, and biopharmaceutical properties of the parent APIs.
Fluorinated Ionic Liquids(IL) Application as drug delivery systems.
Enhanced tunability afforded by aqueous biphasic systems and ILs.
IL – gas hydrate (GH) based systems for clean energy (transportation/ storage) and climate change (CO2 capture)

DEEP EUTETIC SOLVENTS (DES)

Fundamental studies on DES: Physico-chemical and thermodynamic properties, molecular dynamic simulations
DES for polymer processing and modification
DES as stabilizing agents and bioavailability enhancers in pharmaceutical applications.
DES for the production of stable nanoemulsions using novel membrane emulsification approaches;
DES as alternative solvents for extraction and recovery of bioactive compounds

SUPERCRITICAL FLUIDS (SCF)

Supercritical fluid carbon dioxide for extraction and separation:
Extraction of TCA from cork in collaboration with corticeira Amorim.

Collaboration contract with the company EXMCeuticals Portugal for the use of this technology for the extraction of cannabinoids and cannabis oil from cannabis.
Scale-up and design of an industrial plant for the supercritical purification of omega-3 fish oil, financed by Brudy Technologies

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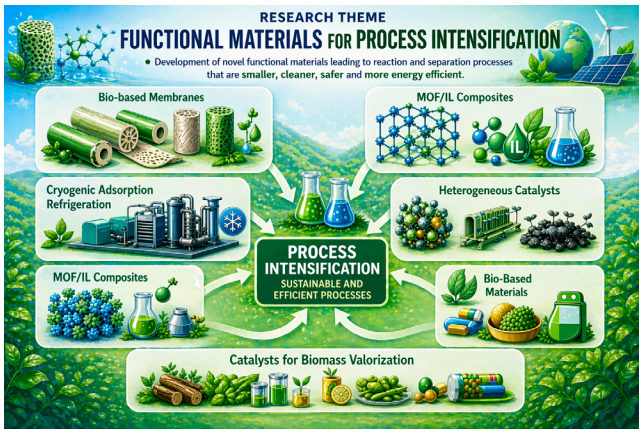
RESEARCH THEMES/
FUNCTIONAL MATERIALS FOR PROCESS INTENSIFICATION

BCPE is committed to the development of novel functional materials leading to reaction and separation processes that are smaller, cleaner, safer and more energy efficient.

- Development of new membrane materials, namely: membranes produced from biopolymers for organic solvent drying and gas drying; membranes with photocatalytic activity for degradation of organic micropollutants and inactivation of pathogens (disinfection); membranes with modulated magnetic response for fouling control; controlled release of bioactive compounds; membrane-like-cell scaffolds for tissue culture and regeneration; membranes with designed topography for locally induced crystallization of proteins.
- Development of advanced hybrid metal organic frameworks-ionic liquids composites to be used as adsorbents with very large specific surface area and finely tuned porosity that enables increased selectivity, to optimize gas separation processes.
- Development of bio-based materials with enhanced porosity for application as catalysts, as adsorbents for water treatment and as adsorption materials from renewable sources for medical applications;
- Development of bio-based materials tailored to act as delivery systems for agriculture purposes, pharmaceutical applications, and food supplements;
- Development of catalysts for biomass valorisation via chemical reactions, using bio-platform molecules such as furfural within the biorefinery concept;
- Process intensification of the catalytic reaction using membrane reactors with bio-based catalysts particularly for biomass valorisation reactions and biodiesel production.
- Development of a cryogenic refrigeration system without vibration or mobile components, using an innovative technology based on adsorption organo-metallic pumps.
- Development of heterogeneous catalysts consisting of homogenous complexes anchored on carbon supports and metal nanoparticles deposited on oxide supports for reactions of industrial importance.



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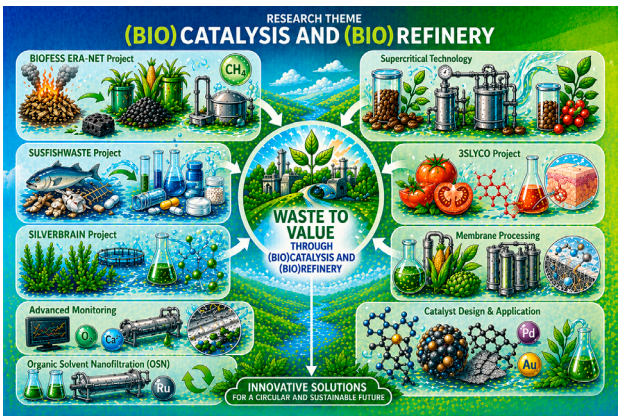
RESEARCH THEMES/
(BIO)CATALYSIS AND (BIO)REFINERY

BCPE is committed to the valorisation of waste materials by recovery and/or (bio)catalytic transformation into value added compounds:

- The slash and burn of maize wastes or the organic fraction of municipal solid wastes are urgent problems that need efficient and fast solutions. BioFESS ERA-NET project produces high-quality activated carbon (AC) from biomass residues, used as adsorbent of impurities in liquid/gaseous media and to recover CH4 from biogas.
- Extraction and fractionation of added-value compounds using supercritical technology: i) valorisation of spent coffee grounds and ii) decaffeination of coffee beans (DELTA Cafés)
- The "Susfishwaste" project aims to develop a sustainable strategy for the valorisation of fish waste into high added value products in key areas such as biomedicine, pharmaceuticals, cosmetics and food.
- The "3SLYCO" project aims to valorise the presence of carotenoids such as lycopene in the residues of the tomato industry for the treatment of inflammatory skin disorders.
- The "Silverbrain" project, aims at the extraction of bioactive compounds from macroalgae from integrated multitrophic aquaculture harvested on the Portuguese coast.
- Use of membrane processing for the recovery, transformation and fractionation of target added-value compounds from harvesting of microalgae (EC projects D-Factory and SaltGae) and their biorefining (EC projects D-Factory and Multi-Str3am), the valorization of corn wastes (funded by COPAM) and the recovery of bioactive compounds from Cynara cardunculus.
- Advanced monitoring approaches based on the use of membranes sensitive to O2 and Ca2+ for in situ and non-invasive detection of early stage fouling and scaling phenomena in membrane processes. Use of Organic Solvent Nanofiltration (OSN), for recovery and reuse of Ru-based catalyst. OSN and membrane pervaporation processes are also used for a continuous removal of reactions by products.
- Design and application of organometallic complexes, such as palladium and gold compounds, and novel metal oxide/carbon nanocomposites as efficient catalysts for several reactions of industrial importance and bio-applications.



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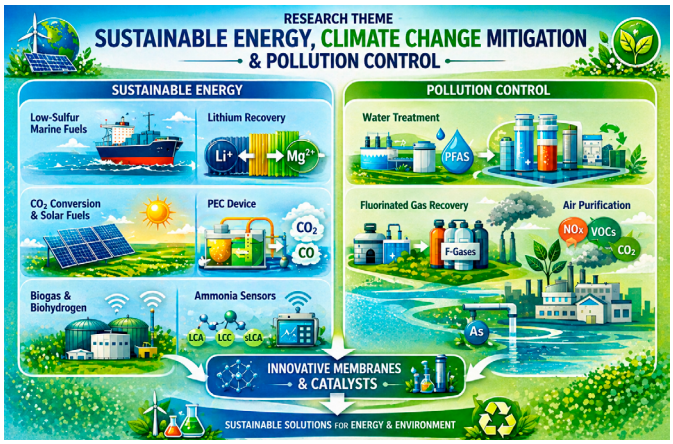
RESEARCH THEMES/
SUSTAINABLE ENERGY, CLIMATE CHANGE MITIGATION AND POLLUTION CONTROL

SUSTAINABLE ENERGY

BCPE is focused on the development of novel processes for energy production and/or for decreasing the environmental footprint of fossil fuels:

- To create a sustainable and cost-effective solution to produce low-sulfur marine fuels (Heavy Fuel Oil)
- Development of new membrane materials and processes for the recovery of lithium from seawater, saltworks and brine streams, promoting its separation from magnesium and from sodium.
- Development of a Lithium Membrane Flow Electrode Capacitive Deionisation prototype, using flow electrodes.
- In the SunStorage project, conversion of solar energy into chemical and electrochemical energies and respective storage. The CO2 conversion is a strong focus, particularly the development and characterization of photoelectrochemical (PEC) devices for solar photoelectroreduction of carbon dioxide to CO.
- CO2usE project focuses on the direct reaction between CO2 and diols for the production of organic carbonates, using hydrophobic ionic liquids (with high CO2 up-take), as solvents for metal-based catalysts.
- The CO2RED project investigates co-electrolysis of CO2 and water to produce syngas as a platform to produce renewable fuels and sustainable chemicals.
- In the M-ECO2 – Industrial cluster for advanced biofuel production, sustainable processes for hydrogen and CO production by CO2 and water co-electrolysis are investigated.
- Projects developed with industries focus on the optimisation of biowaste treatments and operational parameters for biogas/biomethane and biohydrogen production.
- Development of electrospun membrane sensors allowing for a non-invasive detection of ammonia, in low concentrations, in gas phase, intended for agricultural and livestock farming applications - OPTIMA (PTDC/CTA-AMB/31559/2017)
- LCA, LCC and sLCA allows assessing the sustainable dimension of new products and processes developed in BCPE.



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RESEARCH THEMES/
CLIMATE CHANGE MITIGATION AND POLLUTION CONTROL

WATER TREATMENT/VALORIZATION/REUSE

BCPE is committed to the development of water and air treatment processes and technologies for pollution control:

- ALERT-PFAS proposes real-time detection and monitoring of PFAS to prevent these substances from entering the water cycle, with pilot actions planned in natural parks and protected areas that have recently suffered from wildfires.
- LIFE REAMINE, which seeks to develop, implement, and industrially validate the use of an advanced amine recovery technology in core manufacturing operations.
- Use of membrane processes for water treatment aiming the improved quality of water for domestic use or for reuse in urban and industrial applications. These projects involved the design, construction, implementation and validation of dedicated membrane equipment at a pilot scale, operated on-site.
- Wastewater treatment combining membrane filtration (ultrafiltration and/or nanofiltration) with photocatalytic degradation of rejected pollutants.
- Membrane wastewater treatment aiming its reuse for irrigation in the production of fruits.
- Ion-exchange membrane reactor for the removal and recovery of arsenic from drinking water supplies. BCPE is involved in the development of real-time, online techniques that allow for process monitoring, (RESURGENCE), use of molecular probes and online mass spectrometry.
- Construction, demonstration and optimization of an innovative installation to selectively recover fluorinated gases (F-gases) from refrigerant blends allowing the F-gas reutilization in novel environmentally-friendly refrigerant mixtures with low-GWP.
- Development of air treatment processes and technologies for pollution control, focusing on the search for novel functional materials to clean air from contaminants such as nitrogen oxides (NO and NO_2), volatile organic compounds (VOCs, e.g., toluene), and carbon dioxide (CO_2), through advanced photocatalytic and catalytic approaches.

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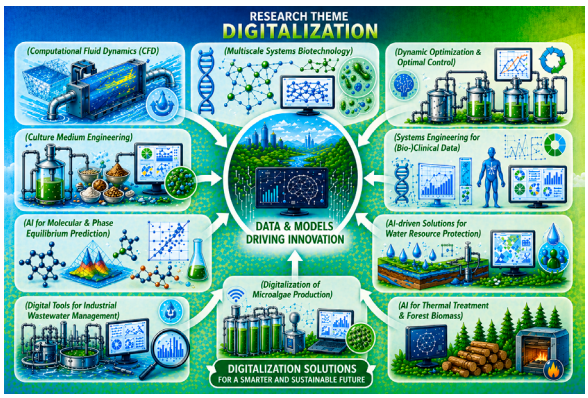
99 M. Yu et al., Sep. Puri.Tech. 2025, 354, 128695. **doi: 10.1016/j.seppur.2024.128695**

100 L. Ma et al., Chin. J. Struct. Chem. 2024, 43 (11), 100416. **doi: 10.1016/j.cjsc.2024.100416**

RESEARCH THEMES/ DIGITALIZATION

BCPE is committed to the development and application of Data Science and systems analysis for product & process engineering, covering the emerging Artificial Intelligence/Machine Learning topics, but also the traditional First Principles, mechanistic phenomenological approaches:

- Computational Fluid Dynamics (CFD) to model flow patterns in membrane applications for sustainable water desalination and resource recovery.
- Hybrid AI/genome-scale modelling: novel multiscale systems biotechnology methods, integrating molecular, subcellular, cellular, community microbiomes and the macroscopic process scales through the combination of AI and genome-scale reconstructed metabolic networks.
- FASTPROCESS: Dynamic optimization/optimal control algorithms supported by hybrid AI/engineering models are used for iterative batch-to-batch process improvement and iterative batch-to-batch parallelization.
- SILICOMEDIA: Novel systems approaches for culture medium engineering to grow cells for more efficient and sustainable bioprocesses engineering (funded by GlaxoSmithKline).
- Development and application of new systems engineering techniques (ML algorithms, data analytics and computational modelling) for (bio-) clinical data analysis and decision-making.
- AI approaches for phase equilibrium prediction and comprehension, modelling of physico-chemical properties of ionic liquids, deep eutectic systems and organic molecules.
- MAR2PROTECT project is an Artificial Intelligence-driven tool that processes real-time data and integrates technological solutions and societal engagement preferences to enhance groundwater quality and quantity.
- Development of digital tools for industrial wastewater management based on multivariate data analysis to achieve real-time, online performance prediction and enabling optimized process control and cost reduction.



- Optimizing microalgae production through digitalization: focus on developments in sensor-based real-time monitoring and control, process simulation, automation and data analytics to enhance resource efficiency and product consistency.
- Use of AI approaches to control thermal treatment and produce high-quality forest wood biomass.

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104 K. O. Klimenko et al., Molecular Informatics, 2020, 2000001. **doi: 10.1002/minf.202000001**

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106 P. Reynolds-Brandão, et al., Bioresour. Technol. 2025, 418, 131988. **doi: 10.1016/j.biortech.2024.131988**

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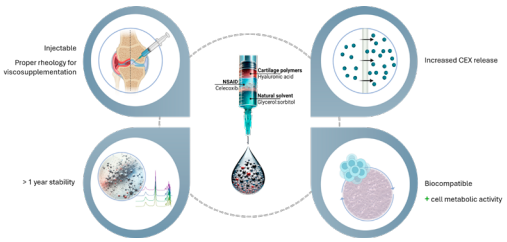
HIGHLIGHTS

OSTEODUAL

Osteoarthritis (OA) is an inflammatory disease, characterized by cartilage loss, pain and loss of joint function. It is a leading cause of disability worldwide, affecting 7% of the population. Portugal is the European leader of prevalence (8.5%) and the 3rd worldwide. Current therapies include pain relief with oral non-steroidal anti-inflammatory drugs (NSAID) such as celecoxib (CEX), and intra-articular injections of hyaluronic acid (HA), to restore the joints' lubricant and protective properties. OsteoDUAL is a patented injectable formulation able to combine HA+CEX, and this combination is only possible due to the proprietary knowledge of the group on eutectic systems, namely on eutectic systems (DES). OsteoDUAL takes advantage of the properties of DES, rendering a gel for viscosupplementation with: 1) increased lubricant properties; 2) improved CEX solubility, incorporated for local anti-inflammatory action; and 3) compatibility with HA, for cartilage protection and as a regenerative building block.



The effect of a low transition temperature mixture for enhanced bioavailability of celecoxib in combination with hyaluronic acid in a rat model with post-traumatic knee osteoarthritis.

Biomedicine and Pharmacotherapy, 189, 118239, 2025

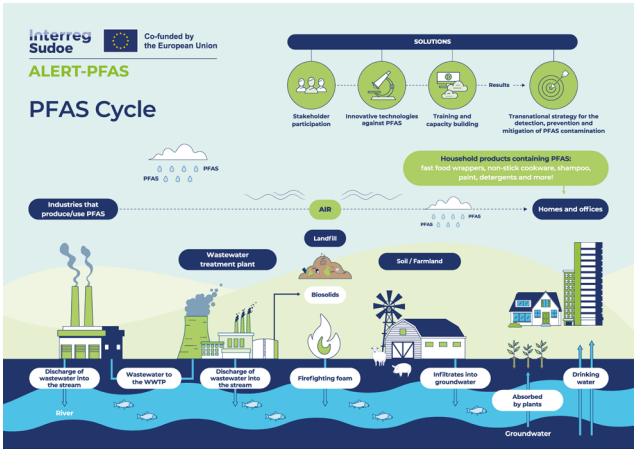
A Low Transition Temperature Mixture-based viscosupplementation complemented with celecoxib for osteoarthritis treatment.

International Journal of Pharmaceutics, 656, 124088, 2024

International Patent Application: PCT/IB2024/056817

TRANSNATIONAL STRATEGY TO DETECT AND PREVENT PFAS CONTAMINATION

Climate change is causing an increase in more intense and aggressive wildfires in the SUDOE area (Spain, Portugal, and France). The wildfires severely affected natural parks and protected areas, endangering biodiversity and ecosystems. To fight these fires, the use of fire-fighting foams containing flame retardants has increased. However, these foams contain PFAS (per- and polyfluoroalkyl substances), known as "forever chemicals", which are highly persistent, mobile, and harmful to both human health and the environment. ALERT-PFAS (2024-2026) aims to detect, prevent and mitigate PFAS contamination, highly persistent pollutants, using innovative technologies from natural parks across the SUDOE region. In addition, it raises awareness and trains key stakeholders to reduce environmental impact and tackle climate change.

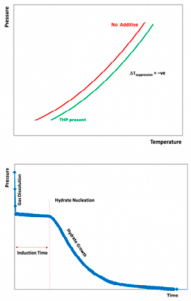


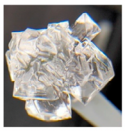
HIGHLIGHTS

FUNCTIONAL IONIC LIQUIDS FOR IMPROVED GAS HYDRATE TECHNOLOGY

Chemicals used as GHs inhibitors (GHIs) to mitigate the flow assurance issues in the oil/gas industry are generally toxic, flammable, volatile and need to be used in high quantities (up to 50 wt%). The development of environmentally friendly functional ionic liquids (ILs) that can act as low dosage hydrate inhibitors (LDHIs) without posing the problems mentioned earlier is a good strategy because of their designer nature.
Moreover, ILs can also be used as GH promoters and may replace the conventional promoters (surfactants that lead to foaming in the reaction vessel) to enhance the formation rate of hydrates for rapid gas storage and capture. We aim to convert natural gas into solid pellets so that they can be transported easily across borders in a compact form. Development of environmentally friendly ionic liquid (IL) – gas hydrate (GH) based biocompatible systems (semiclathrates) to address some of the societal challenges, namely clean energy (transportation/storage) and climate change (CO2 capture) is ongoing.

CO_2 Hydrates





THF Hydrates

Evaluating Amino Acid-Based Additives and Ionic Liquids as Sustainable Kinetic Hydrate Inhibitors: Nucleation Behavior and Toxicity Assessment..

Energy and Fuels, 39 (2025) 19849

Effect of Thiouronium-Based Ionic Liquids on the Formation and Growth of CO2 (sI) and THF (sII) Hydrates.

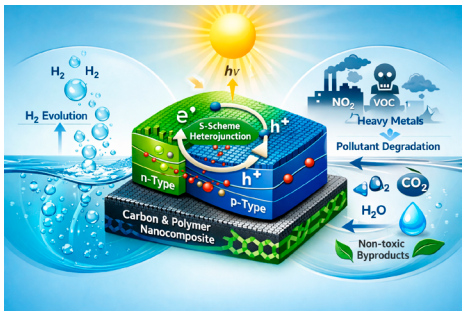
International Journal of Molecular Sciences 23 (2022) 3292

Insights into CO2 hydrates formation and dissociation at isochoric conditions using a rocking cell apparatus.

Chemical Engineering Science 249 (2022) 117319

ADVANCED NANOMATERIALS FOR GREEN HYDROGEN PRODUCTION AND ENVIRONMENTAL REMEDIATION

The conversion of solar energy into sustainable solutions for clean fuel production and environmental remediation has attracted increasing scientific interest. Semiconductor-based photocatalysis stands out as a promising strategy for both green hydrogen generation and the degradation or removal of organic and inorganic environmental pollutants. However, the development of highly efficient photocatalysts remains challenging, as a single material rarely combines broad light absorption, efficient charge separation, and strong redox capability. Recent advances in photocatalyst design—such as step-scheme (S-scheme) heterojunctions, defect engineering strategies, and the construction of Ohmic junctions—have proven effective in enhancing light absorption, interfacial charge transfer, and overall photocatalytic efficiency for hydrogen evolution and efficient removal of air and water pollutants.



Electrocatalytic Synthesis of C-N Coupling Compounds from CO 2 and Nitrogenous Species.

SusMat 2024, 4, e193

Understanding the unique Ohmic-junction for enhancing the photocatalytic activity of CoS2/MgIn2S4 towards hydrogen production,

Applied Catalysis B: Environment and Energy 2024, 351, 123950

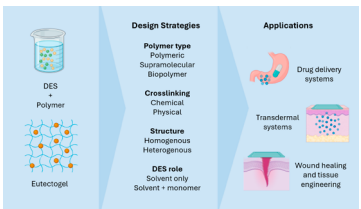
Enhanced photocatalytic efficiency through oxygen vacancy-driven molecular epitaxial growth of metal-organic frameworks on $BiVO_4$.

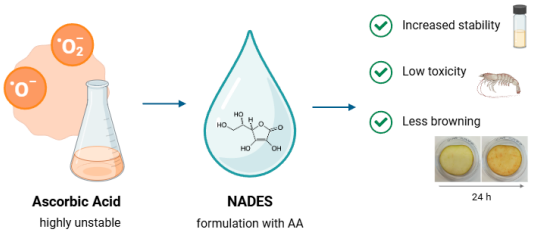
Advanced Materials 2025, 37, 2417589

HIGHLIGHTS

NATURAL DEEP EUTECTIC SYSTEMS (NADES)

Natural deep eutectic systems (NADES), are a new class of green solvents that consist of the mixture of two or more natural metabolites, normally solid at room temperate, that a certain ratio suffers a high melting point depression being liquid at the room, or near room temperature. Their production consists only of a mixture process, reducing drastically process complexity and environmental load, with no waste produced. There are several applications for NADES, from biocatalysis, where NADES act as both solvent and substrate, to extraction solvent, where NADES can be part of the final formulation, circumventing the need to complex downstream processing for the separation and recovery of the solvent, while at the same time avoiding additional processes for the formulation of the extract. When a therapeutic agent is used in the production of NADES, they can be used for many pharmaceutic applications, increasing the bioavailability of the API with no need for chemical modifications or complex formulations. NADES may also present several properties that open opportunities in the industry; as anti-biofilm agents, cryoprotective agents, solvents for carbon capture and utilization and food preservatives.



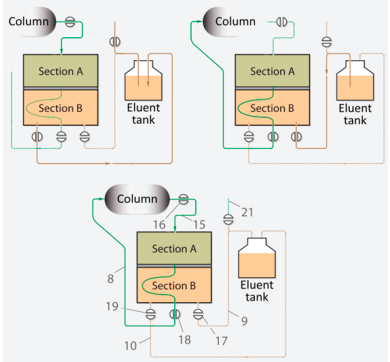


Terpene-Based Natural Deep Eutectic Systems as Efficient Solvents To Recover Astaxanthin from Brown Crab Shell Residues.

ACS Sustainable Chemical Engineering, 2020, 8, 5, 2246–2259.

PROCESS INTENSIFICATION IN DOWNSTREAM BIOPROCESSING

New low-carbon adsorption-based technologies, underlined for wide-spread (or horizontal) industrial applications, are attempted to oppose the well-known problems of resource limitations and severe environmental impacts. These goals are within the Sustainable Development Objectives of the 2030 EU Agenda. This research includes the advance of environmentally clean technology for biogas to biomethane from a biorefinery concept, the production & storage of natural gas, and the recovery of gas/liquid wastes and high-value streams, capable of competing advantageously with the already existent conventional techniques, in terms of production costs and environmental sustainability. In parallel, a strong commitment is being given to the development of novel functional materials leading to adsorption separation processes that are smaller, cleaner and more energy efficient. To reach this goal, the search for 1) new adsorbents (metal-organic-frameworks, nanotubes, carbons, hybrid composites) in the topical materials era, combined with ionic liquids and new manufacturing approaches for their formulation (3D printing), are presently emphasized in the research.



Batch chromatography with recycle lag. I—Concept and design and II—Physical realization and experimental validation.

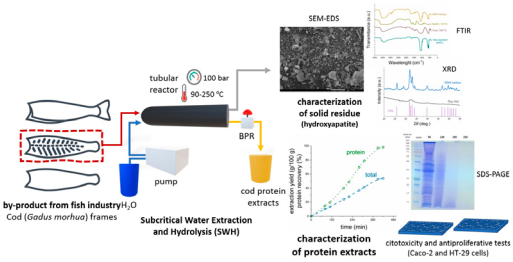
Journal of Chromatography A, 2020, 1623, 461199 & 461211

HIGHLIGHTS

INTEGRATED BIOREFINERY: FRACTIONATION OF FISH CANNING INDUSTRY WASTES BY GREEN SOLVENTS

The world fish production is estimated nowadays to be around 200 million ton. About 70% is processed before sale, producing a significant amount of fish waste of which only a small amount is used for low-value fish silage and animal feeds, the rest being landfilled or incinerated. Yet, fish industry wastes are a valuable source of lipids, proteins, pigments, bioactive peptides, amino acids, inorganics, etc.

Supercritical carbon dioxide and subcritical water were used in a sequential order to fractionate fish canning industry wastes (sardines, cod fish) into different useful fractions, within the concept of integrated biorefinery. Specific extracts rich in lipids and proteins were obtained showing favorable bioactivity and good potential as functional ingredients in food and nutraceutical products. Concurrently, a final residue was obtained, consisting of nearly pure, crystalline hydroxyapatite, that may find applications in biomedical field and hard tissue engineering.



Frames to Produce Bioactive Protein Extracts.

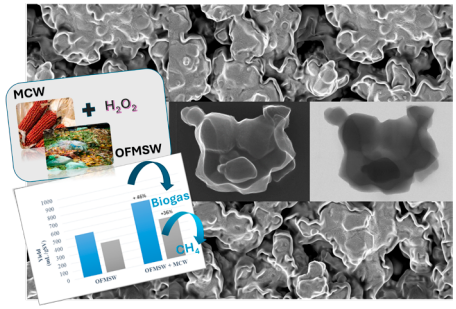
Foods 10 (2021) 1222.

Supercritical CO2 extraction of bioactive lipids from canned sardine waste streams.

Journal of CO2 Utilization 43 (2021) 101359.

(BIO)CATALYSIS & (BIO)REFINERY/FUNCTIONAL MATERIALS FOR PROCESS INTENSIFICATION

New low-carbon adsorption-based technologies, underlined for wide-spread (or horizontal) industrial applications, are attempted to oppose the well-known problems of resource limitations and severe environmental impacts. These goals are within the Sustainable Development Objectives of the 2030 EU Agenda. This research includes the advance of environmentally clean technology for biogas to biomethane from a biorefinery concept, the production & storage of natural gas, and the recovery of gas/liquid wastes and high-value streams, capable of competing advantageously with the already existent conventional techniques, in terms of production costs and environmental sustainability. In parallel, a strong commitment is being given to the development of novel functional materials leading to adsorption separation processes that are smaller, cleaner and more energy efficient. To reach this goal, the search for 1) new adsorbents (metal-organic-frameworks, nanotubes, carbons, hybrid composites) in the topical materials era, combined with ionic liquids and new manufacturing approaches for their formulation (3D printing), are presently emphasized in the research.



Carbons for Biorefinery (BioFESS, ELAC2014/BEE0367). Right: Porous MOF@IL hybrid sorbents (CMILE,PTDC/CTM-CTM/30326/2017)

Boosting CO2 selectivity by mono- and dicarboxylate-based ionic liquids impregnation into ZIF-8 for post-combustion separation.

Carbon Capture Science and Technology, 2024, 13, 100282.

Carbon materials derived from cyano-based IL@ZIF-8 composites for CO2 sorption separation systems.

Materials Today Sustainability, 2023, 22, 100353.

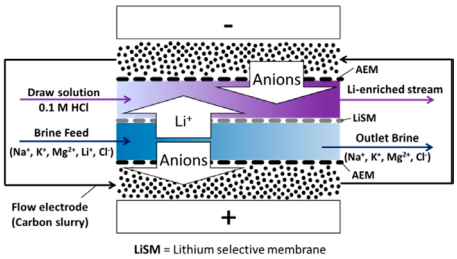
Biocompatible Ammonium-based Ionic Liquids/ZIF-8 Composites for CO2/CH4 and CO2/N2 Separations.

Sustainable Materials and Technologies, 2023, 35, e00558

HIGHLIGHTS

SUSTAINABLE RECOVERY OF LITHIUM FROM SALINE STREAMS AND END-OF-LIFE LI-ION BATTERIES

Lithium is an essential metal in the global economy due to its application in Li-ion batteries (LIBs). Apart from environmentally harsh hard-rock mining, potential sources of lithium include natural and industrial brines, as well as end-of-life LIBs. A new process, Lithium-Membrane Flow Electrode Capacitive Deionization (Li-MFCDI), was developed to achieve sustainable lithium recovery. For this purpose, polymeric membranes with target selectivity for lithium were synthesized and the composition of the non-Newtonian flow electrodes was optimized. As proof of concept, lithium was successfully recovered from a sodium-rich geothermal brine with a Na^+/Li^+ mass ratio of 650. The process demonstrated stable operation and exhibited very high selectivity for lithium compared to other monovalent cations: 141 for Li^+/Na^+ and 46 for Li^+/K^+. Furthermore, the composition of flow electrodes is being optimized and novel membranes are being prepared, based on molecular dynamics simulation insights, to separate lithium from cations such as cobalt, nickel and manganese, all present in the LIBs cathode material. To recycle lithium from LIBs, these membranes will be incorporated into the Li-MFCDI prototype which was meanwhile constructed.



LiSM = Lithium selective membrane

Lithium recovery from brines by lithium membrane flow capacitive deionization (Li-MFCDI) – A proof of concept.

Journal of Membrane Science Letters (2023) 3 (2), 100059

The influence of flow electrode channel design on flow capacitive deionisation performance: Experimental and CFD modelling insights.

Desalination 578 (2024) 117452

Deep eutectic solvent flow electrodes for high-voltage desalination via flow electrode capacitive deionization.

Desalination 614 (2025) 119218.

MITIGATION OF THE ENVIRONMENTAL IMPACT OF FLUORINATED GASES

The main objective of LIFE-4-Fgases (2021-2025) is to develop alternative, environmentally-friendly separation processes for recycling/recovery of the fluorinated gases (F-gases) used in a wide number of industrial applications. LIFE-4-Fgases contributes to improve the sustainability of the RAC sector through the demonstration, with an innovative concept-based prototype, of the efficient recovery of value-added pure F-gases from refrigerant blends with high global warming potential (GWP) contained in end- of-life equipment, for re-utilization purposes in novel environmentally friendly refrigerant blends with low-GWP, applying circular economy.

This main objective enshrines the construction, demonstration and optimization of an innovative installation to selectively recover F-gases, being the first installation of this type worldwide, and its operation in a real environment at the industrial waste management facilities of Ambigroup Reciclagem, S.A. in Seixal (Portugal). LIFE-4-Fgases is the continuation of the European project KET4F-Gas (2018-2021) which aimed at the design and optimization of systems for the separation of azeotropic mixtures of refrigerant F-gases into their individual components using different multi-Key Enabling Technologies.

Life 4 F-gases

KET4F-Gas Launch Event
LISBON 11th June 2018

Design of Ionic Liquids for Fluorinated Gases Absorption..

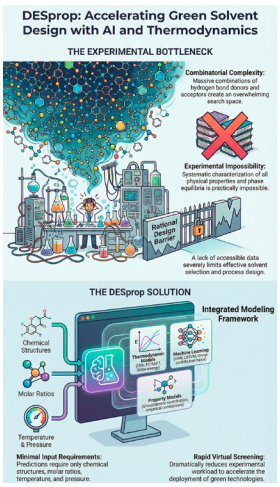
Environmental Science & Technology, 2022, 56, 5898−5909

HIGHLIGHTS

PREDICTIVE THERMODYNAMIC & AI MODELS FOR DEEP EUTECTIC SOLVENTS

This work was financed by national funds by CEEC IND5ed (DOI 10.54499/2022.05803.CEECIND/CP1725/CT0003).

Deep eutectic solvents (DESs) are emerging as highly versatile green solvents, formed from an enormous combinatorial space of hydrogen bond donors and acceptors. This makes systematic experimental characterization of their physical properties and phase equilibria practically impossible, and severely limits rational process design and solvent selection.

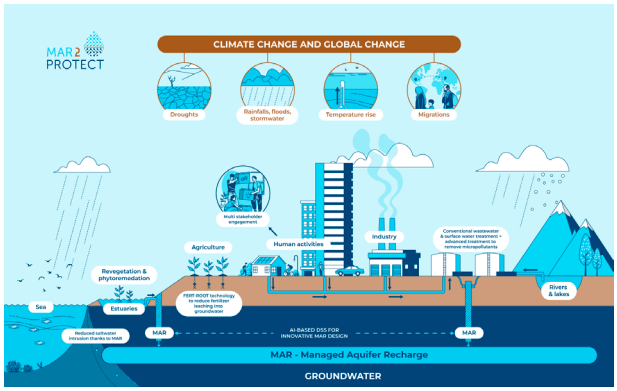


We are developing a comprehensive thermodynamic and machine learning framework, implemented in a user-friendly software package named DESprop. DESprop integrates an extensive DES databank with four complementary classes of models: (i) advanced associating equations of state (CPA, PC- SAFT) and Gibbs-energy models for phase equilibria; (ii) group/atomic contribution models for critical and transport properties; (iii) accurate empirical correlations; and (iv) machine-learning models (ANN, LSSVM) built on a group- contribution basis. By combining rigorous thermodynamic modelling with state-of-the-art AI in a single accessible tool, DESprop will allow engineers and researchers to virtually screen and optimize DESs for targeted applications, dramatically reducing experimental workload and accelerating the deployment of green solvent technologies in industry.

PREDICTIVE THERMODYNAMIC & AI MODELS FOR DEEP EUTECTIC SOLVENTS

MAR2PROTECT project provides a holistic approach to prevent groundwater contamination from global and climate change impacts based on a new-generation Managed Aquifer Recharge (MAR). The core of this project is M-AI-R Decision Support System that incorporates technological and societal engagement information using an AI-based approach to improve groundwater quality and quantity.

Seven demo sites were selected to be representative of a wide panorama in terms of climatic conditions, type of groundwater pollution, water source used for Managed Aquifer Recharge and political /societal context, and to maximize the potential replication of the MAR2PROTECT holistic approach and impact. All demo sites include a coastal aquifer affected by salinity intrusion and the demo sites were also carefully chosen by their degree of maturity from previous successful projects developed by the partners. The MAR2PROTECT LivingLabs integrates technological innovations and strong engagement of stakeholders to explore different socio-economic, political, geographical, climatic and technological settings, to cocreate and uptake the proposed technologies and to promote a behavioural transition towards the prevention of contamination.



This project has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No GA 101082048

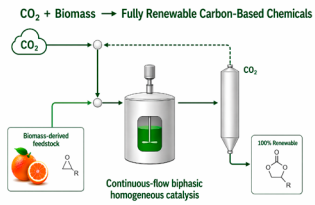
Funded by the European Union

HIGHLIGHTS

CO_2 UTILIZATION AS RENEWABLE FEEDSTOCK FOR THE CHEMICAL AND ENERGY SECTORS

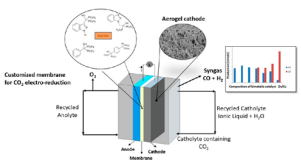
The group is involved in different projects for CO2 utilization as chemical feedstock bringing carbon back into the value chain for the production of sustainable chemicals, materials and fuels. This allows the CO2 valorization, contributing to the substitution of fossil carbon, to the net reduction of global CO2 emissions, and to the increase of circularity in production systems. Ongoing research is focusing on the combination of CO2 with substrates derived from biomass in the production of 100% renewable building blocks for the chemical and materials industry. CO2 will further be a key pillar in the new paradigm of energy systems comprising it reductive conversion into energy vectors. Ongoing project has been focused in the: (i) development of a pressurized process for syngas production near room temperature; (ii) the optimization of the design of a pressurized membrane electrolyser; (iii) the development of an ionic-liquid based electrolyte to integrate CO2 capture with CO2 conversion; (iv) development of 3D porous electrodes; (v) process simulation of integration of photovoltaics-electrolysis for the production of solar fuels.

This work has been funded by Fundação para a Ciência e Tecnologia through projects CO2 Value (MIT-EXPL/CS/0052/2021) and CO2RED (PTDC/EQU-EPQ/2195/2021).



Limonene carbonate synthesis from CO2: Continuous flow catalysis with integrated product separation.

J. Supercrit. Fluids, 2023, 193, 105827



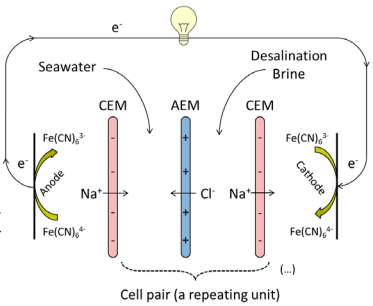
Imidazolium and picoline-based electrolytes for electrochemical reduction of CO2 at high pressure.

Energy Advances, 2022, 1, 277 - 286

HARVESTING OF SALINITY GRADIENT ENERGY FROM DESALINATION BRINES BY REVERSE ELECTRODIALYSIS

The brines resulting from desalination are a severe environmental problem associated with the extensive practice of seawater reverse osmosis (RO) desalination technology, exacerbated by the relatively low water recovery factor (40-50%) of current plants. Furthermore, the energy consumption of these processes is still high (3-4 kWh per m3 of desalted water). Since the brines need to be discarded, it is possible to harvest the salinity gradient energy which is released when two solutions with different salinity mix. The theoretical amount of extractable energy is about 4500 kJ when mixing 1 m3 of seawater (0.5 M NaCl) and 1 m3 hypersaline brine (5 M NaCl). To convert this energy into electricity, Reverse Electrodialysis (RED) electro-membrane technology will be employed. This process is being optimized through 1) the development of ion exchange profiled membranes using 3D printing technology, either directly, either by preparation of supports/molds with a low cost, 2) optimization of stack channels' geometry based on CFD studies, and 3) development of monitoring methods and molecular probes for online tracking of fouling onset and development.

This project receives funding from the European Union's Horizon Europe research and innovation programme under the Marie Skłodowska-Curie grant agreement No 101072449. (EXBRINER: Next-generation membrane technologies for sustainable exploitation of seawater brine resources: transition towards a circular blue industry — HORIZON-MSCA-DN-2021).



Development of cation-exchange membranes using solvent-free 3D printing: towards customised surface topographies.

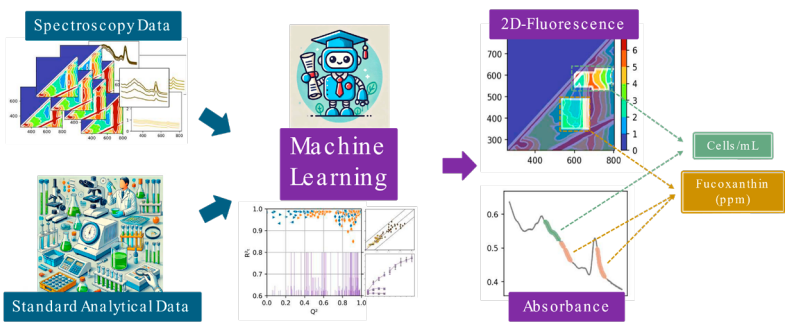
Separation and Purification Technology, 378 (2025) 13456

HIGHLIGHTS

DEVELOPMENT OF SOFT SENSORS FOR MONITORING (BIO) CHEMICAL PROCESSES

Monitoring of (bio)chemical processes involves a high number of off-line and time-consuming analytical techniques required to assess process performance and ensure quality standards. Furthermore, for process control, it is essential to know the process status in order to act immediately. Soft sensors, based on input data acquired online, can be used to estimate at real-time relevant performance parameters that are usually difficult to measure and are obtained with a significative time delay. In the European project AQUAMONITRIX, we developed 14 soft sensors for monitoring water quality in wastewater treatment plants to be integrated with the monitoring device produced (actually being commercialized as AQUAMONITRIX®), widening the number of parameters that can be monitored.
Furthermore, the use of fluorescence and UV-vis spectroscopy to collect online information from biological production systems combined with computational data analysis (both supervised and unsupervised tools) is being used to develop monitoring and control tools for the production of different microalgae (MULTI- STR3AM, MULTIPLY, Phyco-µ-Biome, BioFluSens), for biological performance of bioplastic production and for industrial wastewater monitoring aiming at water reuse (RESURGENCE).

This work has been funded by European projects AQUAMONITRIX (LIFE17 ENV/IE/000237), MULTI-STR3AM (Horizon 2020, Contract No. 887227), MULTIPLY (HORIZON-JU-CBE-2024, Contract No 101214894) and RESURGENCE (HORIZON EUROPE, Contract No 101138097), and national projects Phyco-µ-Biome (FCT, PTDC/BAA-BIO/1262/2020) and BioFluSens (FCT, 2023.14928.PEX).



Acidogenic Fermentation of Brewers' Spent Grain Monitored through Two-Dimensional Fluorescence Spectroscopy.

ACS Sustainable Chemistry & Engineering. 11 19 (2023): 7398-7406

Learning from fluorescence: A tool for online multiparameter monitoring of a microalgae culture.

Computers & Chemical Engineering 179 (2023): 108452

Integration of spectroscopic techniques and machine learning for optimizing Phaeodactylum tricornutum cell and fucoxanthin productivity.

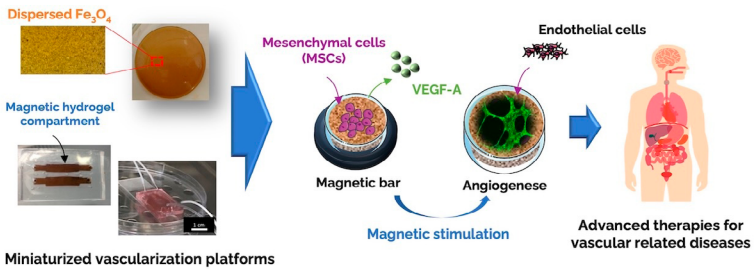
Bioresource Technology 418 (2025): 131988

HIGHLIGHTS

MAGNETIC-RESPONSIVE 3D VASCULAR PLATFORMS FOR IMPROVED DEVELOPMENT OF RELIABLE VASCULAR CELL MODELS

The use of renewable solar energy to produce green chemical fuels is considered a promising method to mitigate the effects of the increasing environmental pollution and energy crisis. Semiconductor photocatalysis has been widely applied to produce hydrogen and to obtain renewable fuels. It is difficult for a single photocatalyst to simultaneously meet the requirements of wide light absorption and strong redox ability. Stepscheme (Sscheme) heterojunction models, coupling an oxidation photocatalyst and a reduction photocatalyst, is an interesting approach that stimulates the spatial separation of the photogenerated charge carriers and maintains the strong reduction/oxidation ability of the photocatalyst. The introduction of atomic-level vacancies on semiconductor photocatalysts is another promising alternative that can effectively improve the separation of photogenerated carriers and enhance light absorption, improving the process efficiency.

This project has received funding from FCT-MCTES project PTDC/EDM-EDM/30828/2017, (BeLive – Suportes celulares eto-sensiveis 3D para estudos de vascularização.



Design of Blood Vessel Models using Magnetic-Responsive Vascular Platforms.

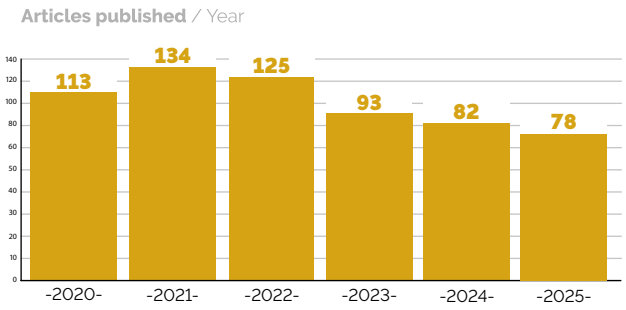
Advanced Materials Technologies (2023) 2300617

Heparinized Acellular Hydrogels for Magnetically Induced Wound Healing Applications

ACS Applied Materials & Interfaces 2024, 16, 9908−9924

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION



H-index: **50**

625 articles*
12643 citations

***01/2020-12/2025**
From WOS core collection

FUNDED PROJECTS

(Representative projects)

- **ERC Proof of Concept Grant – CryoDES 101067844– 2021.**
  Ana Rita C. Duarte (PI)
  Total Funding: € 150,000.00
- **ERC Proof of Concept Grant – ImproVita 101138403– 2023.**
  Ana Rita C. Duarte (PI)
  Total Funding: € 150,000.00
- **AQUAMONITRIX - Enhanced Portable Sensor for Water Quality Monitoring, moving to genuinely integrated Water Resource Management.**
  LIFE17 ENV/IE/000237, João G. Crespo (Local PI). 2018-2021
  Total Funding: € 237,581.00
- **KET4F-Gas - Reduction of the Environmental Impact of Fluorinated Gases in the Sudoe space using Key Enabling Technologies.**
  Interreg Sudoe Programme, SOE2/P1/P0823, 2018-2021, Ana B. Pereiro and João M. M. Araújo (Coordinators).
  Total Funding: € 1,742,800.00, Funding for lab: € 436,175
- **MAR2PROTECT: Preventing Groundwater Contamination related to Global and Climate Change through a Holistic Approach based on Managed Aquifer Recharge.**
  Horizon Europe, HORIZON-CL6-2022-ZEROPOLLUTION-01, GA No 101082048, 2022-2026, Ana B. Pereiro and João M. M. Araújo (Coordinators).
  Total Funding: € 4 143 681.25, Funding for lab: € 710,007.2
- **LIFE-4-Fgases: Towards a circular economy for refrigerants: novel hybrid approach to selectively recycling F-gases.**
  LIFE Programme, LIFE20 CCM/ES/001748, 2021-2025, Ana B. Pereiro and João M. M. Araújo (Portuguese Coordinators).
  Total Funding: € 1,359,702, Funding for lab: € 259,796
- **EXBRINER - Next-generation membrane technologies for sustainable exploitation of seawater brine resources: transition towards a circular blue industry.**
  Call HORIZON – MSCA – 2021 – DN, (Marie Sklodowska-Curie grant agreement No 101072449), João Crespo, Cláudia Galinha, Sylwin Pawlowski. 2022-2026.
  Total Funding € 2.617.264; Funding for institution € 243.403
- **TwiNSol-CECs – Twinning for enhancing the scientific excellence of faculty of technology Novi Sad for innovative solutions to protect environmental resources from contaminants of emerging concern.**
  European Union, GA 101059867, João Crespo. 2022-2025.
  Total Funding € 1.432.937
- **MULTI-STR3AM - A sustainable multi-strain, multi-method, multi-product microalgae biorefinery integrating industrial side streams to create high value products for food, feed and fragrance.**
  U Horizon 2020, Contract No. 887227, João Crespo. 2020-2025.
  Total Funding € 6.588.732;
  Funding for Lab € 774.250
- **ALERT-PFAS - Transnational Strategy to Detect and Prevent PFAS Pollution.**
  FInterreg Sudoe Programme, S1/2.4/P0099-ALERT-PFAS, 2024-2026, João M. M. Araújo and Ana B. Pereiro (Coordinators).
  Total Funding: € 1,845,945, Funding for lab: € 355,872.

FUNDED PROJECTS

(Representative projects)

- **LIFE REAMINE: Sustainable Solutions for NMVOC Emission Reduction in Foundries through Advanced Amine Recovery**
  LIFE Programme, LIFE24-ENV-ES-LIFE REAMINE/101216139, 2025-2029, João M. M. Araújo and Ana B. Pereiro (Portuguese Coordinators).
  Total Funding: € 2,593,879, Funding for lab: € 463,723.

- **MULTIPLY – Multiplying feasible microalgae-derived products at scale.**
  Call HORIZON-JU-CBE-2024 — Circular Bio-based Europe Joint Undertaking, Contract No 101214894, 2025-2029, Cláudia Galinha,
  LAQV Budget: € 285.517

- **SEArcularMINE - Circular Processing of Seawater Brines from Saltworks for Recovery of Valuable Raw Materials.**
  European Union Horizon 2020, No. 869467, Sylwin Pawlowski (Local PI).
  Total Funding € 636.750

- **RESURGENCE - Industrial water circularity: reuse, resource recovery and energy efficiency for greener digitised EU processes.**
  HORIZON EUROPE, Contract No. 101138097, 2023 – 2027, João Crespo, Cláudia Galinha

- **CHIMSEP - Chemists and Chemical Engineers for the Chemical Factory of the Future.**
  DN-MSCA-Horizon Europe-Grant N°101119277, João Crespo (WP leader), Carla Portugal (Team Member).
  Total Funding: € 3 379 543.20, Budget FCT.NOVA: € 500 000.

- **MEMFAST – Membranes as Enablers for Future Biorefineries: from Fabrication to Advanced Separation Technologies.**
  DN-MSCA-Horizon n.º: 10112026, João Crespo (WP leader), Carla Portugal (Team Member). Total Funding: € 2 697 926.40,
  Budget FCT.NOVA: € 250 000

- **ValorCannBio- Valorização de subprodutos da planta de canábis medicinal como biopesticida para o olival,.**
  Ana Rita C. Duarte (Local PI)
  Total Funding: € 150,000.00

- **Solvent Engineering in Microfluidics/ CounterCurrent Chromatography Hybrids for the Purification of Viral Vectors: Bioprivileged Ionic-Liquid-based Aqueous Biphasic Systems.**
  PTDC/EQU-EQU/2223/2021, João M. M. Araújo (PI).
  Total Funding: € 249.839,00

- **CO2VAluE: Ionic Liquids and Porous Structures for CO2 Valorization.**
  CFCT, MIT-EXPL/CS/0052/2021, Ana Nunes (PI).
  Total funding € 49.876,10.

- **CO2-RED: Understanding CO2 electroreduction in porous materials.**
  FCT, PTDC/EQU-EPQ/2195/2021, Ana Machado (PI).
  Total funding € 249.653,15.

- **BIOELA: A green chemistry approach to the catalytic synthesis of fuel bioadditives.**
  FCT, EXPL/EQU-EPQ/1039/2021, Malgorzata Zakrzewska (PI).
  Total funding € 49.950,32

- **Phyco-µ-Biome: Understanding and harnessing the power of the microalgae microbiome aiming the maximization of marine microalgae production**
  FCT, PTDC/BAA-BIO/1262/2020, Cláudia Galinha (Co-PI). 2021-2024.
  Total Funding € 249.792; Funding for institution € 92.662

- **Se(L)ect(i)vity - Design of tailored composite membranes for lithium recovery from brines and seawater.**
  FCT, PTDC/EQU-EQU/6193/2020, Sylwin Pawlowski (PI).
  Total Funding € 208.999,40

- **NGS - New Generation Storage.**
  PRR, João Crespo (PI).
  Total Funding € 100.000

- **AntiviralNADES - Design of tailored green nanoemulsions for delivery of hydrophobic antiviral bio-compounds prepared by membrane technologies within a biobased economy.**
  FCT, 2022.08919.PTDC. Carla Brazinha (PI).
  Total Funding € 49 998,80

- **ZeroFishWaste: Valorisation of fish processing residues by green and sustainable technologies.**
  FCT, IP (2023.14690.PEX); LAQV budget: € 49,327.32

- **Print3D4Capture - 3D-printed Nitrogen-rich Nanoporous Carbons for CO2 capture by Electric Swing Adsorption.**
  FCT, IP – UT Austin Portugal Program (2022.15637.UTA), Rui Ribeiro (PI)
  LAQV Budget: €49 824

- **SWMOF - A smart process for water harvesting from air and water distribution based on eco-friendly MOFs.**
  FCT, IP – Water4All Partnership (Water4All/0004/2022), Rui Ribeiro (PI)
  LAQV Budget: € 39 858

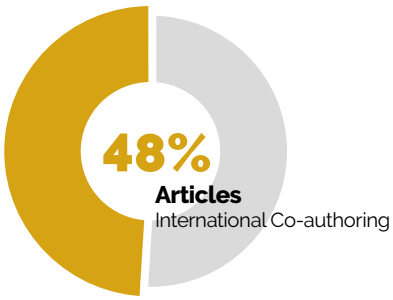
FUNDED PROJECTS

(Representative projects)

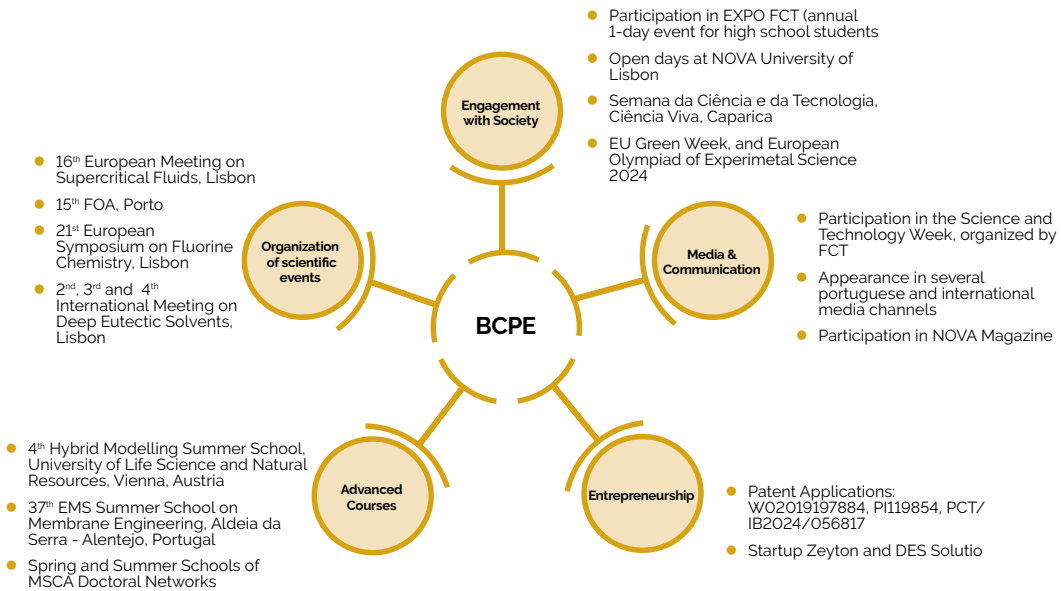
- **Desalination, resource recovery and power generation with ionically conductive membranes.**
  Funded by MIT Portugal. (Total project funding: 400 000.00 $ - managed by MIT), João Crespo (Local PI)
- **SkinBioPOl - Tailor-made bio-based polymeric structures for skin drug delivery.**
  RESTART Program from FCT, Luísa Neves (PI), Reference: 2024.05177.RESTART.
  Total Funding: 48 111,00€
- **Agri-Plast – Organização da Produção e Inovação para a Redução de Plásticos Agrícolas.**
  PRR-C05-i03-I-000167-LA10.2, Paulo Lemos (team member)
  Funding for NOVA FCT € 241.523,70
- **RObUST – Circular Economy Applied to Spent Tyre Rubber: Conversion into energy, chemicals and materials.**
  Industrial project funded by Valorpneu, S. A., Coordinated by Nuno Lapa (LAQV-REQUIMTE).
  Total funding: 22.5 k€; Funding for Lab: 16.25 k€
- **Study of the Contribution of Low-Carbon Liquid and Gaseous Fuels from Renewable Sources to the Transport Sector towards the 2030 National Targets.**
  Industrial project funded by the Low-Carbon Fuels Platform (Plataforma para os Combustíveis de Baixo Carbono – PCBC) and the Association of Portuguese Fuel and Lubricant Companies (Empresas Portuguesas de Combustíveis e Lubrificantes - EPCOL), Coordinated by Nuno Lapa (LAQV-REQUIMTE).
  Total funding: 25 k€; Funding for Lab: 8.5 k€
- **Life Cycle Assessment of AmpliAqua plant.**
  Industrial project funded by BGI, S. A., Coordinated by Nuno Lapa (LAQV-REQUIMTE).
  Total funding/Funding for Lab: 7.5 k€
- **Boehringer Ingelheim industrial project.**
  Ana Rita C. Duarte (PI)
  Total Funding: € 80,000.00

INTERNATIONAL COOPERATION AND NETWORKING

- EUDIME: Erasmus Mundus Doctorate in Membrane Engineering
- CATSUS - Catalysis and Sustainability Ph.D. program
- EM3E-4SW: Erasmus Mundus Master in Membrane Engineering for a Sustainable World;
- MESD – Erasmus Mundus Master in Membrane Engineering for a sustainable development
- EIT RawMaterials activities (as members of Core partner of Co-location Centre CLC West);
- INTERREG Project (EMPORIA 4KT)
- Cooperation with IFREMER- Centre Bretagne, Brest, France in a PhD program.
- MEMCLEARWINE- Development of cellulose-based ion-exchange membranes for wine proteins removal, IEA-International Emerging Actions, CNRS-FCT, France-Portugal
- COST Actions: CA18224; EU4MOFs; CA22134; CA21146; CA21159
- Member of several international clusters, hubs and societies



DISSEMINATION & OUTREACH



LABORATÓRIO ASSOCIADO
PARA A QUÍMICA VERDE

Charm

CULTURAL HERITAGE AND RESPONSIVE MATERIALS

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

Group Coordinator:

A. Jorge Parola

The Cultural Heritage And Responsive Materials (CHARM) group focus the design of responsive molecules and materials where external stimuli enable control over the direction and outcome of chemical and photochemical reactions and on the science of sustainable conservation of Cultural Heritage. Photochemistry and physical chemistry tools and models and the principles of supramolecular chemistry are applied to:

- The study of photo, electro, and thermal-induced reactions in a range of responsive materials commercially important for chromogenic displays, DSSCs, luminescent glasses, alternative solvents, and luminescent probes;
- The preservation of materials incorporated in Cultural Heritage objects (i.e. from Illuminated Manuscripts to Contemporary Art and Photography) that requires research to determine their original chemical and physical state, and to identify agents and mechanisms of change and degradation.

State-of-the-art analytical instrumentation and expertise from a wide range of disciplines is available for the identification of complex aged materials and to address questions of context and meaning in their use, as well as the impact of previous and contemporary interventions. Innovations for preservation treatments include research and application of Liquid and Supercritical CO_2 and Ionic Liquids.

The interdisciplinary environment conveys an integrated approach in which state-of-the- art materials and techniques are applied in conservation, and the knowledge over how ancient materials have endured inspires the design or development of materials with enhanced properties and up and down conversion emitting glasses to increase energy efficiency.

RESEARCH OBJECTIVES [2025-2029]

Over the next five years, the CHARM group is committed to developing sustainable solutions in energy conversion and storage. Research will focus on optimizing solar energy conversion using natural and synthetic dyes; designing ionic liquids, eutectic systems, porous ionic polymers, and metal nanoparticles for redox flow batteries, supercapacitors, and CO_2-to-fuel conversion; and creating up- and down-conversion emitting glasses to enhance efficiency, particularly in hydrogen carrier systems (e.g., NH_3).

CHARM's strong background in responsive systems provides the foundation for advancing photoresponsive switches with applications in photopharmacology, bioimaging, and adaptive systems and materials. Central to this work is CHARM's expertise in electro-, thermo-, and photochromic materials, harnessed to design and optimize systems operating in the near-infrared (NIR) region.

We aim to strengthen our role within LAQV@REQUIMTE, connecting Chemistry and Art through interdisciplinary research. Our focus includes Medieval Iberian Heritage and the preservation of 18th, 19th-century, and contemporary materials, exemplified by the ERC SCARLET project led by Paula Nabais (reviving textile dyeing techniques), the InBloom project directed by Susana Sá (conserving polyurethane fabrics), and initiatives to preserve historic photographic collections. CHARM also collaborates with the Winsor & Newton 19th-century archive, offering online access to over 17,000 records on artists' materials, supporting both national (DCR Master's, CORES PhD) and international students

RESEARCH TEAM

SENIOR RESEARCHERS

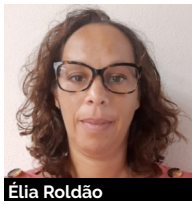
Ana Ferreira

A. Jorge Parola

Artur Moro

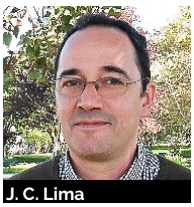
César Laia

Cristina Cordas

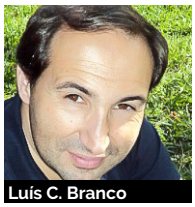

Élia Roldão

Fernando Pina

Isabel Cardoso

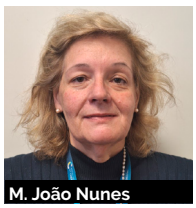

J. C. Lima

João Avó


Luís C. Branco

M. João Melo

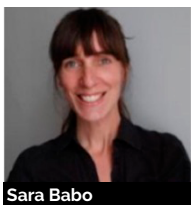
Maria Casanova


M. João Nunes

Nuno Basílio

Paula Nabais

Sandra Gago


Sara Babo

Susana F. de Sá

Vanessa Otero

RESEARCH TEAM

OTHER DOCTORATE RESEARCHERS

Catarina Esteves
Karolina Zalewska
Raquel Marques
Sara Sá
Sunny Freitas

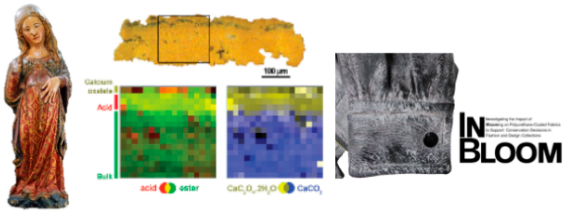
PhD STUDENTS

Afonso Bernardes
Ana Tourais
Carolina Viana
Dário Silva
Diogo Madeira
Dominik Jammal
Ekaterina Pasnak
Gabriel Valério
Hanieh Mahmoodi
Joana Nunes
Paulo Martins
Joana Devesa
Joana Ferreira
Laura-Cassandra Valean
Lénia Fernandes
Liliana Gomes
Luís Pereira
Luis Filipe
Malihe Sotoudeh
Mara Santo
Mariana Costa
Mila Crippa
Miriam Colaço
Sunil Beherra
Victoria Paz

RESEARCH THEMES/ CULTURAL HERITAGE

CAUSES AND MECHANISMS OF ALTERATION

- Medieval illuminated manuscripts.[1-8]
- Material culture studies in polychrome sculpture and the codex.[9-13]
- Amadeo de Souza-Cardoso and 19th century artists' paints.[2]
- 19th century, Modern & Contemporary Cultural Heritage.[14-19]
- Photographic and Audiovisual Materials: Films, Papers and Mixed-Media Artworks.[20,21]
- Polyurethane-based materials in fashion and design collections.[22-24]



HISTORICAL RECONSTRUCTIONS DATABASE

- The book on how to make colours.[4]
- The Winsor & Newton artist materials supplier, 19th century archive.[14,15]
- Natural Dyes and Inks.[25,26]

SUSTAINABLE INNOVATIVE METHODS

- Applications of ionic liquids and nanomaterials in conservation.[16]
- Responsive materials for cultural heritage.[20-24]
- Historical dyes: applications & advanced methods of analysis.[1,3,7,17,26]

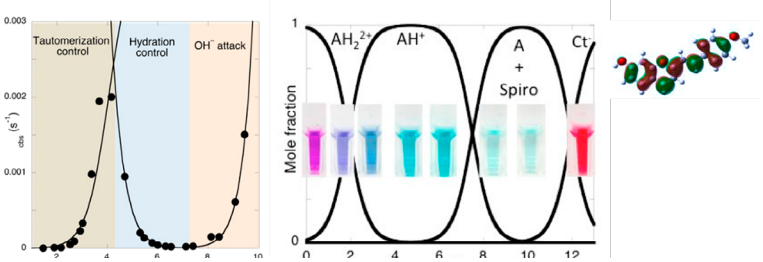
SELECTED PUBLICATIONS

1 M J. Melo et al., 2026. doi: 10.1016/j.talanta.2025.129245
2 M. J. Melo et al., 2024, . doi: 10.3390/heritage7100259
3 M. Vieira et al., 2023. doi: 10.1186/s40494-023-00863-1
4 M. Vieira et al., 2024. doi: 10.3390/su16125027
5 M. J. Melo et al., 2024. doi: 10.1002/cphc.202400859
6 R. Hidalgo et al. 2023. doi: 10.1186/s40494-022-00823-1
7 M. J. Melo et al., 2025. doi: 10.3390/heritage8070261
8 H. Grigoryan et al., 2023. doi: 10.3390/heritage6030170
9 C. Barreira et al. 2022. doi: 10.5565/rev/medievalia.572
10 C. Casanova et al., 2022. doi: 10.23925/2178-2911
11 T. Palomar et al., 2023. doi: 10.1186/s40494-023-01048-6
12 I. Pombo Cardoso, 2024, in C.Barreira et al. (Eds.), Cistercian Horizons Collected Essays.
13 I. Pombo Cardoso et al. (Eds.), 2025. doi: 10.14568/cp49
14 V. Otero et al.,2025. doi: 10.1038/s40494-025-02128-5
15 V. Otero et al., 2025. doi: 10.1016/j.culher.2025.06.008
16 V. Otero et al., 2025. doi: 10.1016/j.culher.2025.06.008
17 S. França de Sá et al. 2025. doi: 10.3390/gels11120954
18 R. Marques et al. 2023. doi: 10.1140/epjp/s13360023-04330-5
19 C. R. Pires et al. 2023. doi:10.1080/01971360.2023.2172130
20 A. Neves et al. PNAS Nexus, 2023, 2, 1–11. doi: 10.1093/pnasnexus/pgad360
21 L.-C. Vâlean et al.,2025. doi: 10.3390/heritage8090361
22 S. França de Sá et al., 2025. doi: 10.1080/00393630.2025.2472457
23 S. França de Sá et al., 2025. doi: 10.3390/heritage8120511
24 S. França de Sá et al., 2024. doi: 10.14568/cp47fm2
25 P. Nabais et al., 2025. doi: 10.3390/heritage8090375
26 P. Nabais et al., 2023. doi: 10.1186/s40494-023-01020-4

RESEARCH THEMES/ RESPONSIVE MATERIALS

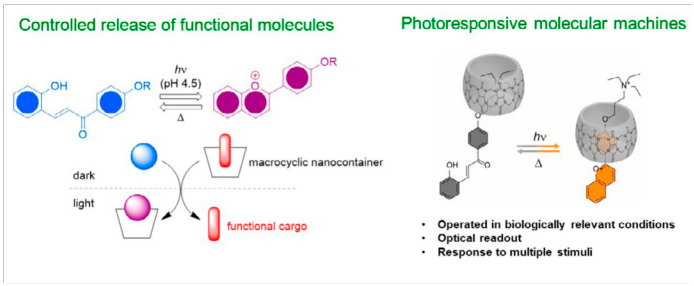
ANTHOCYANINS AND FLAVYLIUM SALTS

- Uncovering color mechanisms in anthocyanins.[27-30]
- New dyes for DSSCs.[31]
- Isomeric styrylflavylium systems.
- New flavylium-based dyes.[32, 33]



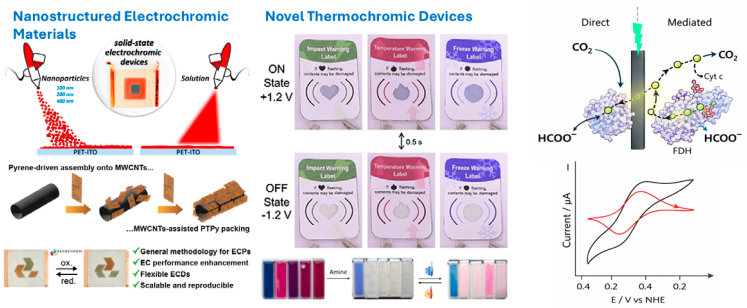
PHOTOCHROMIC AND PHOTOSWITCHING SYSTEMS

- Stimuli-responsive soft materials for delivery applications.[34,35]
- Molecular machines based on flavylium photoswitches.[36-39]
- Host-guest functional systems.[40-43]



ELECTROCHROMIC AND THERMOCHROMIC SYSTEMS

- Development of electrochromic polymer nanoparticles.[44,45]
- Novel thermochromic devices for responsive smart labels.[46]
- Electrochemistry for sustainability and energy transition.[47]



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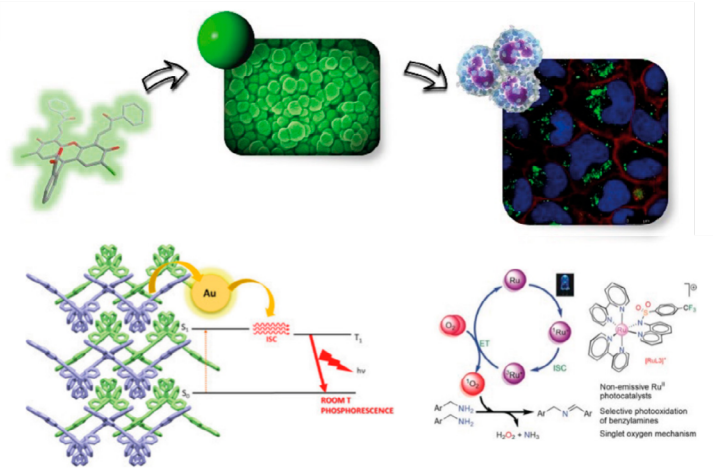
27 A. Camuenho et al. 2022. doi: 10.1021/acsomega.2c02571
28 A. Seco et al., 2022. doi: 10.1021/acs.jafc.2c03879
29 F. Pina et al., 2023. doi: 10.1016/j.dyepig.2022.110925
30 J. Oliveira et al. 2025. doi: 10.1039/d5cc03251b
31 A. L. Pinto et al., 2023. doi: 10.1016/j.dyepig.2023.111495
32 P. Araújo et al., 2022. doi: 10.1039/D2CP01966C
33 A. Camuenho et al., 2023. doi: 10.1016/j.jphotochem.2023.114658
34 D. Moreira et al., 2023. doi: 10.1016/j.jcis.2023.07.129
35 D. Moreira et al., 2025. doi: 10.1039/D5TB01908G
36 J. Chen-Wu et al., 2023. doi: 10.1039/D3CC00384A
37 P. Máximo et al., 2022. doi: 10.1039/D2QO00423B
38 A. Seco et al., 2021. doi: 10.1002/chem.202102343
39 M. Colaço, M. et al., 2025. doi: 10.1021/jacs.4c13353
40 J. N. Martins et al., 2023. doi: 10.1021/jacs.3c01829
41 M. Paulino et al., 2022. doi: 10.1021/acs.joc.2c01875
42 B. González et al., 2024. doi: 10.1002/anie.202317553
43 A. Trevisan et al., 2024. doi: 10.1002/ijch.202300143
44 R. Ferreira et al., 2024. doi: 10.1021/acsaenm.4c00534
45 E. L. Howard et al., 2024. doi: 10.1007/s10800-023-01991-z
46 M. Spirache et al., 2023. doi: 10.1016/j.dyepig.2023.111208
47 N. Paul et al., 2025. doi: 10.1002/celc.202500100

RESEARCH THEMES/ RESPONSIVE MATERIALS

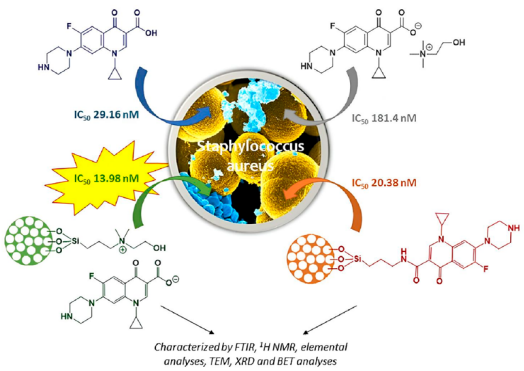
LUMINESCENT MATERIALS AND SENSORS

- Zeolite photoluminescence for LEDs and light management applications.[48,49]
- Organometallic complexes for Photodynamic Therapy.[50-53]
- Fluorescence sensors for biological and catalytic applications.[54-63]



FUNCTIONAL MATERIALS BASED ON IONIC LIQUIDS

- Innovative active pharmaceutical drugs based ionic liquids.[64-66]
- Functional Materials for energy[67] and ionic liquids for electrochromism and solar cells.[68-70]
- Alternative lubricants based on ionic liquids for silicon surfaces.[71, 72]
- Task-specific Ionic liquids for sustainable synthesis[62] & catalysis.[73, 74]



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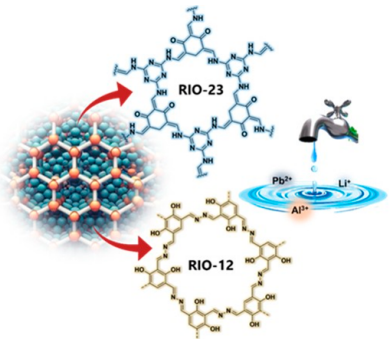
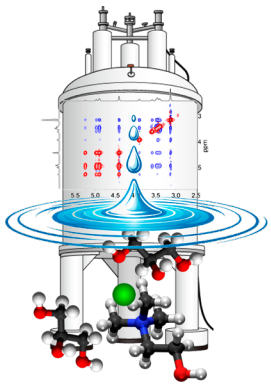
48 C. Viola et al., 2023. doi: 10.1016/j.mtchem.2023.101514
49 C. Viola et al., 2025. doi: 10.1039/d5tc02810h
50 C. Yagüe et al. 2020. doi: 10.1002/chem.202001460
51 J. Sanz-Villafruela et al.2024. doi: 10.1039/d4dt00390j
52 J. Sanz-Villafruela et al., 2025. doi: 10.1039/d5qi00924c
53 C. Bermejo-Casadesús et al., 2025. doi: 10.1039/d5qi00775e
54 A. J. Moro et al, 2020. doi: 10.3390/bios10090129
55 L. J. Gomes et al. 2022. doi: 10.1016/j.dyepig.2021.109845
56 G. D. Teixeira et al., 2024. doi: 10.1016/j.snb.2024.135726
57 R. Bisauriya et al., 2024. doi: 10.1016/j.colsurfa.2024.135061
58 M. A. Bento et al., 2024. doi: 10.1021/acs.inorgchem.4c03091
59 A. M. Diniz et al. 2024. doi: 10.1002/adom.202402063
60 M. Tosolini et al., 2023. doi: 10.1002/chem.202301597
61 A. Cerqueira et al., 2024. doi: 10.1016/j.jphotochem.2024.115490
62 A. de Aquino et al., 2025. doi: 10.1021/acs.inorgchem.4c04964
63 L. J. Gomes et al., 2026. doi: 10.1002/ceur.202500431
64 D. Silva et al., 2025. doi: 10.1039/D4MD00960F
65 L. Filipe et al., 2023. doi: 10.3390/pharmaceutics15071934
66 F. Faisca et al., 2025. doi: 10.1021/acs.molpharmaceut.5c00310
67 A. C. Amorim et al. Mat. Advances 2025. doi: 10.1039/D5MA00761E
68 F. Leitão et al. 2025. doi: 10.1002/elsa.70006
69 H. Cruz et al. 2025. doi: 10.1021/acsomega.5c04216
70 A. F. M. Santos et al., 2023. doi: 10.1016/j.molliq.2023.121456
71 M. Donato et al., 2023. doi: 10.3390/molecules28062678
73 J. Afonso et al., 2024. doi: 10.1021/acssusresmgt.3c00057
74 S. Messias et al., 2022. doi: 10.1039/D2YA00001f

RESEARCH THEMES/ RESPONSIVE MATERIALS

DEEP EUTECTIC SOLVENTS AS GREEN SOLVENTS

- Water purification using hydrophobic DES.[70]
- Eutectic Systems based on alkali metals as green electrolytes for electrochromism and solar cells.
- Extractive desulfurization of fuels using eutectic systems and solvent-free processes.
- NMR-based investigation of structure–property–function relationships. [75,76]





SELECTED PUBLICATIONS

75 A. Ferreira et al., 2021. doi: 10.1016/j.molliq.2021.117463
76 H. Monteiro et al., 2026. doi: 10.1016/j.molliq.2025.129169

HIGHLIGHTS

PHOTOSWITCHABLE CALIXARENE ACTIVATORS FOR CONTROLLED PEPTIDE TRANSPORT ACROSS LIPID MEMBRANES

Supramolecular synthetic transporters are crucial to understand and activate the passage of hydrophilic effector molecules across lipid membranes, being useful as active pharmaceutical ingredients or drug-delivery systems. In this work we introduced the first photoswitchable amphiphilic counterion activators for the transport of cationic peptides across lipid membranes and inside living cells. Our design combines a high-affinity oligoarginine binding unit, based on a sulfonatocalixarene macrocyclic host decorated with azobenzene pendants, whose lipophilicity can be remotely controlled by light-induced interconversion between the more hydrophobic, extended E and the more polar, bent Z configuration. The transport efficiency of these light-sensitive counterion activators was significantly enhanced for the E azobenzene isomers, which allows their application as photomodulated carriers for hydrophilic cargos. Based on the robust performance and response to light stimulation of these molecular photoswitches, we envisage possibilities in conceptually new stimulus-responsive transport systems for biological, pharmaceutical, and analytical applications.

Photoswitchable Calixarene Activators for Controlled Peptide Transport across Lipid Membranes

J. Am. Chem. Soc. 2023, 145 (24), 13126–13133

COVALENT ORGANIC FRAMEWORKS AS PROMISING MATERIALS FOR THE REMOVAL OF METAL AND ORGANIC POLLUTANTS FROM WATER

Polythiophenes (PTs) are among the most common electrochromic systems used to assemble electrochromic devices (ECDs) in industry. Apart from PEDOT, that was engineered to become water soluble by using PSS as counterion, most PTs (necessary to confer electrochromism new colours) require organic solvents to be industrially processed.
In this work, an electrochromic PT (P3HT) was used to prepare aqueous suspensions of nanoparticles (NP) of different sizes that were assembled into ECDs. These devices show enhanced performance (shorter switching times, higher cyclability, similar coloration efficiency) when compared to those assembled from chloroform solutions of the pristine polymer, providing an environmentally sustainable strategy towards ECDs with improved properties.

Covalent organic frameworks as promising materials for the removal of metal and organic pollutants from water

Materials Today Sustainability 2023, 21, 100279

HIGHLIGHTS

PROJECT PRR INSECTERA

"Agenda Mobilizadora InsectERA" (PRR Program-Contract of Financing of the Recovery and Resilience Plan); Timeframe: 2023-2025; Budget: 55M€; 1M€ for FCT-NOVA. (Coordinator of the project: Daniel Murta, Entogreen; 44 partners)
https://www.insectera.pt/

The InsectERA Agenda brings alternative food/nutritional solutions that will respond to the sector's new needs, such as the increase in the world's population, climate change and food waste. It thus contributes to the green transaction towards environmental sustainability, based on a circular economy.
It was in this context that the InsectERA Mobilising Agenda was created, bringing together players from across the value chain who want to explore the potential of insects as a bioindustrial tool and bioindustrial solutions and covers the entire innovation cycle, from Research & Development to the manufacture and commercialization of products on the market, based on technologically advanced production methods. During the Agenda's implementation period, from 2023 to 2025, multiple projects and initiatives will be developed to foster the circular economy and leverage the development of new products, processes and services with high added value.

A 1000-year-old mystery solved

THE MOLECULE BEHIND THE MEDIEVAL BLUE FROM *CHROZOPHORA TINCTORIA*, ALSO KNOWN AS *FOLIUM*

To understand why color is fading in precious artworks, the reproduction of ancient colors is a vital ingredient. This know-how was lost at the turn of the 20th c. with the rise of industrially-produced synthetic dyes.
The retrieving of this "lost knowledge" has been an important line of research within our group and enabled us solving the mystery of the medieval blue named folium whose molecular structure remained elusive until now. As it turned out to be in a class of its own, this outcome was recently published in a high impact journal, by the Science group. The discovery was widely covered by the media and celebrated by the scientific community
10.1126/sciadv.aaz7772.

A 1000-year-old mystery solved: Unlocking the molecular structure for the medieval blue from *Chrozophora tinctoria*, also known as *folium*

Science Advances, 2020, 6, eaaz7772

HIGHLIGHTS

A SUSTAINABLE APPROACH TOWARD LONG-LASTING SOLID-STATE ELECTROCHROMIC DEVICES

Polythiophenes (PTs) are among the most common electrochromic systems used to assemble electrochromic devices (ECDs) in industry. Apart from PEDOT, that was engineered to become water soluble by using PSS as counterion, most PTs (necessary to confer electrochromism new colours) require organic solvents to be industrially processed.

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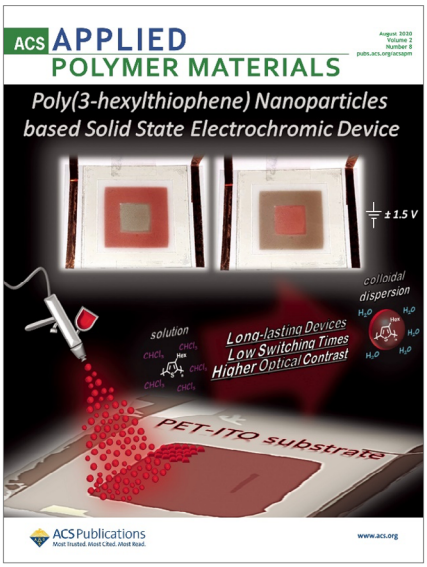


Semicrystalline polythiophene-based nanoparticles deposited from water on flexible PET/ITO substrates as a sustainable approach towards long-lasting solid- state electrochromic devices

ACS Appl. Polym. Mater., 2020, 2, 3301-3309

ERC STARTING GRANT "SCARLET:", FUNDED BY THE EUROPEAN COMMISSION – EUROPEAN RESEARCH COUNCIL, REFERENCE 101219122, TIMEFRAME: 2026-2030. BUDGET: 1,5M€, PROJECT COORDINATOR: PAULA NABAIS

The SCARLET project aims to revolutionise the textile sector by optimising historical recipes for eco-friendly applications in response to the growing demand for sustainable practices and the European Union's SDGs. SCARLET's research will explore centuries-old dyeing techniques meticulously documented by master dyers to create a bridge between traditional craftsmanship and contemporary sustainability standards. This investigation will validate the environmental benefits of these practices and provide actionable solutions for SMEs, designers, artists, and the wider textile community seeking alternatives.

By weaving historical insights with cutting-edge research, SCARLET addresses the sustainable transformation of textile production and fosters a deeper appreciation for cultural heritage.

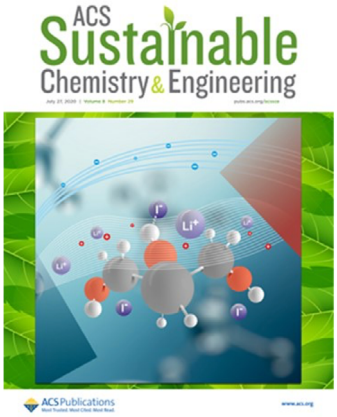
erc
European Research Council

SCARLET
Study and interpretation of historical natural dye formulations for the modern textile design

HIGHLIGHTS

DEEP EUTECTIC SOLVENTS FOR ELECTROCHEMICAL APPLICATIONS

Deep eutectic solvents (DES) composed of lithium, sodium, or potassium iodide salts in suitable combination with ethylene glycol (EG), glycerol (Gly), or polyethylene glycol (PEG) have been developed. All prepared DES were characterized by thermal analysis (DSC and TGA) and its complex conductivity (*) and impedance (Z*) frequency were evaluated through dielectric relaxation spectroscopy (DRS). Two- and three-electrode electrochemical studies of all DES have been performed. All DES avoid crystallization, exhibiting conductivity values in a range from 10−4 to 10−2 S cm−1 at room temperature and electrochemical windows higher than 1 V (on the order of 3−4 V), fulfilling the usual suitability criteria for utilization in electrochromic devices (ECD). The most promissory DES as electrolytes were tested for ECD. Being suitable candidates for further application in batteries.

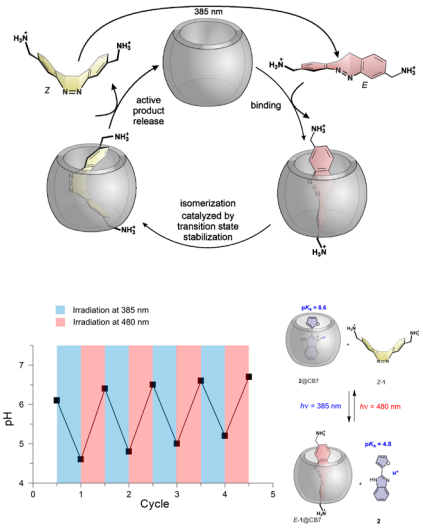


Alkaline Iodide-Based Deep Eutectic Solvents for Electrochemical Applications

ACS Sustainable Chem. Eng. 2020, 8, 29, 10653−10663

LIGHT-DRIVEN BINDING AND DISSOCIATION OF HOST-GUEST BINDING PAIRS IN WATER

The discovery of light-responsive non-covalent binding pairs that can assemble in water with high affinity and selectivity is critical for the development of remotely controlled molecules and materials. Such systems enable precise spatiotemporal control over molecular recognition and assembly, with potential applications in areas such as targeted drug delivery, molecular machines, and dynamic supramolecular systems.



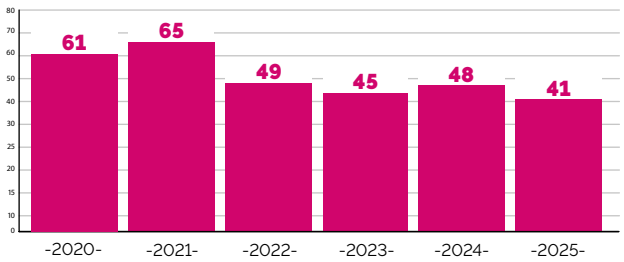
This work reported a new and exceptionally efficient water-soluble binding pair based on a diazocine photoswitch and the synthetic barrel-shaped macrocyclic receptors cucurbit[n]urils (n = 7 and 8). We show that the smaller receptor, CB7, strongly binds the E-diazocine isomer generated under UV irradiation and releases the Z isomer in the dark, exhibiting a binding selectivity of more than four orders of magnitude. In contrast, the larger receptor CB8 binds both isomers with high affinity while maintaining good selectivity (1000-fold) for the Z isomer.

The extraordinary properties of this system were further used to introduce the concept of supramolecular photoacids, which exploit the increased basicity of a photochemically silent guest upon binding to CB7 together with the extremely high affinity of the E isomer. Upon irradiation, the E isomer displaces the acid from CB7, thereby triggering a change in the pH of the solution.

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION

Articles published / Year



H-index: **27**

309 articles*
4125 citations

***01/2020-12/2025**
From WOS core collection

FUNDED PROJECTS

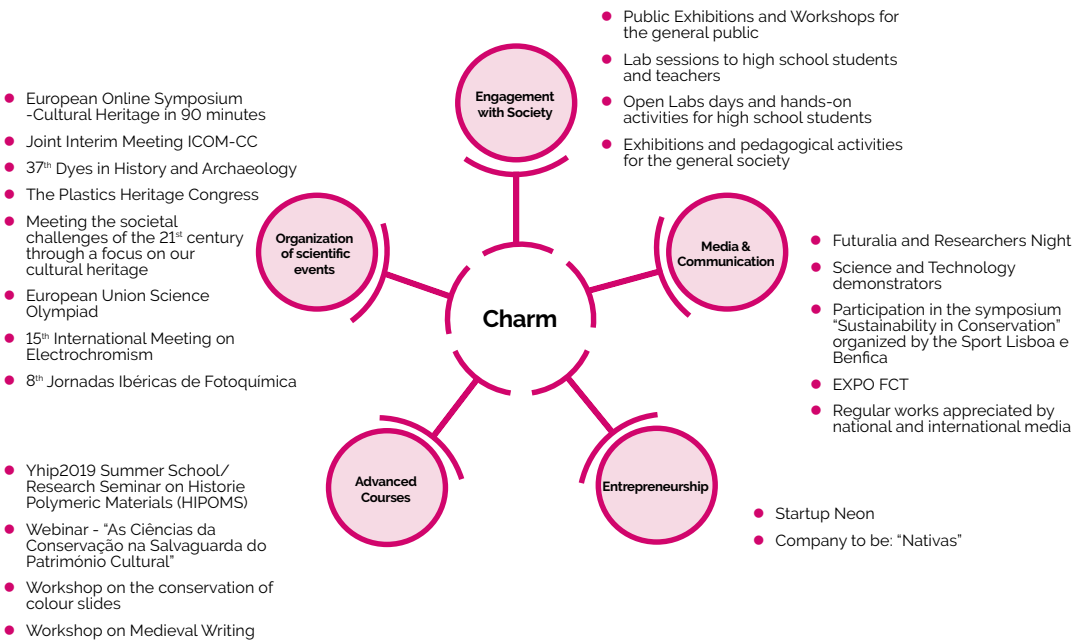
(Representative projects)

- Agenda Mobilizadora "InsectERA"
  PRR Program, Timeframe: 2023-2025; Budget: 55M€; 1M€ for FCT-NOVA. (Coordinator of the project: Daniel Murta, Entogreen; 60 partners)
- Archaeology of Colour: a comparative material culture study on Portuguese medieval polychrome sculpture. (PTDC/ART-OUT/5992/2020)
  (PI) Isabel Pombo Cardoso Total funding: € 236,501. 38
- LUMCEL – Cellulose Materials with Circularly Polarized Luminescence (FCT Exploratory Project 2023.12086.PEX)
  Total Budget: 49,812 €; LAQV Budget: 49,812 €; LAQV Coordinator: João Avó
- MicroDOS – Dual-Dye Optical Smart Sensor for Microplastic Monitoring (FCT/MIT Exploratory Project 2024.13013.MIT)
  Timeframe: 2025-2026; Total Budget: 49,968 €; LAQV Budget: 49,968 €; LAQV PI: João Avó
- MoPRA. "The Plastics Metamorphoses – the reality and the multiple approaches to a material" (2022.05086.PTDC)
  Timeframe: 2023-2025; Total Budget: 250 k€; LAQV Coordinator: Maria João Melo
- MULTIDNA - Multivalent Synthetic Receptors for the Recognition, Transport and Controlled Delivery of Nucleic Acids (FCT-ICDT Project 2023.16144.ICDT)
  Timeframe: 2025-2028; Total Budget: 249 955.20 €; LAQV Coordinator:
  Nuno Basílio
- NATURIST project (2022.07089.PTDC)
  Timeframe: 2023-2026; Total Budget: 249,871.15€; LAQV Budget: 90,705€
- Photonia - Photocatalytic Conversion of Nitrogen to Ammonia for On-Site Fertilizer Production
  HORIZON EIC Grants, Grant agreement ID: 101223328 Timeframe: 2025-2029; Total Budget: 3,760,073.36 €; LAQV Budget: 443,643.24 €; LAQV Coordinator: César A.T. Laia
- REDiscovering madder colours. (2022.02909.PTDC)
  Timeframe: 2023-2024; Total Budget: 49,997.50 €; LAQV Budget: 49,997.50 €; LAQV PI: Vanessa Otero
- REVALGAE - Restoration of Damaged Ecosystems and Valorisation of Invasive Algae and Salt-Tolerant Plants
  Interreg Atlantic EAPA 0130/2024
  Timeframe: 2026-2028; Total Budget: 2,063,505.85 €; LAQV Coordinator: Luís C. Branco
- The threads of the past weaving the future: The colors from the Royal Textile Factory of Covilhã, 1764-1850" (2022.01243.PTDC)
  Timeframe: 2023-2026; Total Budget: 249,430.38 €; LAQV Budget: 249,430.38 €; LAQV PI: Paula Nabais
- VALOR2FUELS - Sustainable Catalytic valorization of CO2 and plastic waste into fuels using alternative solvents
  FCT Exploratory Project 2024.17945.PEX)
  Timeframe: 2026-2027; Total Budget: 59,994.69 €; LAQV Budget: 59,994.69 €; LAQV Coordinator: Luís C. Branco
- VIT, Polymer engineering via molecular design: embedding electrical and optical properties into VITrimers
  European project H2020-MSCA-RISE-2020 N. 101008237
  Portuguese Coordinator: António Jorge Dias Parola
  Coordinator: Roberta Pinalli, University of Parma, Italy
  Total funding: €1,352,400.00

INTERNATIONAL COOPERATION AND NETWORKING

- INFUSION - Engineering optoelectronic INterfaces: a global action intersecting FUndamental conceptS and technology implementatION of self-organized organic materials (H2020-MSCA-RISE-2014).
- International Scientific Coordination Network (GDRI) – Photographs: Perception and Changes.
- International Advisory Committee member on the Restoration of the Ghent Altarpiece.
- Paint (Paint Alterations in Time), Science4Arts, Netherlands Organization for Scientific Research (NWO).
- The Cleaning of Modern Oil Paintings (CMOP), Collaborative European Research Project (Heritage Plus Project).
- Glossy Surfaces - The Conservation of TPU-coatings in Fashion Collections; MoMu & Centexbel (BE), MET (US) e MUDE & DCR FCT NOVA (PT)

DISSEMINATION & OUTREACH



LABORATÓRIO ASSOCIADO
PARA A **QUÍMICA VERDE**

MatSusWell

MATERIALS FOR SUSTAINABILITY AND WELLNESS

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

Group Coordinator:

Ana Aguiar-Ricardo

The Materials for Sustainability and Wellness (MatSusWell) group is composed of researchers with combined complementary expertise in Green Chemistry, Materials Science, Nanotechnology, Chemical Engineering, Pharmacy, and Biomedical Sciences, with the objective of developing advanced multifunctional (nano)materials using sustainable methodologies. The overall purpose of MatSusWell, in line with the aforementioned background, is to promote a science-based approach complementary for core scientific areas, in particular: i) (Bio)Materials Engineering and Production; ii) Sustainable Environment: Catalysis for a Sustainable Environment, Renewable Energy and Climate Change Mitigation, and Green Metric Tools; iii) Drug Delivery and Tissue Regeneration; and iv) Wearable Technologies and Devices.

MatSusWell research work has a strong emphasis on innovation, encompassing research in fundamental physicochemical properties and composition *vs.* functionality *vs.* performance relationships, essential to the rational design of materials for target applications, and the development of environmentally friendly processes using supercritical CO_2 and deep eutectic systems. A considerable volume of intellectual property has been produced within the group, which is fostering the upscale of laboratory research to pilot scale in collaboration with industry through the creation of University spin-offs, with the goal of contributing to innovative products/technologies for society.

RESEARCH OBJECTIVES [2025-2029]

MatSusWell remains committed to address the Global Grand Challenges in order to achieve a better and more sustainable world through the rational design, production, and characterization of advanced materials by innovative green strategies, namely:

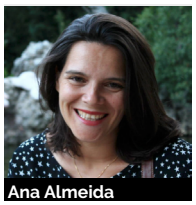
- Carbon-based materials from waste biomass for sustainable production of biofuels and bulk/fine (bio)chemicals based on the concept of biorefinery and circular economy.
- Innovative hybrid metal organic frameworks (MOFs), mesoporous silicas, carbon-based, and magnetic nanomaterials as recyclable catalysts and/or adsorbents in sustainable catalysis, wastewater treatment, fuels desulfurization and gas separation and capture.
- Efficient electrocatalysts for energy storage/conversion and CO_2 conversion.
- Novel optical sensors for the detection of heavy metal ions in water and toxic gases in the air.
- New biomimetic affinity materials for capture and sensing.
- Innovative therapeutic solutions for drug loading and delivery systems, biomimetic biomaterials for enhanced bone regeneration, craniofacial and dental disorders, and periodontal regeneration.
- New calcium phosphate cement with tailored individual components to ensure sustainable drug delivery.
- Nanoplatforms for biosensing and environmental applications with improved analytical performance and signaling of multiple analytes; (bio)sensors inclusion in portable and/or disposable devices.
- 3D Textile-based structures for tendon/ligament repair.
- High-performance light-responsive textiles for sensing and protection.
- New electromagnetic radiation shielding textiles.
- Self-powered smart textiles and flexible devices with energy production and storage properties for IoT applications.
- Development of (multi)functional nanomaterials for textile-based anticounterfeiting sensors.
- Development of sustainable translational new approach methodologies (NAMs) aligned with the "3Rs Principle" (Replacement, Reduction, Refinement) to minimize animal experimentation

Researchers from MatSusWell group will proceed in promoting funding procurement and knowledge transfer/technological valorization taking advantage of well-established collaborations with other Academic and Industrial partners at national and international levels. MatSusWell group will continue to enthusiastically participate in science dissemination in strict alignment with society demands and needs.

RESEARCH TEAM

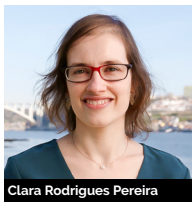
SENIOR RESEARCHERS

Ana Aguiar-Ricardo


Ana Almeida

Andreia Peixoto

Carlos Granadeiro


Clara Rodrigues Pereira

Cristina Freire

Diana Fernandes

Francisco Correia

Honorato Vidal

Inês Matos

Isabel Fonseca

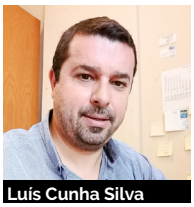
Jelena Vladic

João Sotomayor

José Domingos Santos

Liliana Grenho

Ligia Gomes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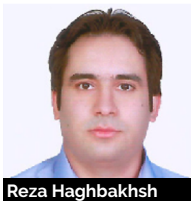
Maria Bernardo

Pedro Sousa Gomes

Raquel Viveiros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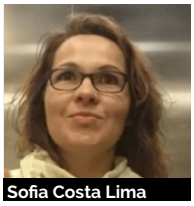
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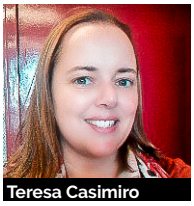
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RESEARCH THEMES/
(BIO)MATERIALS ENGINEERING AND PRODUCTION

MatSusWell uses the long-term expertise in Materials Science to design and produce new advanced (nano)materials to support the different target applications. A special emphasis is always given to cost-effective, scalable, and sustainable synthetic strategies to allow scaling-up.

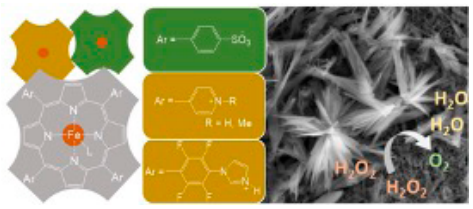
• **Magnetic nanomaterials** (transition metal ferrites), **2D/3D metal oxides and sulfides** with tailored morphology, textural, chemical and/or magnetic properties through coprecipitation in aqueous media using organic alkaline agents, hydrothermal/solvothermal processes and thermal decomposition.

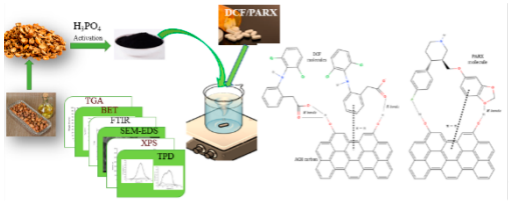
• **Carbon-supported, core-shell silica or gold-coated magnetic nanoparticles** for sensing applications. [1,2]

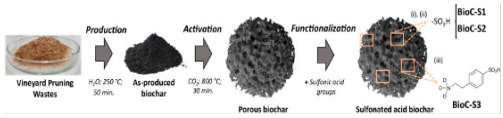
• **Light-responsive hybrid silica nanoparticles** with tailored photochromism and wider color palette based on silylated naphthopyran dyes (microwave-assisted synthesis) or polyoxometalates.

• L**ight-responsive hybrid tungsten oxide nanomaterials** with tailored morphology, particle size, and photoswitchable properties through hydrothermal and solvothermal processes. [3]

• **Multifunctional hybrid carbon/metal oxide or sulfide nanomaterials** with fine-tuned morphological, chemical (redox), electrical, and/or magnetic properties through coprecipitation, hydrothermal and ball milling processes for catalytic and energy applications.[4,5]







• **Tripodal metallic complexes with catalytic activity by one-pot three-step mechanically assisted synthesis**.[6]

• **Biochar-based materials** to prepare carbon-based catalysts by heteroatom doping and metal/sulfonic acid functionalization.[7,8]

• **Doped bismuth-based dielectric ceramic materials** produced by mixed oxide method and sintering by pressureless sintering method.[9]

• **Lanthanide luminescent-based POMs and MOFs** for application in optical sensing.[10,11]

• **Photoluminescent carbon quantum dots** with fine-tuned color emission features produced by hydrothermal and microwave approaches for application in security and anticounterfeiting inks.

• **Magnetic porous, nanoporous and nanostructured adsorbents** for the removal of organic contaminants, recovery of metals and rare-earth elements, and CO2 capture.[12-16]

• **Binuclear nanozymes as catalytic antioxidants and (photo)catalysts** prepared by ionic self-assembly of oppositely charged metal complexes.[17-20]

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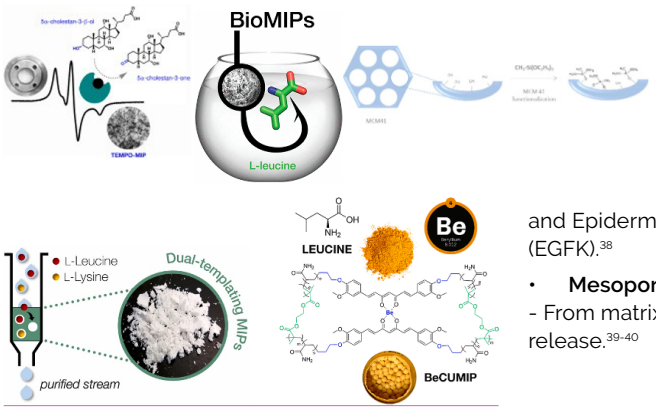
RESEARCH THEMES/
(BIO)MATERIALS ENGINEERING AND PRODUCTION

- **Molecularly imprinted polymers (MIP)** for drug delivery systems and catalytic processes using supercritical fluid technology. [21] An enzyme-inspired molecularly imprinted polymeric (MIP) catalyst was designed for fast and selective oxidation of a cholesterol derivative with easy catalyst regeneration. [22]
- **Polymeric particles with affinity for 4-dimethylaminipyridine (DMAP)** were developed by molecular imprinting using supercritical carbon dioxide (scCO2) technology, for cleanup of this potentially genotoxic impurity from crude mixtures of active pharmaceutical ingredients. [23]
- **Biomolecular Fishing**: Design, Green Synthesis, and Performance of l-Leucine-Molecularly Imprinted Polymers. LEU-MIPs were synthesized for the first time by supercritical carbon dioxide (scCO2) technology and mechanochemistry.[24] A significant imprinting factor of 12 and a binding capacity of 27 mg LEU/g polymer were obtained.
- **Development of plastic antibodies with affinity for biomolecules** under the scope of the ongoing project BioMIPs.
- **Sustainable development of dual–templating molecularly imprinted polymers for biopurification**.[25,26]
- **Biosensing by green, switchable photochromic molecularly imprinted polymers.**[27]
- **Natural deep eutectic systems (NADES)** – alternative green solvents formed after the mixture of two or more natural occurring molecules (from sugars, aminoacids or organic acids).[28-33]
- **Natural polymers extracted from plants for the production of bioinspired materials** with high biocompatibility for tailored drug delivery.[34-37]
- **Hemi-synthesis of novel (S)-carvone hydrazone from the natural (s)-carvone** by reacting oxalyldihydrazide with caraway's seeds essential oil extracted by conventional and supercritical fluid technology: Structural and crystal characterization, targeted bioassays and molecular docking on human protein kinase (CK2) and Epidermal Growth factor Kinase (EGFK).[38]



- **Mesoporous Silica Matrices** - From matrix synthesis to drug release.[39-40]

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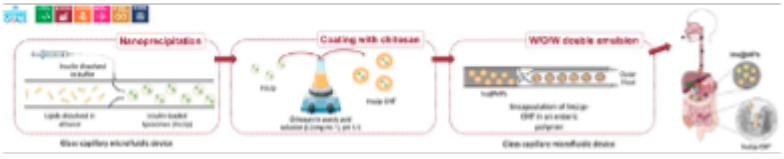
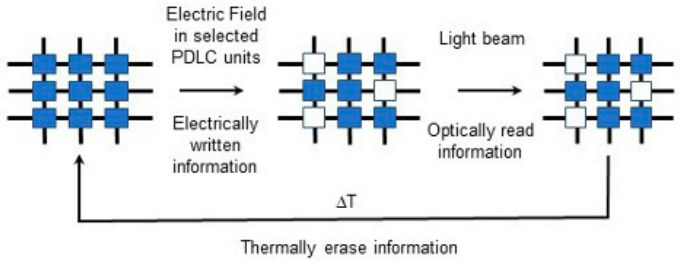
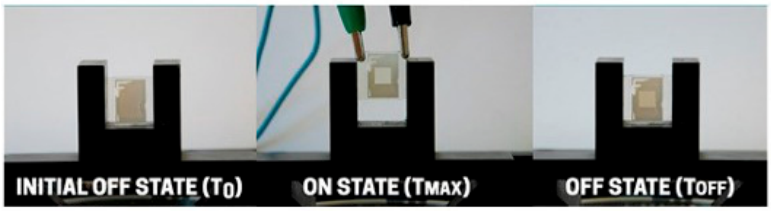
RESEARCH THEMES/
(BIO)MATERIALS ENGINEERING AND PRODUCTION

- **Nano-in-micro dry powder formulations** based on polyurea dendrimers, trehalose, PLGA and cholesterol with excellent biocompatibility prepared using super supercritical fluid technology.[41]
- **Microfluidics production of biopharmaceutical-loaded lipidic particles** for the efficient treatment of diabetes and inflammatory diseases.[42,43]
- **Photocatalytic Composite Nanomaterial and Engineering Solution for Inactivation of Airborne Bacteria.**[44]
- **The AEROPILs Generation: Novel Poly(Ionic Liquid)-Based Aerogels for CO2 capture.**[45]
- **Polymer Dispersed Liquid Crystals in non-volatile memory devices** for applications in digital memories, particularly in non-volatile memory systems where data retention is essential.[46-56]







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RESEARCH THEMES/
SUSTAINABLE ENVIRONMENT

CATALYSIS FOR A SUSTAINABLE ENVIRONMENT

MatSusWell has a mature knowledge on sustainable catalysis & catalysts development in line with the huge challenges in this area: i) advanced design of novel catalysts for industrial application; and ii) use of natural resources as alternative to fossil fuels expanding catalysis concepts to biorefinery and sustainability.

Selective homogeneous and heterogeneous chemical catalysis[57]

• **Nitroaromatics reduction** including 4-nitrophenol (a prevalent pollutant found in wastewater) to 4-aminophenol with great industrial interest for the synthesis of bulk and fine chemicals using recyclable nanocatalysts: Au/Ag-based TiO2 nanocomposites, carbon-based materials hybridized with metal oxides or magnetic ferrite nanoparticles, magnetic Fe-rich coal fly ashes.[58-60]

• **Photocatalytic degradation of organic water pollutants** including dyes, highly toxic nitroaromatics and pharmaceuticals under UV/simulated sunlight using metal oxide ceramics or carbon-based materials (undoped or heteroatom-doped) hybridized with metal oxides and sulfides or with TiO2 as photo- and/or photo-Fenton catalysts and oxygen or H2O2 as oxidant.[61-63]

• **Functional porous carbons**: Synthetic strategies and catalytic application in fine chemical synthesis.[64-66]

• **Phenol hydroxylation to catechol** (important intermediate with great industrial interest for the production of perfumes, dyes, medicines, pesticides, rubbers and other chemicals) using Fe(II) and Cu(II)-based complexes encapsulated in NaY zeolite as heterogeneous catalysts.[67]

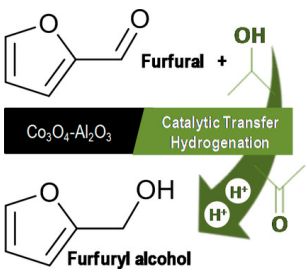
Biorefinery and biomass conversion into value-added products

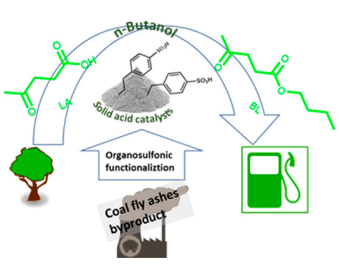
• Marine waste biorefinery: from biomass to bioactive molecules and functional catalytic materials[68]

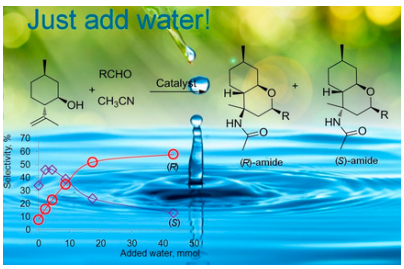
• Preparation of ZrO2-supported copper nanoparticles (Cu NPs/ZrO2) under different pH (4, 7 and 9) and evaluation in glycerol dehydration reaction. [69-70]

• Furfural production and valorization: catalytic transfer hydrogenation (CTH) production of trans-4,5-Diamino-Cyclopent-2-Enones under continuous flow conditions.[71-73]

• HSO3-functionalized derived catalysts as a new strategy to produce solid acid catalysts for industrial catalytic applications: i) biodiesel and biofuels production,[74] and ii) amides, including highly valuable chromenols.[75,76]







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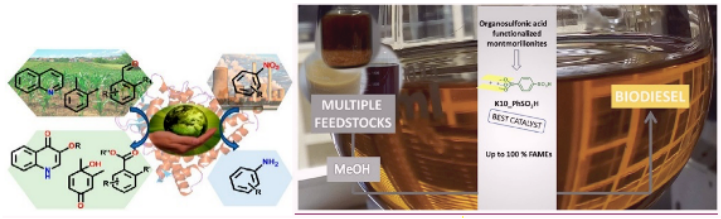
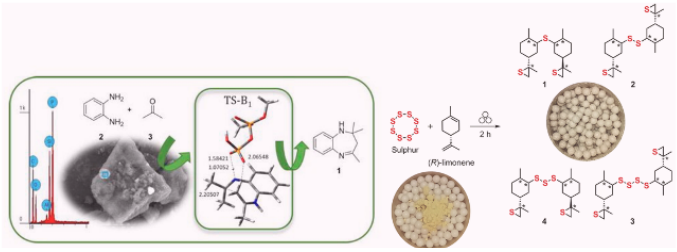
RESEARCH THEMES/ SUSTAINABLE ENVIRONMENT

- **Bioinspired circular processes**: biomimetic catalysis for valorization of biomass derivatives (benzofuran, aldehydes, inert aromatics from biomass pyrolysis) and pollutants upcycling.[77-79]
- **Wood fiber functional materials and membranes for water remediation** from dyes and microplastics.[80,81]
- **Desulfurization of biofuels** based on active heterogeneous catalysts having polyoxometalates as active centres, in collaboration with Galp Energia, IBEROL and Green Energy companies.[82-86]
- **Biodiesel production** using waste shells derived catalysts;[87] using sulfonic-acid natural montmorillonites/ silica particles as catalysts (real feedstocks, *e.g.* waste oils);[88,89] using membrane reactors for sustainable production.
- Design of active and selective heterogeneous catalysts based on MOFs (Au@MOF, Au/Pt@MOF and Heteropolyacids@MOF) for glycerol oxidation and acetalization to form valuable fuel additives.
- **Eco-sustainable and recyclable porous carbon catalysts:** a new series of promising porous catalytic carbon materials functionalized with Lewis and Brønsted acid sites for the green synthesis of 2,3-dihydro-1H-1,5-benzodiazepine,[90-92] selective oxidized carbon nanotubes and graphene flakes carbocatalysts for the mild oxidation of cis-cyclooctene.
- **Eco-sustainable processes for carbon materials recovery from electronic waste.**[93]
- **Valorization of crude glycerol**: bulk and membrane catalytic materials for the transformation of diesel production waste, crude glycerol, into add-valuable products for cosmetic and pharmaceutical industries via oxidative reactions. Futhermore, glycerol is converted in (bio)fuel additives via acetalization.[94,95]
- **Mechanosynthesis using zirconium oxide reactors** explored as a promising methodology to produce high-added-value products from abundant raw materials such as sulphur and limonene.[96]





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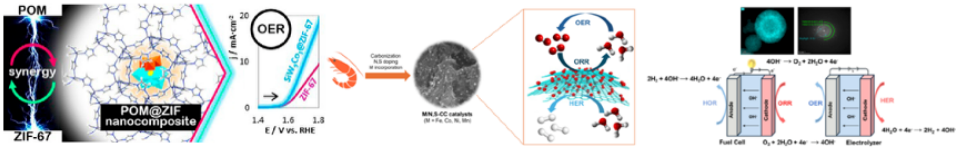
RESEARCH THEMES/
SUSTAINABLE ENVIRONMENT

RENEWABLE ENERGY & CLIMATE CHANGE MITIGATION

MatSusWell is committed with the transition to a Sustainable and Circular Economy based on secure, clean, and renewable energy against the current excessive consumption/combustion of fossil fuel resources (coal, nature gas, and petrol), which are the main contributors to the global climate changes, air pollution, and greenhouse effect.
MatSusWell is also committed in advancing green and sustainable chemistry, by developing metrics and dynamic scoring tools to evaluate products and processes.
Therefore, research work has been developed in the following topics:

- **Energy conversion:** noble metal-free POM@MOF nanocomposites, MOF-derived nanocarbons, activated carbons from biomass, POM-based composites, mixed-valence Co and Mn oxides@doped-graphene nanocomposites, 3D carbon nanotube/graphene nanocomposites and carbon-based materials derived from industrial residues valorization for application in electrochemical energy-related reactions – hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and oxygen reduction reaction (ORR).[97-109]
- **CO_2 conversion and valorization:** nitrogen-doped metal-free carbon catalysts for CO_2 electrochemical conversion and CO_2 valorization to cyclic carbonates, useful fuels and chemicals, with a focus on the results underlying their mechanistic behavior, advantages and limitations.[110]



GREEN METRIC TOOLS

- **Quantitative framework for measuring greenness and/or sustainability** of chemical products and processes.[70]

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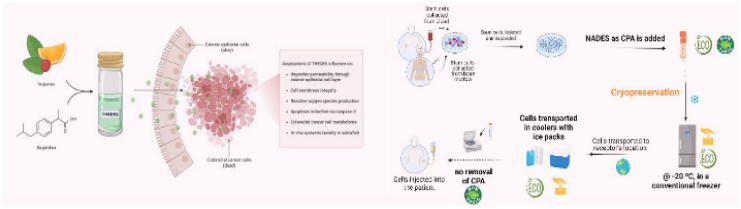
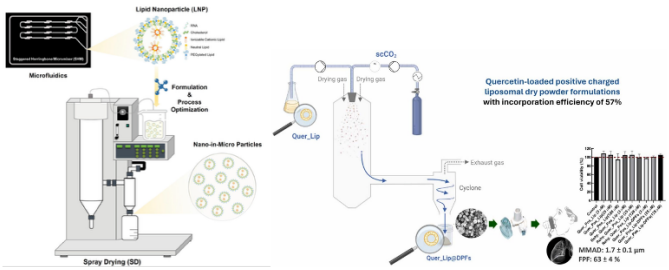
RESEARCH THEMES/
DRUG DELIVERY AND TISSUE REGENERATION

MatSusWell focus on the integration of neoteric solvents, nanotechnologies, and quality-by-design to generate advanced drug delivery platforms and smart constructs for tissue healing. Strong emphasis is set on the materials characterization and biocompatibility assessment, established through distinct in vitro, ex vivo, and in vivo models of either physiological or pathological conditions:

- **Layer-by-layer nanosystems micronized in chitosan aerosols** using the supercritical CO2-assisted spray drying (SASD) enabled the design and production of effective systems for pulmonary delivery of siRNA.[111]
- **Cyclodextrin host-guest complexation by SASD for HIV drug delivery**.[112]
- **Therapeutic deep eutectic systems (THEDES) based on natural terpenes and anti-inflammatory agents explored as anticancer therapeutic** pharmaceutical ingredients.[113-115]
- **Natural deep eutectic systems (NADES) based on sugars and polyols** explored as cryoprotectant agents.[116]
- **Innovative Drug Repurposing Strategies (DRS)** as therapeutic approaches for inflammation and immune response modulation in organ-specific and systemic conditions.[117-119]
- **Advances in oral implantology**: pre-clinical and clinical trials. [120-122]
- **Next Generation Hydrogel Systems** for enhanced skin delivery of bioactive compounds. [123,124]
- **Curcumin-Loaded Lipid Nanoparticle Hydrogel** for safer and enhanced root canal disinfection. [125,126]
- Mitigation of shear stress in **spray drying for the production of RNA-loaded lipid nanoparticles through process and formulation optimization**.[127]



- Optimization of **quercetin–liposomal dry powders for pulmonary delivery using supercritical CO_2-assisted spray drying**.[128]
- **Proof-of-concept production of Cu, Zn-Superoxide dismutase liposomal dry powder formulations** using supercritical CO2-assisted spray-drying.[129]
- Development of a **new inhalation-based theranostic approach for metabolism-targeted therapy in non-small-cell lung carcinoma** using lactate-functionalized nanoparticles loaded with selenium and chrysin.[130]



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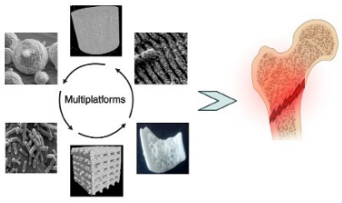
RESEARCH THEMES/
DRUG DELIVERY AND TISSUE REGENERATION

- **Dry Dosage Forms of Add-Value Bioactive Phenolic Compounds by Supercritical CO2-Assisted Spray-Drying.** SASD has proven to be an efficient encapsulation technique for phenolic compounds gallic acid and resveratrol, preserving their antioxidation potential after three months in storage.[131]
- **Solid Dosage Forms of Biopharmaceuticals in Drug Delivery Systems Using Sustainable Strategies**.[132]
- **Inhalable hydrophilic molecule-loaded liposomal dry powder formulations** using supercritical CO2-assisted spray-drying a synergy between pharmaceutical and supercritical carbon dioxide technologies to assist in liposome drying. [133]
- **Biocompatible oligo-oxazoline crosslinkers:** advanced chitosan for controlled dug release. [134]
- **Multifunctional biomimetic and antibacterial materials for enhanced tissue healing/regeneration.** [135-143]
- **Oral rehabilitation.** [144-149]
- **Hollow structured porous ceramic spheres for bone tissue repair** aiming dual release of antimicrobial and osteogenic drugs to prevent infections/ film formation in the outer and promote bone regeneration from the inner.[150]



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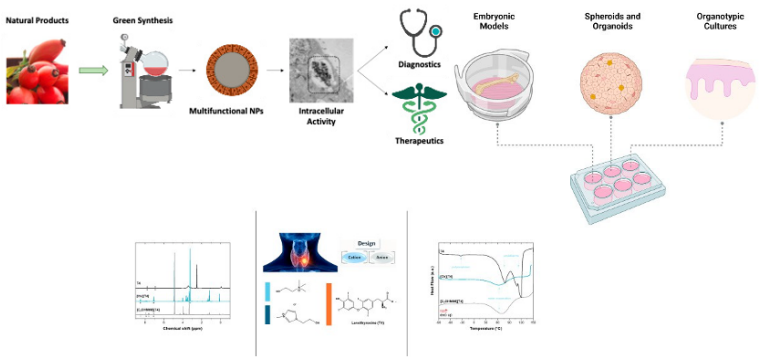
RESEARCH THEMES/
DRUG DELIVERY AND TISSUE REGENERATION

- **Development of customized 3D structures for bone regeneration.** [151-160]
- **Green-synthesized multifunctional nanoparticles for diagnostic and therapeutic applications** [161,162]
- **Development of sustainable translational research methodologies** aligned with the "3Rs Principle" (Replacement, Reduction, Refinement) to minimize animal experimentation. [163,168]
- **Micro- and nano-scaled particles designed as drug carriers for antimicrobial activity, osteogenic promotion, and immunomodulation.** [169,170]
- **Ionic levothyroxine formulations** as an alternative to the commercial levothyroxine sodium salt with promising bioavailability.



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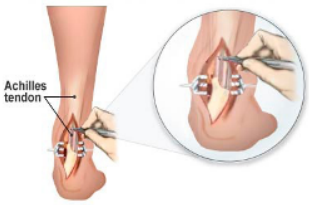
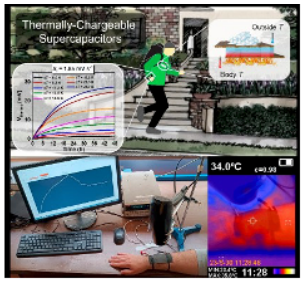
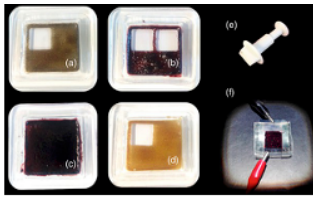
RESEARCH THEMES/
WEARABLE TECHNOLOGIES AND DEVICES

MatSusWell has been fostering innovation on the development of smart and wearable technologies for the benefit of Society, targeting applications ranging from healthcare and personal protection to fashion, sports, and energy,[171] namely:

- **Healthcare and medical devices:** 3D Textile-based structures for tendon/ligament repair with improved mechanical performance using innovative textile technology. A worldwide patent application (PCT) has been published and multinational companies that operate in the medical sector have demonstrated a great interest in these developments.[172-180]
- **Smart wearable & flexible energy harvesting & storage technologies for IoT applications:** multifunctional electrochromic and "glow-in-the-dark" supercapacitors and self-chargeable energy harvesting/storage textiles and flexible devices based on hybrid carbon/metal oxide or sulfide electrode nanomaterials and redox-active polyelectrolytes to power miniaturized electronic sensors and devices integrated on clothes for IoT applications.[181-186] An international patent application under EU evaluation has been published.[187]
- **Radiation protection textiles:** Functional textiles with improved protection against X-rays, radio frequency, or microwave radiation and enhanced comfort through their coating/functionalization with metal oxide and/or carbon-based nanomaterials.[188,189]
- **High-performance light-responsive smart textiles** by printing technologies: Photochromic textile fabrics and fibers under UV and/or sunlight exposure featuring tunable photoresponse, high photoswitching reversibility, high thermal stability, and a wider color palette through the incorporation of hybrid tungsten oxide nanoparticles.[190]
- **Anticounterfeiting textiles**: development of innovative smart security labels based on multifunctional inks that combine the conventional QR-readable information with additional physical security features embedded in the functional inks, thereby enhancing coding versatility and security potential
- **A new class of donor-acceptor dedrimers with photodiode-like behavior** was developed.







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RESEARCH THEMES/
TECHNOLOGY TRANSFER AND ENTREPRENEURSHIP

MatSusWell research work fosters scientific knowledge transfer and product & technology valorization through collaboration with other companies or entrepreneurship start-up projects.

Collaboration with companies and technological centres

- **Porous functionalized carbons derived from spent tire rubber –** Collaboration with Valorpneu, the Portuguese Management Company of Used Tires, and GENAN for the development of new products (nanoporous carbon materials) for innovative applications (recovery of critical rare earth elements, H2 production).[191]
- **Platform for the promotion of low-carbon fuels (Plataforma para a promoção dos combustíveis de baixo carbono, PCBC) –** Collaboration with PCBC which represents a group of associations and organizations operating at different stages of the value chain, from raw materials to fuel production, including its supply, distribution, and use, forming a substantial part of the sustainable renewable fuels sector in Portugal. Additionally, this collaboration resulted into a cooperation agreement with EPCOL – Empresas Portuguesas de Combustíveis e Lubrificantes.[192]
- **Enhancement of Solubility of APIs using Deep eutectic Systems** in collaboration with Boheringer Ingelheim (2021)
- **Footwear, Advanced Materials, Equipment, and Software Technologies**
- **New textile solutions for electromagnetic shielding:** project RFProTex - Innovative Textiles for Radiofrequency Radiation, in collaboration with the portuguese textile company Cottonanswer S.A., and the technological center CITEVE (Co-Promotion Project POCI-01-0247-FEDER-039833).
- **All-in-one energy harvesting & storage smart textile technologies:** project BoostEnergy4Tex, in collaboration with the portuguese textile company TINTEX S.A., and the technological center CITEVE (R&TD project PTDC/CTM-TEX/4126/2021, funded by FCT)
- **Innovative multifunctional smart labels for anticounterfeiting textiles:** project SafeTex - Smart security labels for anti-counterfeiting textiles using multifunctional technologies, in collaboration with the Portuguese textile company SMARTEX.AI (PEX project 2023.13995.PEX, funded by FCT).
- **Novel catalytic processes based on active composites for simultaneous desulfurization and denitrification of real fuels:** in straight collaboration with Galp, crucial to achieve the best results conciliating fuels quality and cost-efficiency.[193-197]
- **Scale-up of catalysts and functional materials production and natural compounds extracttion using advanced technologies**[198] in collaboration with INNOVCAT company.
- **New Nanotechnology-Based Cosmetic Products** Obtained Through Advanced Technologies for Extraction and Valorisation of Marine Biomass in collaboration with Nueva Pescanova group and Mesosystem company.
- **CATALVALOR**[199]**, WEStoreOnTEX**[200] projects were awarded with 30,000 euros to support proofs of concept under the BIP Proof - Business Ignition Programme, promoted by U.Norte Inova, University of Porto, 2018 and 2023.
- **Enhancing microalgae biomass growth towards food and feed supplementation:** Exploring the micronutrients role interaction and gamma radiation effect. In straight collaboration with Allmicroalgae and C2TN-IST.177.[201,202]
- **Valorization of cork-based industrial residues** in collaboration with J.A. Veiga de Macedo S.A
- **Intellectual Property and Translational Valorization of Perioceutic Nanotechnologies:** under the NanoTec4Perio project (PTDC/BTM-SAL/2022.06464), key technology-transfer outcomes were achieved through the filing of two patents (PT119901 and EP24220085.5) protecting an innovative nanosystem for controlled local delivery of repurposed immunomodulatory drugs in periodontal therapy.

SELECTED PUBLICATIONS

191 M. Nogueira, et al., Waste Manag., 2024, 174, 451. **doi: 10.1016/j.wasman.2023.12.025**

192 N. Lapa, et al., Estudo sobre Combustíveis de Baixo Carbono em Portugal – Perspetivas para 2030, Relatório Técnico, PCBC, 2025.

193 D. Julião et al. J. Mol. Liq., 2020, 309, 113093. **doi: 10.1016/j.molliq.2020.113093**

194 D. Julião et al. Appl. Catal. A, 2020, 589, 117154. **doi: 10.1016/j.apcata.2019.117154**

195 F. Mirante et al. Fuel, 2020, 259, 116213. **doi: 10.1016/j.fuel.2019.116213**

196 D. Julião et al. Appl. Organomet. Chem., 2020, 34(4), e5490. **doi: 10.1002/aoc.5490**

197 D. F. Silva, et al., Sust. Chem., 2021, 2, 382–391 **doi: 10.3390/SUSCHEM2020022**

198 O. Dorosh et al. Molecules, 2020 25(7), 1739 **doi: 10.3390/molecules25071739**

199 https://upin.up.pt/pt-pt/content/catalysing-greener-future

200 https://upin.up.pt/pt-pt/tecnologias/flexible-thermoelectric-supercapacitors

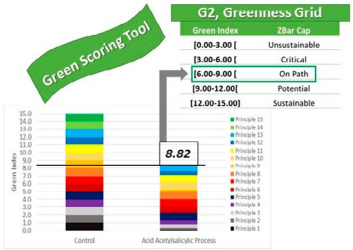
201 R. Pires, et. al., Algal Research, 2022, 68, 102876 **doi: 10.1016/j.algal.2022.102876**

202 M. Trovão, et al., Sci. Rep., 2025, 15, 23325 **doi: 10.1038/s41598-025-05913-1**

HIGHLIGHTS

GREENNESS GRID (G2): A GREEN CHEMISTRY SCORE TOOL

GeoSoil in collaboration with MatSusWell researchers proposed a green chemistry score tool, composed of 15 metrics based on principles and guidelines of green chemistry. This was possible to achieve through a series of steps, starting with: a) the existing 12 principles of green chemistry; b) introducing additional principles; c) defining new metrics and associating existing ones for each principle; d) collecting and analyzing published results from other studies (*i.e.* average E-factor of different industries); e) laws (*i.e.* half-life of a biodegradable substance) to normalize the generated outputs from each metric; f) formulating an overall index score for each process in a close normalized range and finally, g) associating a green qualitative scale to the score. G2 can also assist in product or process evaluation and/or comparison, independently of the development stage, such as: (i) process design, (ii) process development, and (iii) process delivery.

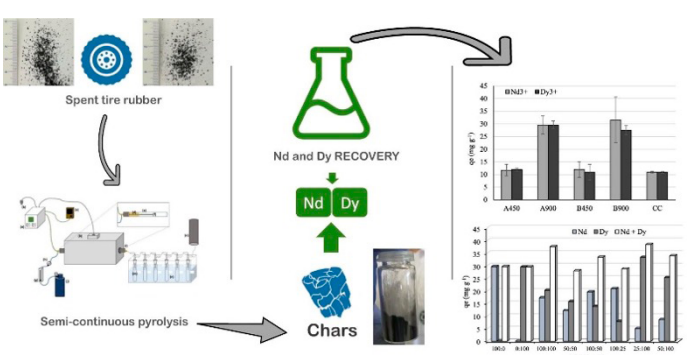


Towards a new, green and dynamic scoring tool, G2, to evaluate products and processes.

J Clean. Prod. 2020, 276, 123079

RECOVERY OF RARE EARTH ELEMENTS (ND^{3+} AND DY^{3+}) BY USING CARBON-BASED ADSORBENTS FROM SPENT TIRE RUBBER

Two samples of spent tire rubber (rubber A and rubber B) were submitted to thermochemical conversion by pyrolysis process. A450, B450 and A900, B900 chars were obtained from rubber A and rubber B at 450 ˚C and 900 ˚C, respectively. The chars were then applied as recovery agents of Nd^{3+} and Dy^{3+} from aqueous solutions in mono and bicomponent solutions, and their performance was benchmarked with a commercial activated carbon. The chars obtained at 900 ˚C were the most efficient adsorbents for both elements with uptake capacities around 30 mg g^{-1}. The chars obtained at 450 ˚C presented uptake capacities similar to the commercial carbon (≈ 11 mg g^{-1}). A900 and B900 chars presented a higher availability of Zn ions that favored the ion exchange mechanism. It was found that Nd^{3+} and Dy^{3+} were adsorbed as oxides after Zn was released from silicate structures (Zn_2SiO_4). A900 char was further selected to be tested with Nd/Dy binary mixtures and it was found a trend to adsorb a slightly higher amount of Dy^{3+} due to its smaller ionic radius. The uptake capacity in bicomponent solutions was generally higher than for single component solutions due to the higher driving force triggered by the higher concentration gradient.



Recovery of rare earth elements (Nd_3+ and Dy_3+) by using carbon-based adsorbents from spent tire rubber

Waste Management, 2024, 174, 451–461

HIGHLIGHTS

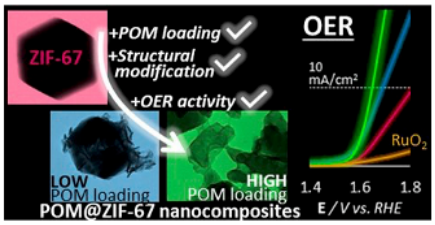
VINEYARD PRUNING EXTRACTS AS NATURAL ANTIOXIDANTS FOR BIODIESEL STABILITY: EXPERIMENTAL TESTS AND PRELIMINARY LIFE CYCLE ASSESSMENT

Biodiesel is prone to oxidation depending on the process production, feedstocks used, especially those from low-grade sources, and storage conditions, among others. The addition of natural extracts obtained from biomass rich in polyphenols represents a promising alternative to synthetic additives (fossil fuel derivatives). This work demonstrated the suitability of VPW extracts obtained by SWE as an antioxidant additive to promote the oxidative stability of biodiesel. The VPW extract showed comparable antioxidant activity as the commercial antioxidant butylated hydroxytoluene (BHT) typically used in biodiesel. The assessment of the environmental impacts associated with the development of this novel VPW-based additive, clearly show that VPW extract is environmentally competitive with BHT up to its drying, also thanks to the energy integration step included in the design of the process of VPW extraction.

Vineyard Pruning Extracts as Natural Antioxidants for Biodiesel Stability: Experimental Tests and Preliminary Life Cycle Assessment.

ACS Sustainable Chemistry & Engineering, 2023, 11(21), 8084-8095

POM@ZIF-67 NANOCOMPOSITES AS HIGHLY EFFICIENT EVOLUTION REACTION ELECTROCATALYSTS



Advanced nanocomposites were produced through the encapsulation of Co-containing polyoxometalates (POMs) inside the Co-based zeolitic imidazole framework (ZIF-67) cavities via *in situ* synthesis. All POM@ZIF-67 nanocomposites showed bidirectional synergy regardless of the POM substitution degree. Moreover, they revealed intrinsic OER activities higher than those developed by the expensive state-of-the-art electrocatalysts (RuO_2 and IrO_2) especially in the case of $SiW_9Co_3[h]$@ZIF-67, with an overpotential of 0.42 V for a current density of 10 mA/cm² and a Tafel slope of 93.9 mV/dec. This work contributed to the design/preparation of new and highly efficient OER electrocatalysts based on POMs and MOFs produced at room temperature, avoiding solvothermal processes hard-conditions. Work chosen for the Themed Collection of HOT Papers of Journal of Materials Chemistry A

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Advanced framework-modified POM@ZIF-67 nanocomposites as enhanced oxygen evolution reaction electrocatalysts.

Journal of Materials Chemistry A, 2020, 8, 13509–13521

HIGHLIGHTS

CU,ZN- SUPEROXIDE DISMUTASE LIPOSOMAL DRY POWDER FORMULATIONS PRODUCTION USING SUPERCRITICAL CO_2-ASSISTED SPRAY-DRYING

Enzyme-based inhalable therapeutics for lung inflammation are gaining interest as an alternative to long-term corticosteroids treatments. However, enzymes have poor pharmacokinetics. Encapsulating enzymes in liposomes can increase their half-live and modify their biodistribution Also both liposomes and enzymes are susceptible to destabilization during storage. This drawback can be surpassed, by converting liposomal suspension into solid dosage forms for different administration routes, including inhalation. Cu, Zn-superoxide dismutase (SOD) was encapsulated in liposomes, then dried using scCO2-assisted spray-drying to make SOD-loaded liposomal dry powder formulations (SOD_Lip-DPFs). Upon resuspension in water, liposomes maintained structural integrity, with 99% SOD encapsulation efficiency and preserved enzymatic activity. Stability studies showed that SOD_Lip-DPFs maintained liposomal and enzyme stability for 50 days at 40% relative humidity. This offers a stable and efficient delivery system for enzyme-based inhalable therapeutics.

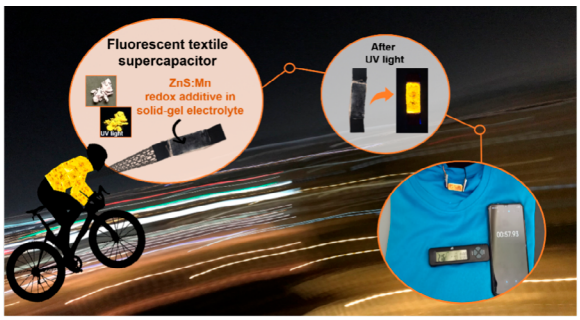
Cu,Zn- Superoxidise dismutase liposomal dry powder formulations production using supercritical CO2-assisted spray-drying.

Journal of Supercritical Fluids, 2023, 200, 105991.

HIGHLIGHTS

SMART DUAL-FUNCTIONAL ENERGY STORAGE/FLUORESCENT TEXTILE DEVICE

A dual-functional textile supercapacitor merging enhanced energy storage performance with optical properties was fabricated using a new redox-active electrolyte based on fluorescent Mn(II)-doped ZnS combined with carbon nanotube-coated textile electrodes. The device was able to store energy and power supply electronic/illumination systems, while simultaneously exhibiting intense yellow-orange fluorescence under UV light irradiation.



The fluorescent hybrid textile supercapacitor exhibited enhanced energy storage performance relative to a similar device containing the undoped electrolyte, namely 20% higher working voltage (1.64 V vs. 1.37 V), 48% higher energy density (1.63 W h kg-1 vs. 1.10 W h kg-1) and 74% higher power density (641.6 W kg-1 vs. 369.2 W kg-1). Additionally, it presented excellent cycling stability (100%) after 8000 charge/discharge cycles.

This work demonstrated the versatility of this type of technology for dark environment applications, namely in reflective/safety electronic clothing for night time users.

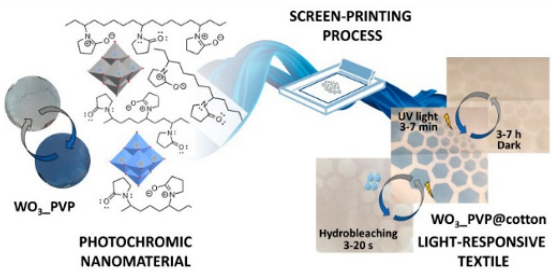
Smart dual-functional energy storage/fluorescent textile device based on a new redox-active Mn-doped ZnS solid-gel electrolyte.

Chemical Engineering Journal 2021, 426, 131274.

HIGH-PERFORMANCE LIGHT-RESPONSIVE TEXTILES BASED ON SMART WO3 BUILDING BLOCKS

Engineered tungsten oxide-based materials with tunable photochromism were produced by a low-cost, single-step, and scalable solvothermal process using different structure-directing agents, and applied as building blocks in the fabrication of high-performance light-responsive smart textiles.

The WO3-based materials prepared using polyvinylpyrrolidone (PVP) featuring the best photochromic response under both sunlight and UV irradiation, with up to 13× faster coloration than that reported in the literature for this class of materials (7–20 min vs. 60–90 min) and up to 2× higher total color difference (21.4–50.6 vs 25.2–25.8). High-performance UV/sunlight-responsive smart textiles were subsequently produced by screen-printing, changing color from white to blue in 3–7 min and bleaching in 3–7 h, which excelled the results documented in the literature (up to 13× faster bleaching under environmental conditions). Remarkably, the smart textiles presented fast hydrobleaching properties when immersed in water. The best-performing fabric hydrobleached in only 3–20s and could withstand multiple coloration/hydrobleaching cycles. This work opens promising perspectives for the design of engineered UV/sunlight-responsive materials and textiles with hydrobleaching properties, offering potential prospects for smart clothing and optical sensors.



Tuning the Photochromic Properties of WO3-Based Materials toward High-Performance Light-Responsive Textiles.

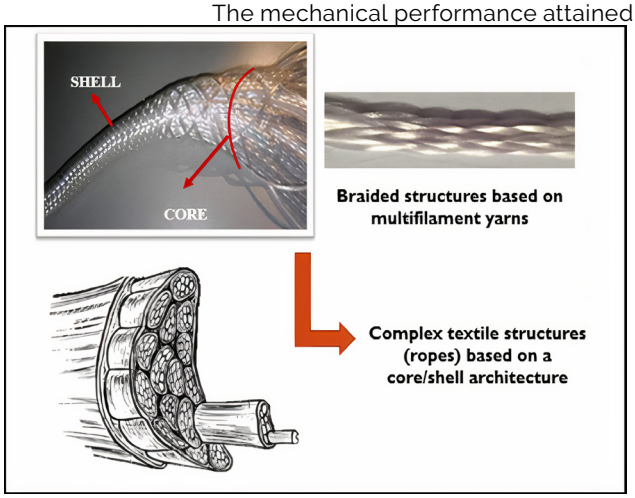
ACS Applied Optical Materials 2023, 1, 8, 1434.

HIGHLIGHTS

3D TEXTILE-BASED STRUCTURES FOR TENDON/LIGAMENT REPAIR

Poly(ethylene terephthalate) biocompatible fibrous structures have been developed for tendon/ligament repair using innovative textile technology. To accomplish the levels of load at failure, strain to failure, stiffness, creep and fatigue resistance observed in native tendon/ligament tissues, core/shell architectures were optimized to mimic those properties.

The mechanical performance attained was shown to be superior to those of the current products in the market, which clinically show a very low success rate in the long-term medical use. A worldwide patent application (PCT) has been published and multinational companies that operate in the medical sector have demonstrated a great interest in these developments



Bio-Functionalized Prosthetic Structure with Core-Shell Arquitecture for partial or total repair of Human Tendons or Ligaments.

PCT/IB2020/053014, International Application No. WO/2020/194280, Publication Date 01.10.2020.

Amination of Polymeric Braid Structures to Improve Tendon Healing: An Experimental Comparison.

Macromolecular Materials and Engineering, 2023, 308(1), 2200426.

Poly(lactic acid) composites with few layer graphene produced by noncovalent chemistry.

Polymer Composites, 2022, 43(11), 8409–8425.

Hybrid structures for Achilles' tendon repair.

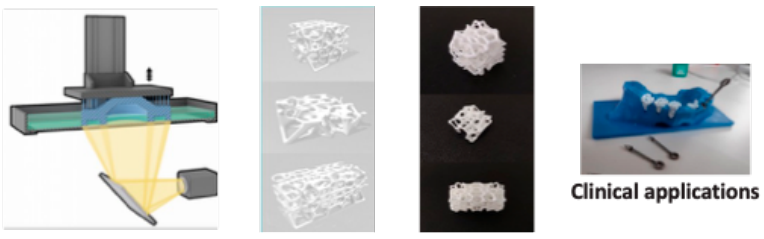
Polymers for Advanced Technologies, 2022, 33(7), 2362–2373.

Engineering hybrid textile braids for tendon and ligament repair application.

Journal of Applied Polymer Science, 2022, 139(17), 52013.

DEVELOPMENT OF CUSTOMIZED 3D STRUCTURES FOR BONE REGENERATION BY ADDITIVE MANUFACTURING USING COMPUTER ASSISTED DESIGN (CAD) MODELS

Using computer assisted designed combined with additive manufacturing processes it is possible to fabricate customized bone substitutes with very complex geometries, total liberty of shape and completely adapted to the host implantation site. It is also possible to simultaneously mimic the external structure of the cortical and trabecular bone structures, the micro and macroporosity and pore interconnectivity.



Additive manufacturing of ceramic alumina/calcium phosphate structures by DLP 3D printing.

Materials Chemistry and Physics, 2022, 276, 125417.

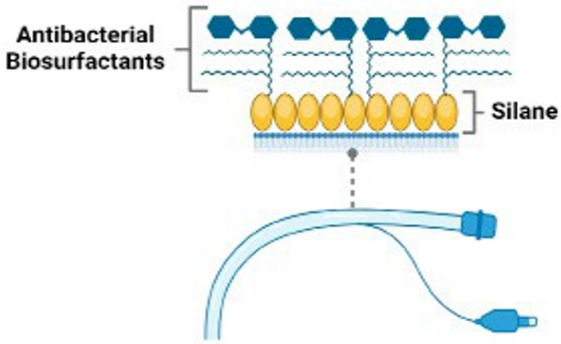
Preparation and characterization of customized bone grafting hydroxyapatite models obtained by digital light processing 3D printing.

Journal of Materials Research, 2022, 37, 784-795.

HIGHLIGHTS

PREVENTING CATHETER-RELATED INFECTIONS BY SURFACE FUNCTIONALIZATION

Silicone venous and urinary catheters are prone to microorganism adhesion, which can lead to catheter-related infections. To prevent this, the functionalization of the silicone surface with antimicrobial compounds rises as a promising alternative. The incorporation of biosurfactants produced by bacteria over the silicone's surface resulted in a substantial reduction of biofilm formation by bacteria and fungi. Additionally, functionalized catheters displayed suitable biocompatibility, hemocompatibility, and a non-irritant profile, assessed in diverse pre-clinical settings. Overall, this research sheds light on novel approaches that rely on natural compounds to avoid infections.



3D-printed biosurfactant-chitosan antibacterial coating for the prevention of silicone-based associated infections.

Colloids and Surfaces B: Biointerfaces, 2023, 230, 113486.

Using plasma-mediated covalent functionalization of rhamnolipids on polydimethylsiloxane towards the antimicrobial improvement of catheter surfaces.

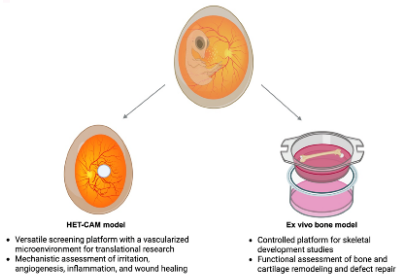
Biomaterials Advances, 2022, 134, 112563.

Assuring the biofunctionalization of silicone covalently bonded to rhamnolipids: antibiofilm activity and biocompatibility.

Pharmaceutics, 2022, 14(9), 1836

CAM-BASED AND ORGANOTYPIC NAM PLATFORMS FOR BIOEVALUATION

To accelerate the safe and responsible translation of innovative biomaterials and drug-based therapies, advanced New Approach Methodologies (NAMs) have been developed based on the chick embryo chorioallantoic membrane (CAM) and ex vivo organotypic bone tissue cultures. These complementary platforms provide biologically relevant, ethically responsible alternatives to conventional animal experimentation for early-stage validation of therapeutic concepts. The CAM model offers a highly vascularized and rapidly responsive environment to assess angiogenesis, biocompatibility, and therapeutic performance in a dynamic in vivo–like setting. In parallel, organotypic bone explant cultures preserve native tissue architecture and cell–matrix interactions, enabling mechanistic evaluation of osteogenesis, biomaterial integration, drug release behavior, and tissue remodeling under controlled conditions. Together, these integrated NAM platforms support predictive, scalable, and cost-effective screening of regenerative biomaterials and advanced drug-delivery systems, aligning with the 3Rs principle (Replacement, Reduction, Refinement) while strengthening the translational pipeline from laboratory innovation to clinical application.



Unveiling metabolic pathways in the hyperglycemic bone: bioenergetics and proteomic analysis of the bone tissue exposed to acute and chronic high glucose.

Molecular Medicine, 2025, 31, 194.

Exploring the Chorioallantoic Membrane (CAM) as a platform for burn wound modelling and analysis.

Methods and Protocols, 2025, 8, 79

Impact of high glucose on bone collagenous matrix composition, structure, and organization: an integrative analysis using an Ex Vivo model.

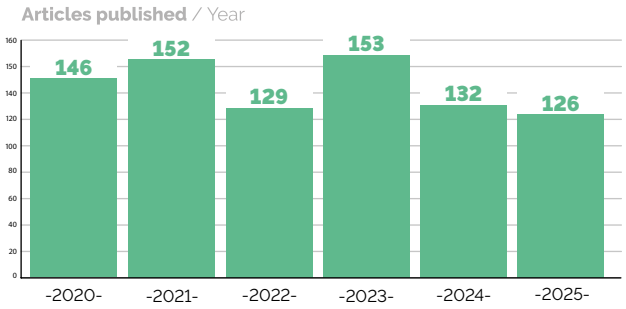
Cells, 2025, 14, 130.

Osteogenic potential of simvastatin and fluvastatin in an organotypic bone model.

Pharmaceuticals, 2025, 18, 939.

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION



H-index: **45**

838 articles*
12297 citations

*01/2020-12/2025
From WOS core collection

FUNDED PROJECTS *(Representative projects)*

- **Des.solve – When solids become liquids: Natural Deep Eutectic Solvents**
  ERC Consolidator Grant - grant 725034, Ana Rita C. Duarte (PI).
  Total funding: €1,877,006.00
- **NanoMed – Nanoporous and Nanostructured Materials for Medical Applications**
  H2020 - MSCA-RISE-2016 – 734641. Svitlana Lyubchyk (Local PI), Funding: € 171,000, Total Funding: € 972,000.00
- **NC-ARS Novel Composites Based on Cerium Oxide Nanoparticles and Carbon Enterosorbents for Acute Radiation Sickness Therapy**
  NATO Science for Peace and Security Programme Multi Year Project MYP G5683. Svitlana Lyubchyk (Coordinator), Funding: € 58,000 Total Funding: € 360,000
- **SSHARE - Self-sufficient humidity to electricity Innovative Radiant Adsorption System Toward Net Zero Energy Buildings**
  Programme "PEOPLE" – H2020-MSCA-RISE-2019- Project ~ 871284 , Svitlana Lyubchyk (Local PI),
  Funding: € 322,00 Total Funding: 1.564,000 €
- **POsTURE – PhOtocrosslinked hydrogels for guided periodontal TissUe Regeneration**
  M-ERA.NET, Maria Helena Fernandes (Co-PI)
  Total Funding: € 604,380.00
- **UniRCell - Unitised Regenerative Fuel Cell for Efficient Renewable Energy Supply: from Materials to Device**
  PAC Portugal 2020, Cristina Freire (Local PI). Funding: € 59,904.71
  Total Funding: € 2,251,685.38
- **TEXBOOST – Less commodities more specialities**
  Mobilizer Programme (COMPETE 2020), POCI-01-0247-FEDER-024523, Clara Pereira (Local PI). Funding: € 61,601.04
  Total funding: € 9,229,676.00
- **SIMPLIFIED – Easy tooth abutment (Pilar Dentário Universal)**
  Co-Development TR&D (POCI-01-0247-FEDER-017982), Maria Ascensão Lopes (Local PI). Total Funding: € 934,337.14
- **FAMEST – Footwear, Advanced Materials, Equipments and Software Technologies - Calçado e tecnologias avançadas de materiais, equipamentos e software**
  Mobilizer Programme (COMPETE 2020), POCI-01-0247-FEDER-024529, Maria Ascensão Lopes (Local PI)
  Total Funding: € 5,848,174.10
- **RFProTex - Innovative Textiles For Radiofrequency Radiation Protection**
  Co-Promotion Project funded by Agência Nacional de Inovação, POCI-01-0247-FEDER-039833, Clara Pereira (Local PI).
  Total Funding: €700,971.51
- **BioMIPs – Green strategy on the development of plastic antibodies for bio-recognition**
  Funded by the Portuguese Foundation for Science and Technology (FCT), PTDC/EQU-EQU/32473/2017, Teresa Casimiro (PI).
  Total Funding: € 236,303.38
- **BoostEnergy4Tex – All-In-One Energy Harvesting & Storage Smart Textiles: Boosting the New Generation of Safe and Sustainable Self-Powered Wearable Electronics**
  Funded by the Portuguese Foundation for Science and Technology (FCT), PTDC/CTM-TEX/4126/2021, Clara Pereira (PI).
  Total Funding: € 244,994.39
- **AIMed - Antimicrobial Integrated Methodologies for orthopaedic applications**
  H2020, 2020-2024, Maria Helena Fernandes (Co-PI), Total funding: ~2.3M€
- **CryoDES- Nature-inspired Cryopreservation Systems using Natural Deep Eutectic Systems**
  ERC PoC Grant - Ana Rita C. Duarte (PI) Total funding: €150,000.00

GROUP IN NUMBERS

FUNDED PROJECTS *(Representative projects)*

- NUTRIMIPS: Green development of antibody-like inspired materials for selective nutrient removal from biological-based aqueous streams.
  Funded by the Portuguese Foundation for Science and Technology (FCT), 2023.18036.ICDT, Teresa Casimiro (PI). Total Funding: €238,075.38
- SUSMATER, Sustainable development of biomaterial–based platforms to avoid the spread of infection diseases: from computational design to green production,
  Funded by RSC, R25–9833776562, Raquel Viveiros (PI), Total Funding: €5593.39.
- NanoTec4Perio - Innovative nanosystems with repurposed drugs for periodontal diseases' treatment.
  Funded by the Portuguese Foundation for Science and Technology (FCT), 2022.06464.PTDC, Pedro Sousa Gomes (PI). Total Funding: 200 m€
- Targeted RNA-Guided Epigenetic Therapy with Zoledronate for Osteosarcoma.
  Project FCT - UT Austin-Portugal: 2024.13302.UTA; 2025-10 - 2026-10, Pedro Sousa Gomes (PI)
- PreservArt – Abordagem Multidimensional à Preservação de Gravações Áudio Históricas: Um Estudo dos Mecanismos de Degradação Química e Microbiológica.
  06/2025-06/2028, Funded by LISBOA2030-FEDER-00819600, João Sotomayor (Local PI). Total Funding: € 249,955.20. LAQV Funding: € 116,380.80
- WFs4Plas- Wood fibers-based active membranes for microplastic capture and conversion,
  FEDER (COMPETE 2030) and FCT/MECI, doi: https://doi.org/10.54499/2023.17901.ICDT, Susana L. H. Rebelo (PI). Total funding: € 249,177.60.
- NANO-AquaFeed - Advanced Nanotechnology for Functional Nutrition in Aquaculture.
  20.02.2025 to 19.08.2026. Funded by the Portuguese Foundation for Science and Technology (FCT), 2023.14508.PEX. Sofia A. Costa Lima (PI). Total funding: 49 975,00 €
- MICAT - Membranes of intrinsic porosity with catalytic properties for advanced processes in Biorefinery
  (2022.05483.PTDC) Funded by the Portuguese Foundation for Science and Technology (FCT). Inês Matos (PI). Funding: 49 545,00 €. Project duration: 01/03/2023 - 28/02/2025.
- Shrimp4NanoCosmetic - New Nanotechnology-Based Cosmetic Products Obtained through Advanced Extraction Technologies and Valorisation of Marine Biomass,
  Co-Promotion Project funded by COMPETE 2030, through Portugal 2030 and FEDER, Andreia Peixoto (Local PI), Funding: € 134 068.00, Total Funding: € 1 115 623.04.
- SelfEnergyDriver - 3-in-1 Self-Powered Hybrid Energy-Driven Wearable Technologies: Unifying Energy Harvesting and Storage.
  ERC Consolidator Grant funded by the European Research Council (Grant agreement ID: 101171793, doi: 10.3030/101171793). Clara R. Pereira (PI) Total funding: € 1,992,329.00

INTERNATIONAL COOPERATION AND NETWORKING

- COST Actions as member/participant: CA19118 - Member of Management Committee; CA17107 - Team Member; CA22160 Team Member; CA21108 - Science Communication Coordinator
- CA18224, "Greenering - Green Chemical Engineering Network Towards Upscaling Sustainable Processes", LAQV role: coordinator, 2019–2023
- SERP+ - International SERP-Chem master with Laboratoire de Chimie Physique, Université Paris-Sud, Paris, France
- Collaborations: Catalysis: FI, ES, CZ, CL, US, PL; Drug delivery: FI, GB, DE, IT, BG, LT, BR, HR, GR, SP, RS; Imprinting materials: GB; DZ. Energy conversion, harvesting and storage: FF, DE, ES, US. Bone/Tissue regeneration: EUA, BR, Japan, SP, UK, IT, FR, BE, DE, HR, SE, LT.

DISSEMINATION & OUTREACH

LABORATÓRIO ASSOCIADO
PARA A QUÍMICA VERDE

NanoPlat

NANOPLATFORMS

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

Group Coordinator:

Salette Reis

The Nanoplatforms group conveys expertise in physical-chemistry, medicinal chemistry, pharmaceutical, and analytical sciences to support research towards the development of innovative nanoplatforms to address current environmental, food industry, and biomedical challenges.

The group's research is focused on the design, synthesis, and optimization of inorganic, organic and hybrid nanoparticles for multipurpose applications, such as the development of plasmonic, electrochemical, and fluorescent (bio)sensors and their incorporation in miniaturized detection devices to enhance analytical automation. Another relevant application value-added by the group is the development of more efficient, targeted, spatially, and temporally controlled delivery systems to carry multiple molecules for the improvement of their (bio)activity. The use of nanoplatforms as bio-mimetic models to study the complex interactions of drugs, bioactive compounds and/or nanoparticles with lipid cell membranes is another topic of interest.

Liposomes, cyclodextrins, micelleplexes, lipid, polymeric, magnetic, and gold nanoparticles are tools to produce innovative nanoplatforms with potential application in Nanomedicine, Biomedical Engineering, Biosensing, Functional Foods, and Industrial Production.

RESEARCH OBJECTIVES [2025-2029]

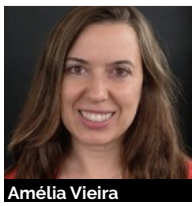
The research activity of the Nanoplatforms group has attracted significant attention to the optimization of innovative nanoplatforms to overcome several clinical, chemical, environmental, and food quality challenges. The main research objectives are the:

- Development of innovative smart materials as sustainable delivery carriers;
- Design of multipurpose nanoplatforms as enhanced analytical automation tools;
- Design and application of multifunctional (bio)sensors for molecular imaging, molecular targeting, and diagnosis;
- Implementation of structured nanoplatforms as biomimetic models;
- Translational research based on the application of knowledge gained through basic research to studies that could support the development of new products, to solve the gap between the discovery of the new nanoplatforms developed and their dissemination to potential users and routine application.

RESEARCH TEAM

SENIOR RESEARCHERS

Alexandra Plácido

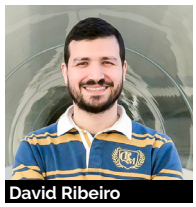

Amélia Vieira

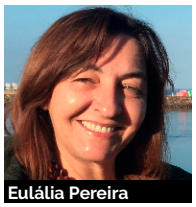
Ana Cláudia Santos

Ana Figueiras

André Pereira

Cláudia Nunes

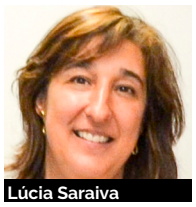

David Ribeiro


Eulália Pereira

Francisco Veiga

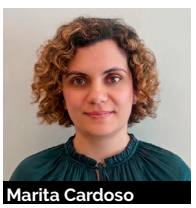
Helena Gonçalves

João Santos


Lúcia Saraiva

Luís Ribeiro

Marieta Passos


Marita Cardoso

Patrícia P. Pires

Paula Gameiro

Rui Carvalho

Salette Reis

 Group coordinator

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Andreia Granja
Andreia Marinho
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Raquel Costa
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Ana Isabel Martins
Raquel Andrade
Susana Neves
Tiago Azevedo

OTHER RESEARCHERS

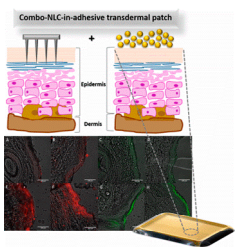
Cátia Domingues
Fátima Mota

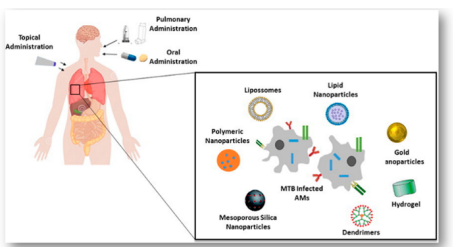
RESEARCH THEMES/ DELIVERY SYSTEMS

SMART MATERIALS AS SUSTAINABLE CARRIERS

The NanoPlatforms group aims the development of more efficient, spatially and temporally controlled drug delivery methods by developing innovative bioactive materials able to be stimulus-responsive activated to: i) guide and trigger the drug release locally at specific locations, ii) generate local hyperthermia to boost the therapeutic effects, iii) act as a contrast agent, iv) theranostic performance and iv) enhance the drug pharmacokinetic behavior. The specific goals involve:

- Nanocarriers development based on a nano multi-approach strategy to eradicate bacterial biofilms
- Biomimetic vitamin E-based nanosystem: red blood cell-pancreatic cancer hybrid cell membrane-coated dual-loaded micelles for synergistic and improved pancreatic cancer therapy.
- Natural product-based biomimetic-coated halloysite clay nanotubes hydrogel with improved efficacy and safety for cutaneous wound treatment.
- Hybrid biomaterials system: hydrogel-containing functionalized halloysite clay nanotubes for melanoma combined gene and photodynamic therapies.
- Targeting tumor cells through theranostic nanoparticles and Micelleplexes.
- Design of a targeted nanotherapy approach for the upgrade of rheumatoid arthritis treatment. Collaboration with Centro Hospitalar do Porto
- Design of a targeted nanotherapy approach for the upgrade of rheumatoid arthritis treatment. Collaboration with Centro Hospitalar do Porto.
- Development of mucoadhesive and pH responsive fucoidan-chitosan nanoparticles for the oral drug delivery.
- Design and characterization of hybrid hydrogels for enhanced skin drug delivery.
- Implementation of polymeric microneedle devices for transdermal drug delivery.
- Dermal delivery of lipid nanoparticles-enriched hydrogels for atopic dermatitis and psoriasis therapy. Collaboration with Centro Hospitalar do Porto.





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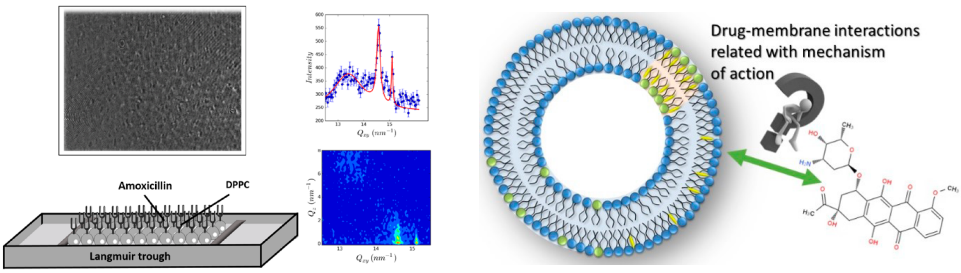
RESEARCH THEMES/
DELIVERY SYSTEMS

NANOSTRUCTURED PLATFORMS AS BIOMIMETIC MODELS

The goal of NanoPlatforms projects is to unravel the physical principles that govern interactions at the molecular level of several clinically relevant compounds with cell membranes using 2D and 3D biomimetic cell systems. The final goal is to improve the knowledge about the mechanism of action of already established drugs and to contribute to the development of new drugs.
Present research topics include the design and development of 2D and 3D biomimetic platforms for the study of:

- Biological and biophysical studies on antibiotic resistance in the context of biofilms.
- Antimicrobial and antibiofilm assessment of new compounds against relevant bacterial pathogens
- Cardiovascular and gastric toxicity related to the interaction between membrane lipids and conventional/recently developed NSAIDs;
- Synergistic effect of anticancer drugs and polyphenols on breast cancer;
- Development of skin mimetic models to evaluate drugs' skin permeation;
- Membrane-active peptides with improved selectivity toward bacterial cells;
- Pleiotropic action of natural compounds as a result of their interaction with different cell membrane lipids;
- Novel anticancer drugs activity potential assessment through biophysical studies;
- New methods and protocols based on biophysical techniques.



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RESEARCH THEMES/
BIOMIMETIC MODELS

MULTIFUNCTIONAL (BIO)SENSORS FOR MOLECULAR IMAGING, TARGETING AND DIAGNOSIS

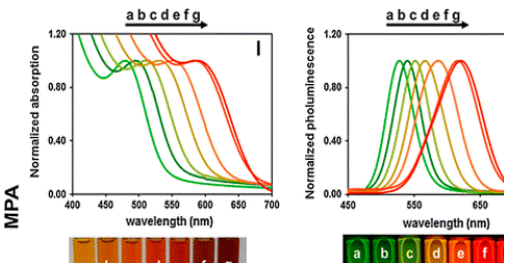
The NanoPlatform group seeks to provide a strong contribution to the development of distinct types of (bio)sensors and analytical devices that exploit the remarkable physical-chemical properties of different nanomaterials, including metallic nanoparticles, semiconductor, and graphene quantum dots, carbon nanotubes, polymeric nanoparticles, silica nanoparticles, nanogumbos, etc. This goal involves: (i) the development and optimisation of new microwave-assisted synthesis protocols that assured the production of large-scale high-quality nanomaterials, with respect to optical and chemical properties; (ii) the modification of the quantum dots (QDs) surface by means of functional groups or ligands to assure the establishment of interactions with the target analyte and, guarantee that these interactions result in dramatic changes of the referred properties, fostering their application in sensing schemes. In this field, we focus on:

- Rationally designed synthesis of bright core/shell ternary quantum dots with emission control.
- Implementation of portable sensors for mycotoxins monitoring in food products.
- Development of multiplexed sensing schemes combined with chemometric tools for improved data processing.
- Development of QDs/MIPs probes for biomarkers screening.

The group is also involved in the development of ultrasensitive low-cost substrates for surface-enhanced Raman spectroscopy (SERS) based on renewable materials and metal nanostars. This is being achieved by optimizing the optical properties with new strategies for the synthesis/deposition/bioconjugation methods of metal nanoparticles. New methods of synthesis of carbon dots (C-dots) from renewable sources has led to several applications, including the development of a low-cost biosensor for SARS-CoV-2 and the use of C-dots in photodynamic therapy.

Another research area is focused on: (i) the development of environment-responsive sensors to track the changes (wound temperature, secretions of exudate, or pH changes) in particular wounds, such as post-operative; (ii) the synthesis of new molecular probes for selected event signalling or analyte targeting based on luminescent detection techniques to develop a disposable sensor device for the screening of poisonous mushrooms.

Within this thematic, we highlight the nano2Prevent project, which aims to prevent SARS-CoV-2 transmission through the development of 3 solutions based on nanoparticles. Thus, this research focus: (i) virus inactivation in locus, namely in PPE and bed linens, upon nanosystems incorporation within the textiles; (ii) specific visual detection of the virus on surfaces, by pulverization; and, (iii) a combination of both solutions in a unique formulation for the simultaneous detection and inactivation of the virus, in medical facilities, enabling the elimination of the virus while identifying contamination outbreaks.



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RESEARCH THEMES/
(BIO)SENSORS AND ANALYTICAL AUTOMATION TOOLS

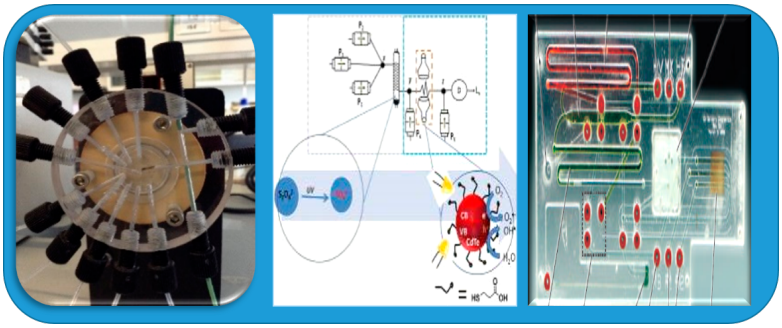
MULTIPURPOSE NANOPLATFORMS AS ENHANCED ANALYTICAL AUTOMATION TOOLS

The NanoPlatforms group has been successfully developing effective analytical tools, capable of responding to multiple desires, and fulfilling requirements such as low cost, easy and rapid operation, friendly use, disposability, and portability. The most promising (bio) sensors developed will be employed to create devices enabling higher selectivity and sensitivity and to develop array platforms for different (bio)assays with different types of nanomaterials such as nanoGUMBOS, multi-colored quantum dots.

Different pathways will be explored, such as bench-top automated systems or portable devices capable of onsite response, resorting to different technologies such as microfluidics, or paper-based platforms. The devices produced may become powerful tools for new challenging applications. As part of the ongoing research projects, NanoPlatforms group aims the development of multipurpose devices such as for clinical chemistry, food quality, and environmental monitoring. In this context, the development of generic tools, based on a battery of miniaturized (bio)assays, for rapid screening of biomarkers or the impact of chemicals on selected biomarkers in the early stage of their development, as a part of their sustainable synthesis.

Molecular and cellular tests are being used as a complement of whole cell organisms to clarify the impact of the (eco)toxicity of compounds, relating with particular structural elements and to guide their modification to reduce their hazardous potential.

So, these evaluations are carried out using enzymes with important biological functions and whole cell organisms (bacteria and yeasts) with advantages as simplicity of laboratory implementation and data interpretation as well as reduction of costs and duration of the assays.



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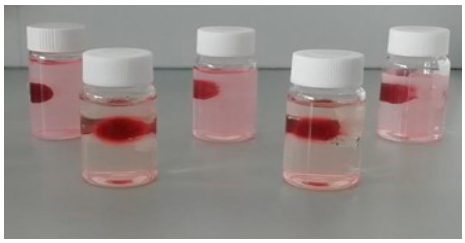
RESEARCH THEMES/
(BIO)SENSORS AND ANALYTICAL AUTOMATION TOOLS

FUNCTIONALIZED NANOPLATFORMS AS DELIVERY SYSTEMS FOR DIFFERENT APPLICATIONS

Research is focused on three main topics with application in the food, textile, and environmental applications:

1 - The biotechnological application of bioactive compounds in functional foods is proposed using a concerted nanotechnological/ agro-food approach to engineer nanoparticles that protect the compounds from degradation and improve their oral bioavailability. The design of novel nutraceutical nanoformulations using bioactive phytochemicals is under development. To achieve these purposes, it is planned the rational design, preparation, and modelling of different nanomaterials taking into account their future applications as nutraceutics. In this field, nanocarriers loaded with essential aminoacids such as lysine to be applied as supplementation in dairy cow nutrition, to improve the milk production, are under development.

2 –Within this thematic, we highlight the nano2Prevent project, which aims to prevent SARS-CoV-2 transmission through the development of 3 solutions based on nanoparticles. Thus, this research focus: (i) virus inactivation in locus, namely in PPE and bed linens, upon nanosystems incorporation within the textiles; (ii) specific visual detection of the virus on surfaces, by pulverization; and, (iii) a combination of both solutions in a unique formulation for the simultaneous detection and inactivation of the virus, in medical facilities, enabling the elimination of the virus while identifying contamination outbreaks.



3 - Microplastic pollution represents a major global environmental concern of the 21st century. In fact, plastic debris may have transboundary distribution and persistence in aquatic ecosystems. Microplastics present in the environment contain other toxic chemicals (e.g. metals) and may contain microorganisms including pathogenic ones, turning up to be their transport vectors, which in literature as an additional potential threat to biota and human health. Considering all this, it is utterly urgent to find new strategies to minimize the impact of microplastics and smaller debris in the nano-size range known as nanoplastics. A new approach, based in magnetic nanoparticles coated with a polymeric shell is being pursued, taking advantage of the magnetization of the metals adsorbed to microplastics surface and also the inherent properties of the coatings to remove microplastics from water.

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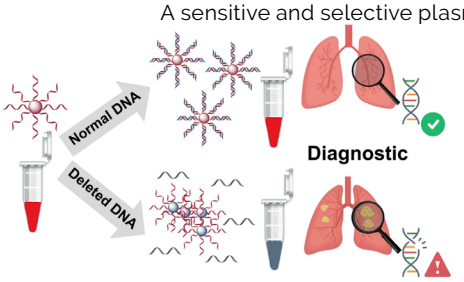
HIGHLIGHTS

GOLD NANOPROBES FOR DETECTION OF A CRUCIAL EGFR DELETION FOR EARLY DIAGNOSIS OF NON-SMALL-CELL

A sensitive and selective plasmonic nanosensor based on gold nanoprobes was developed for the detection of a clinically relevant EGFR deletion associated with non-small-cell lung cancer (NSCLC). The assay enables rapid, straightforward, and cost-effective identification of the mutation, offering strong potential for early diagnosis and improved patient stratification.



Gold Nanoprobes for Detection of a Crucial EGFR Deletion for Early Diagnosis of Non-Small-Cell Lung Cancer.

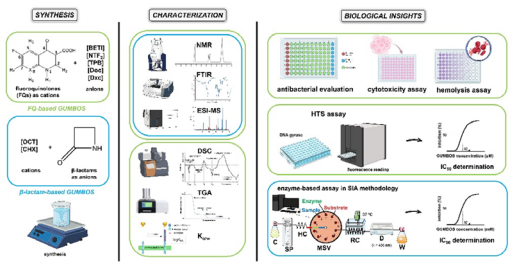
Biosensors 2024, 14, 162

TAILORING GUMBOS FOR ENHANCED ANTIBACTERIAL POTENCY: SYNTHESIS, CHARACTERIZATION AND BIOLOGICAL INSIGHTS

Novel GUMBOS (group of uniform materials of organic salts) were successful synthesized and evaluated as a potential novel therapeutic offer to advance antimicrobial strategies providing a transformative approach to combating AMR. With simple metathesis reactions we get strategic exchange of ionic counterparts between active pharmaceutical ingredients (APIs), including the fluoroquinolones (FQs) ciprofloxacin [Cip], lomefloxacin [Lom] and moxifloxacin [Mox] and the -lactams cefalotin [Cflt], cefoperazone [Cfpz], ceftriaxone [Cftx], oxacillin [Oxa] and cloxacillin [Clox] with distinct adjuvant ions.

Compared to percursors, hydrophobic GUMBOS, particularly those synthesized from non-polar anions such as [TPB] and [Doc] displayed bacterial growth inhibition, exhibiting enhanced membrane penetration capabilities. Conversely, hydrophilic GUMBOS with imide salts displayed aqueous compatibility, offering advantages for specific biological interactions. Cytotoxicity assessed on L929 fibroblast cells and in haemolysis studies, showed higher safety profile.

The antibacterial efficacy of FQ-based GUMBOS exhibited superior inhibitory effects on bacterial DNA gyrase. Notably, [Cip][Doc], [Lom][Dxc], and [Mox][NTF2] demonstrated exceptional potency, with IC50 values ranging from 0.076 to 0.204 µM. Beta-lactam-based GUMBOS effects on -lactamase was performed by an automatic system optimized for beta-lactamase activity, and the ones containing chlorhexidine [CHX] and octenidine [OCT], exhibited significantly improved inhibition. For instance, the most potent IC50 values achieved with each antiseptic were 6.39 mM for [OCT][Cflt] and 0.885 mM for [CHX][Oxa]. These findings underscore their potential to enhance the antibacterial performance of traditional antibiotics.



Exploring beta-lactamase inhibition through automatic analysis of beta-lactam-based organic salts (GUMBOS)

Journal of Molecular Liquids, 437, Part B, 1 (2025): 128478.

Novel fluoroquinolone-based organic salts: Pioneering solutions in targeting bacterial DNA gyrase

Journal of Molecular Liquids 417 (2025): 126654.

Ionic liquids and organic salts with antimicrobial activity as a strategy against resistant microorganisms".

Journal of Molecular Liquids 368 (2022): 120750.

HIGHLIGHTS

TASK SPECIFIC IONIC LIQUIDS-BASED MATERIALS TARGETING RELEVANT BIOMARKERS FOR DIAGNOSTIC AND THERAPY

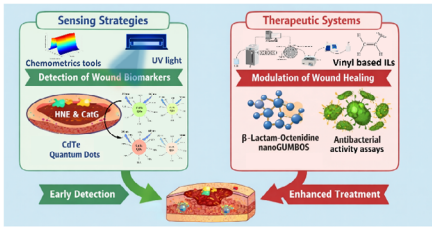
Chronic wound management can benefit from two complementary approaches: the development of sensing strategies for the early detection of relevant biomarkers and the design of therapeutic systems capable of modulating key biological processes that impair healing. In this context, advanced sensing platforms based on optical principles have been explored for the detection of biomarkers associated with inflammation and proteolytic activity. Fluorescence-based systems using CdTe quantum dots combined with chemometric analysis were investigated to enable the discrimination and quantification of important enzymes involved in wound inflammation, such as human neutrophil elastase and cathepsin G. In parallel, automated flow-based analytical methodologies were developed to evaluate the inhibition of cathepsin G by vinyl-based ionic liquids, providing efficient tools for the rapid screening of potential modulators of enzyme activity and enabling molecular insight into inhibitor–enzyme interactions through computational modeling. Complementary therapeutic strategies were also explored through the synthesis of novel -lactam–octenidine nanoGUMBOS, nanoscale antimicrobial systems that exhibited enhanced antibacterial activity and favorable cytocompatibility, highlighting their potential for controlling infections associated with chronic wounds. Together, these sensing and therapeutic approaches contribute to the development of integrated strategies for improved detection and treatment of processes involved in chronic wound progression.

Comparative analysis of electrochemical and optical sensors for detection of chronic wounds biomarkers: A review

Biosensors and Bioelectronics, 2024, 116095

Simultaneous detection of human neutrophil elastase and cathepsin G on a single substrate using a fluorometric quantum dots probe and chemometric models

Biosensors and Bioelectronics: X, 2025, 100571



GLIOBLASTOMA PERSONALIZED THERAPY BASED ON BIOINSPIRED NONLAMELLAR LYOTROPIC COLLOID NANOPARTICLES WITH TUMOR HOMING ABILITY (GLYNT)

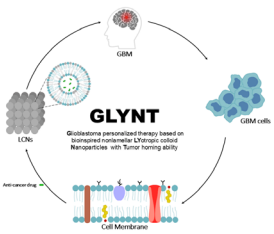
Glioblastoma Multiforme (GBM), a grade 4 brain tumor, is characterized by its aggressiveness and high malignancy [1,2]. Conventional treatments lack efficacy as evidenced by the unfavorable prognosis: a median survival time inferior to 15 months and a 5-year survival rate of less than 5% [2]. Nonlamellar lyotropic Lipid Liquid Crystalline Nanoparticles (LCNS), an emerging type of lipid nanoparticles, have shown distinctive properties, including high stability and complex internal structures [3]. In this study, biomimetic LCNs with tumor homing capabilities were developed for GBM therapy. Mitoxantrone (MITO) was selected as a model anticancer drug for proof-of-concept studies, and three formulations were prepared using the thin film hydration method: unloaded LCNs, MITO-loaded LCNs, and MITO-loaded biomimetic LCNs. All formulations exhibited adequate sizes for brain drug delivery with EE% exceeding 70% and remained stable for at least 3 weeks upon storage. Stability was also maintained in protein-rich biological media for 24 h. A sustained and controlled release of MITO from LCNs was achieved when compared to a drug solution. The LCNs were non-hemolytic and demonstrated high cytocompatibility in L929 fibroblast, bEnd.3 brain epithelial, and U251 glioblastoma cells. MITO-loaded LCNs exhibited dose-dependent anti-cancer activity in U251 cells, which was higher than free MITO. Biomimetic LCNs did not affect the permeation capacity across an in vitro BBB model and exhibited higher cellular internalization in U251 than in L929 cells, demonstrating the tumor homing ability of the developed nanoplatform. Overall, these findings suggest that the produced biomimetic LCNs are promising carriers for targeted GBM therapy.

Mitoxantrone-loaded lipid nanoparticles for breast cancer therapy–quality-by-design approach and efficacy assessment in 2D and 3D in vitro cancer models

Int J Pharmaceutics 2021, 121044

Gold nanostructures as mediators of hyperthermia therapies in breast cancer.

Biochemical Pharmacology, 2021, 114639



HIGHLIGHTS

BRIDGING SKIN AGING MODELS WITH NANOPARTICLE-BASED THERAPEUTICS

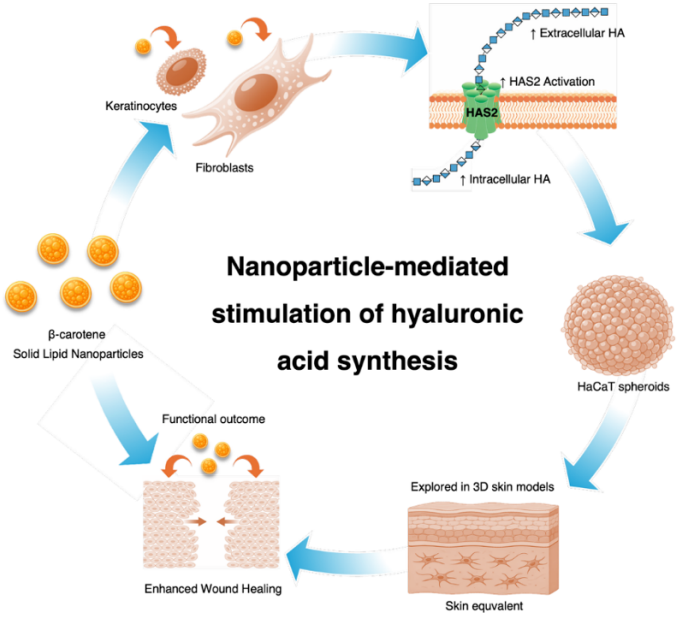
Our work focuses on connecting physiologically relevant skin ageing models with the development of nanotechnology-based therapeutic strategies. To do this, we use a stepwise experimental approach, starting from simple 2D cell cultures and progressing to 3D spheroids and full-thickness reconstructed skin models. This allows us to study ageing-related processes with increasing biological complexity while maintaining experimental control.

Within this framework, we explore solid lipid nanoparticles (SLNs) not just as delivery systems, but as bioactive platforms capable of influencing skin cell behaviour. Rather than relying on the external supply of active molecules, these systems are designed to stimulate intrinsic cellular pathways involved in skin regeneration, such as those related to hyaluronic acid production.

Our models address both intrinsic and extrinsic aspects of skin ageing. Chronological ageing is reproduced through senescence-inducing conditions, while environmental stressors, particularly UV exposure, are used to mimic extrinsic ageing. At the molecular level, we focus on key processes including oxidative stress, extracellular matrix remodelling, wound healing and cellular senescence.

By combining data across different model systems, we aim to minimise the limitations associated with individual models and improve the robustness of our findings. This integrated approach helps to bridge the gap between in vitro studies and more physiologically relevant conditions, strengthening the translational value of the work.

Overall, this research highlights how a deeper understanding of skin ageing biology can guide the design of more effective therapeutic strategies. In particular, it supports a shift towards regenerative approaches that activate endogenous pathways, moving beyond traditional formulations based on passive replacement.



Strategies to make human skin models based on cellular senescence for ageing research.

Ageing Research Reviews, Volume 100, 102430

HIGHLIGHTS

FROM OLIVE POMACE TO SKIN: DEVELOPMENT OF AN ECO-FRIENDLY ANTIOXIDANT NANOCOSMETIC

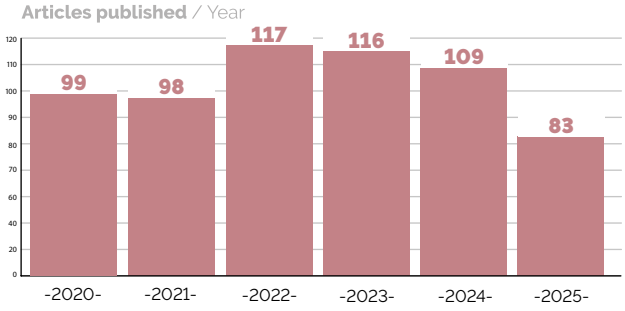
The extraction of olive oil is an activity almost as ancient as time. In the mediterranean countries, like Portugal, this has a marked social and economic value. Improved methods compared to the traditional pressing extraction have been developed over time, but all still have a by-product in common – Olive Pomace.

Olive pomace is rich in polyphenols which are associated with several beneficial effects on health, namely dermatological. Despite, the hydrophilic nature of these compounds is the reason they are not significantly co-extracted with the oils and the main obstacle to their direct application.

This is where nanotechnology comes in handy. Delivery systems, in the form of nanoparticles, are an approach widely studied, that allow to solve pharmacokinetic problems related to solubility and bioavailability. Revising the composition of Olive Pomace, there is a fraction of lipids left from the oil extraction that can be used to produce nanoparticles. With all this in mind, the objective of this project is the production of nanoparticles 100% made up of olive pomace extracts recurring to sustainable, eco-friendly nanotechnological approaches, in the perspective of obtaining an antioxidant nanoformulation for topical application..

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION



H-index: **57**

622 articles*
14102 citations

*01/2020-12/2025
From WOS core collection

FUNDED PROJECTS *(Representative projects)*

- **FOODSENS – Transferência de Tecnologias para reduzir riscos alimentares**
  FEDER, Sara Cunha (PI)

- **PortoBiocide – Avaliação e mitigação da presença de biocidas em águas urbanas: A cidade do Porto como caso de estudo**
  Funded by tPT2030 – Compete 2030 , José Fernandes (PI)

- **ESCAPE-TB – Eutectic Solutions for Controlled and Advanced Pulmonary Enhancement in Tuberculosis**
  Funded by tCOMPETE2030-FEDER and FCT / MCTES , Mafalda Sarraguça (PI),
  Total Funding: € 224,208.00

- **HONEY2KILL – Honey-exosomes to fight superbugs**
  Funded by the Portuguese Foundation for Science and Technology, Catarina Seabra (PI),
  Total Funding: € 49,999.46

- **FOODSENS – "Transferência de Tecnologias para reduzir riscos alimentares"**
  INTERREG POCTEP, 0591_FOODSENS_1_E,
  João Santos (participant),
  Total Funding: € 171,890.00

- **GLYNT – Glioblastoma personalized therapy based on bioinspired nonlamellar LYotropic colloid Nanoparticles with Tumor homing ability**
  Funded by the Portuguese Foundation for Science and Technology , Andrea Granja (PI),
  Total Funding: € 50,000.00

- **Unraveling the structure of innovative bio-based cubosomes (20250340257) – CELLS - ALBA Synchrotron**
  Funded by NEPHEWS, Cláudia Nunes (PI)

- **NanoProMilk – Nanostructured milk for the prevention of hypertension**
  Funded by the Portuguese Foundation for Science and Technology – Salette Reis (PI)
  Total Funding: € 249,972.87€

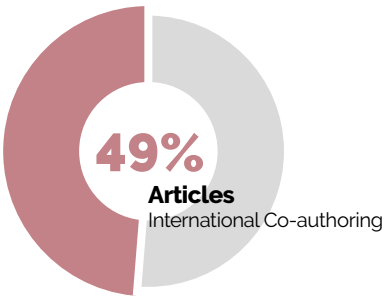
- **PANTHERMICELL – Micelas biomiméticas à base de vitamina E revestidas por membrana celular para nanoteranóstica multimodal do cancro do pâncreas**
  Funded by the Portuguese Foundation for Science and Technology – Ana Claudia Santos (Co-PI)

- **NANO4FILM: Uma abordagem nanotecnológica, seletiva e direcionada para evitar a remoção cirúrgica de implantes infectados com biofilmes**
  Funded by the Portuguese Foundation for Science and Technology – FCT (POCI-01-0145-FEDER-031444), Cláudia Nunes (PI)
  Total Funding: € 239.787,18

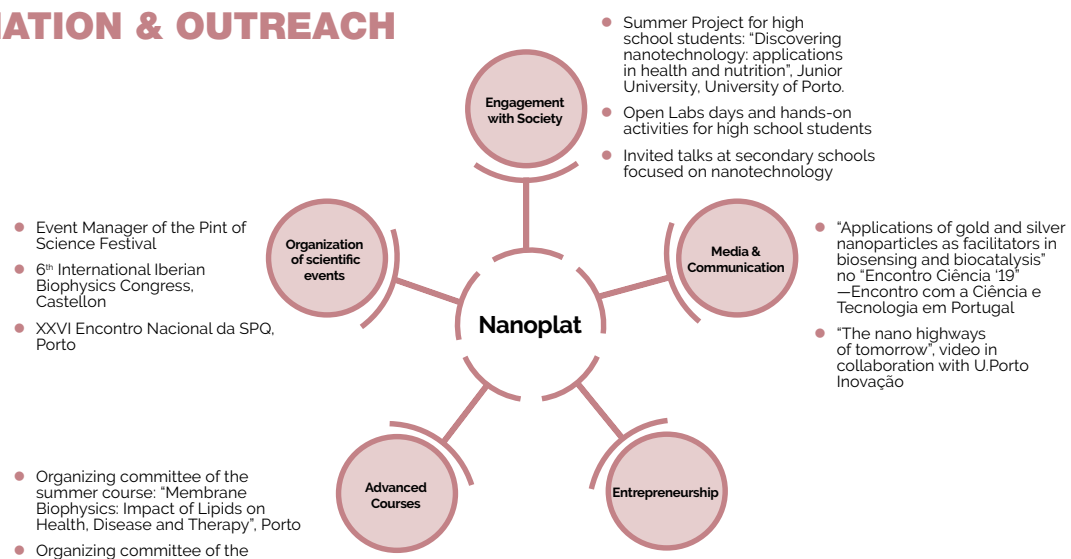
- **NanoBioGel - Natural product-based biomimetic-coated halloysite clay nanotubes hydrogel for cutaneous wound healing**
  Funded by the Portuguese Foundation for Science and Technology - FCT (2022.05270.PTDC), Ana Cláudia Santos, FFUC (PI)
  Total Funding: € 49,958.77

INTERNATIONAL COOPERATION AND NETWORKING

- COST Actions as member/group leader: CA18112; CA18224; CA21164; CA22107; CA21108; CA22103; CA26205; TD1402; CA18233
- Brillouin Light Scattering Microspectroscopy for Biological and Biomedical Research and Applications", 2017-2020 (Working Group Leader).
- I3-4-SEAWEED – Interregional innovation investments for the piloting, demonstration and scale-up of innovative seaweed/algae-based solutions and ecosystem building.



DISSEMINATION & OUTREACH



LABORATÓRIO ASSOCIADO
PARA A QUÍMICA VERDE

4FOOD

FOOD QUALITY AND TECHNOLOGY

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

Group Coordinator:

Victor Freitas

FOOD QUALITY AND TECHNOLOGY is an interdisciplinary group focused on analysis of food composition, development of food complements, novel foods and processing technologies, control of allergens, and advance of strategies for their mitigation, monitoring of genetically modified organisms (GMO), additives, chemical contaminants and adulterants promoting sustainable foods with enhanced safety health and sensorial properties. Food Supplements labelling compliance. Chromatographic and spectroscopic methods for evaluation of nutrients, bioactive compounds, contaminants and DNA-based methods for species identification and allergen/adulterants detection in plant and animal matrices are among the main skills of the Group. Other relevant areas of expertise are the improvement of dairy products, meat and fish quality by the development of animal feeding strategies; the optimization of food processing methods as well as novel methods based on high pressure and hyperbaric storage processes to enhance shelf life; test the activity of beneficial and harmful food compounds by using human cells and tissues in vitro; tailor-make the functionality of food macromolecules, prebiotics, and psicobiotics; and extraction of bioactive compounds from industrial by-products, agricultural and forestry wastes for food supplements and novel technological applications.

RESEARCH OBJECTIVES [2025-2029]

Main research objectives include:

Natural Ingredients, Bioactives, and Healthy Food Development

- Identify new sources of natural colorants with enhanced nutritional value, bioactivity, and safety.
- Clarify and control molecular interactions determining the stability and chromatic performance of anthocyanin based pigments in complex food matrices.
- Sustainably recover polyphenols and biopolymers to develop healthy, palatable foods, including processed products with improved bioactive composition.
- Explore agricultural biodiversity to identify neglected, highly bioactive plant varieties.
- Conduct comprehensive profiling of FODMAPs in Portuguese foods.
- Promote food innovation through enriched products, novel protein sources, and exploration of their functional and bioactive properties.
- Study polyphenol–metal chelation and apply polyphenols as functional and technological ingredients in clean label food formulations.
- Utilize industrial, agricultural, and forestry by products as stable natural colorants and novel material solutions.

Sustainability, Food Technology, and Resource Valorization

- Develop innovative technologies and processes to increase the production of sustainable and nutritionally superior foods.
- Investigate nano enabled strategies to enhance agricultural and forestry production efficiency while reducing the use of toxic pesticides.
- Valorize agri food and forestry residues as sources of functional compounds for new food matrices, textures, sensory properties, and extended shelf-life within circular economy frameworks.
- Advance sustainable food preservation methods, including active/intelligent packaging, hyperbaric storage, and light activated antimicrobial strategies.
- Develop food contact materials and active packaging incorporating natural preservatives and bioactives.
- Create smart labels using pH responsive dyes for real time monitoring of food spoilage.
- Develop efficient antioxidants to protect highly unstable food matrices and biological systems.

Food Safety, Authenticity, and Toxicological Assessment

- Assess consumption patterns and knowledge levels regarding food supplements among different population groups and evaluate labeling compliance with regulatory standards.
- Implement advanced analytical strategies for food quality, safety, and authenticity, including volatilomics, high throughput DNA based identification of adulterants, and species/varietal authentication.
- Evaluate contamination by natural toxins, environmental pollutants, agrochemicals, veterinary drugs, and processing derived contaminants, and develop mitigation strategies.
- Estimate nutrient, bioactive, and contaminant bioaccessibility and intestinal transport through in vitro models.
- Investigate emerging endocrine disruptors and study neurotoxic effects of low level dietary exposures using complex gut–brain models.
- Develop advanced in vitro and human cell based assays

OVERVIEW & OBJECTIVES

to evaluate biological effects of bioactive and toxic food compounds focusing on mechanisms related to developmental and lifestyle related disease prevention.

Advanced Models, Allergens, Microbiota, and Food Physiology

- Develop safer food products through allergenicity mitigation strategies and advanced analytical methods for trace allergen monitoring.
- Build advanced in vitro models to:
- predict taste responses and support development of more acceptable and health driven foods;
- assess digestibility, absorption, and transport mechanisms linked to protein allergenicity;
- simulate allergic reactions using basophil activation tests.
- Investigate polyphenols and polysaccharides as modulators of immune responses to food.
- Uncover structure–function relationships of carbohydrates to enhance traditional foods and support new functionalities.
- Establish links between food composition, microbiota modulation, and psychobiotic production.
- Use microbial bioconversion to generate next generation ingredients improving flavor complexity, functionality, and nutritional value in plant-based foods.
- Develop human microbiota inclusive in vitro models and multi omics approaches to study health effects of bioactive and toxic food compounds.

RESEARCH TEAM

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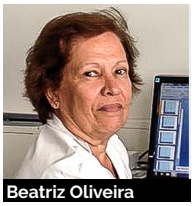
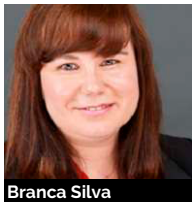

Beatriz Oliveira


Branca Silva

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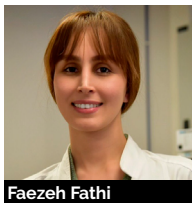
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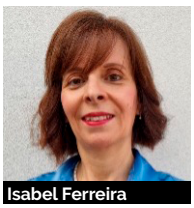
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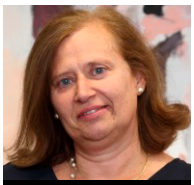
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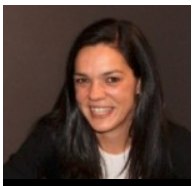
Marta Leite

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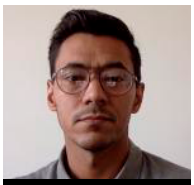
Nelson Andrade

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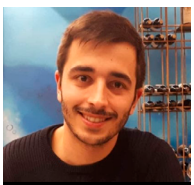
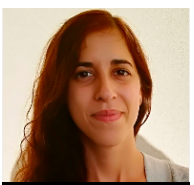

Pedro Fernandes


Rebeca Cruz

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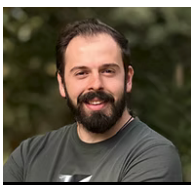

Rui Pereira

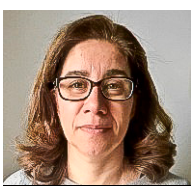
Sara Cunha

Sílvia Petronilho

Sílvia Rocha

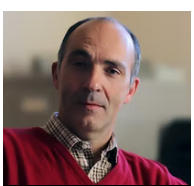
Sofia Duarte

Sónia Ferreira


Susana Casal

Susana Soares

Tânia Albuquerque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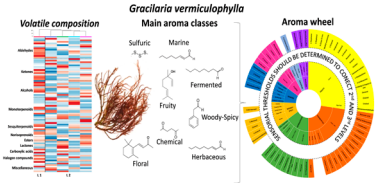
Sara Martins
Susana Machado
Tiago Costa

RESEARCH THEMES/
FOOD COMPOSITION, SENSORY PROPERTIES, AND FOOD AUTHENTICITY

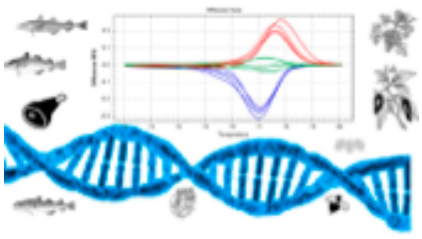
FOOD COMPOSITION, SENSORY PROPERTIES AND FOOD AUTHENTICITY



- Characterizing the chemical components of food to select new or enhanced plant varieties and assess general quality (e.g., coffee, beer, grapes, wine, olive oil, berries, and milk).
- Establishing the relationship between food composition and quality parameters, such as aroma, color, and flavor profile (including astringency and bitterness).
- Evaluating the nutritional composition and quality features of agricultural products and foodstuffs registered under EU quality schemes (PDO, PGI, and TSG).
- Assessing oxidative stability and predicting the shelf-life of various foodstuffs.
- Screening new compounds to modulate and improve overall food quality parameters.
- Sensory analysis and tracking consumer preferences to better understand market trends and consumer choices.

FOOD AUTHENTICATION AND FRAUD FIGHT

- Advanced methods to detect genetically modified organisms in foods;
- Authentication of foods from animal and plant origin based on specific molecular makers;
- New digital nanoplate-based methods for species specific quantitative authetication of foods;
- Identification of adulterants based on chemical and biochemical markers in food matrices: fish products and spices;
- Molecular characterization of agricultural species at the varietal level: hops and olives, grapes;
- DNA barcode markers coupled to High-Resolution Melting (HRM) analysis for species identification in foods, herbal medicines, and plant food supplements;
- Botanical and entomological authentication of honey.



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RESEARCH THEMES/
IMPROVEMENT OF ANIMAL FEEDING AND NUTRITION

- Evaluation of sustainable and alternative feed ingredients in animal nutrition and feeding;
- Valorization of agro-industrial co-products to enhance circular economy practices;
- Use of functional ingredients to modulate gut microbiota and promote immune function and overall health;
- Precision nutrition strategies to improve nutrient-use efficiency and animal welfare;
- Promotion of food security for a growing population through the production of healthier animal-derived foods;
- Improved understanding rumen function to improve ruminant nutrition and production;
- Identification of new biomarkers of rumen function in non-invasive biological samples (e.g., urine, feces, milk) to detect metabolic dysbiosis in dairy cows before clinical symptoms arise;
- Dietary modulation as an effective alternative to the use of antibiotics;
- Enhancement of livestock production sustainability by reducing greenhouse gas emissions and nitrogen excretion.

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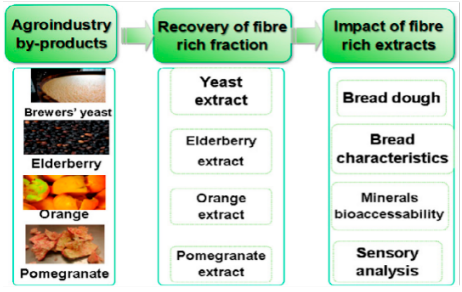
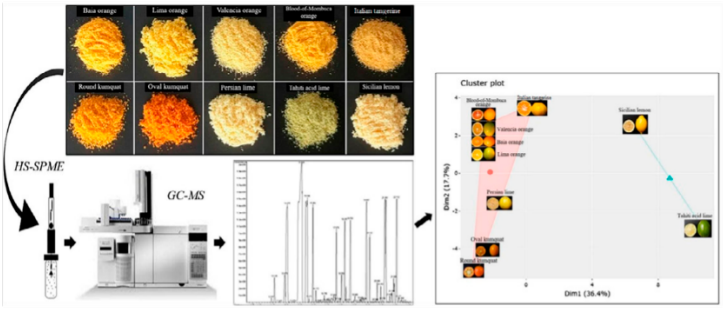
RESEARCH THEMES/
FOOD SUSTAINABILITY

- Valorization of compounds recycled from agro-industrial wastes (brewer's spent grain and spent yeast, fruit peels and pomace, vegetable parts, starch-rich rice and potato by-products, used fried oil, coffee silverskin and spent coffee grounds, olive pomace, eggshell, and canned fish wastes), thereby promoting the sustainability of industrial processes and adding value to the chain production of the industries by developing new and profitable ingredients;
- Development and application of green and sustainable methods of extraction and concentration of bioactive compounds from agrifood wastes;
- Development of rapid and eco-friendly methods for by-products discrimination and valorization;
- Optimization of the extraction of valuable compounds from plant cell walls, seaweeds, yeasts, and marine animals;
- Formulation of new appealing processed products, toward the improvement of preservation, prevention of lipid oxidation, or formation of harmful compounds throughout cooking;
- Chemical synthesis/transformation of new added-value compounds using molecules extracted from by-products.





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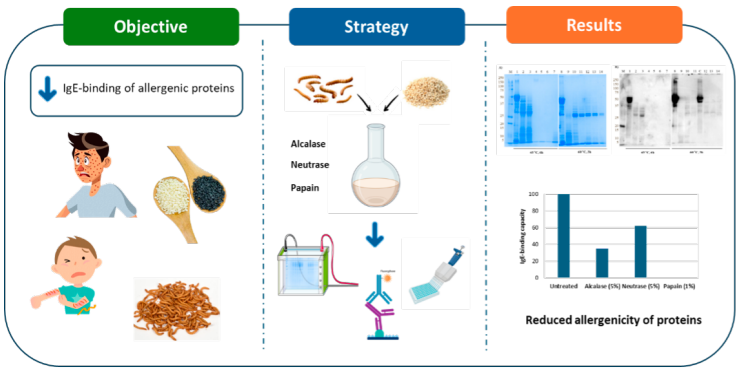
RESEARCH THEMES/ FOOD AND HEALTH

ALLERGENS, ADDITIVES, AND CONTAMINANTS

- Assessment of food allergens from plant and animal origin at trace levels by DNA markers and immunochemical approaches;
- Evaluation of the allergenicity of foods as affected by food processing and matrix; exploiting new strategies to reduce allergenicity;
- Assessment of the allergenicity of novel protein sources;
- Dietary exposure to food additives (sweeteners and dyes) and unhealthy food components (trans fatty acids, salt) from beverages and foodstuffs and daily intake estimation exposure;
- Assessment of the dissemination of a wide range of contaminants;
- Agrochemical residues (e.g. pesticides, antibiotics), heavy metals, and mycotoxins
- "emerging pollutants", such as flame retardants, disinfection by-products, pharmaceuticals, personal care products and biosolids as fertilizers;
- Packaging materials (e.g. bisphenols), micro and nano-plastics;
- Heat generated compounds (e.g. acrylamide, 4-methylimidazole, furans, heterocyclic aromatic amines) in foods or water;
- Assessing the impact of realistic food contaminants mixtures on human health
- Estimate contaminants bioaccessibility, intestinal transport and metabolization using in vitro using human cell models;
- Follow the fate of contaminants by in vitro assays and in the human body through biomonitoring of biological fluids;
- Estimation of human and environmental risk and search for mitigation strategies to decrease food and water contamination.



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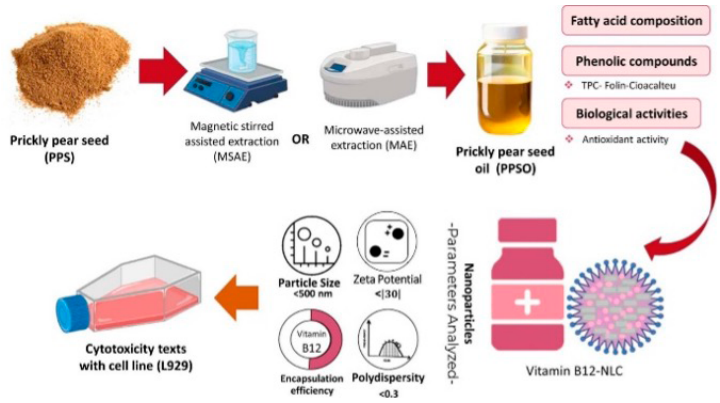
RESEARCH THEMES/ FOOD AND HEALTH

PROCESSING HEALTHIER, APPEALING, AND SAFER FOODS

- Optimization of traditional (grilling, barbecuing, baking, roasting) and advanced food processing methods (oven and osmotic dehydration, low-fat frying, microwave heating and high pressure based) or formulae that preserve food components, while reducing the formation of undesirable compounds;
- Exploiting the effect of novel processing technologies on the allergenicity of foods (e.g. milk and wine);
- Sustainable extraction of food ingredients and development of microencapsulation techniques to add bioactive components, extend food shelf-life, and control taste;
- Microbial fermentation at sub-lethal pressure levels for use in novel products production;
- Increasing food safety and shelf-life by hyperbaric preservation and modified atmosphere packaging;
- Developing more efficient antioxidants and improving the efficiency of the existing ones.



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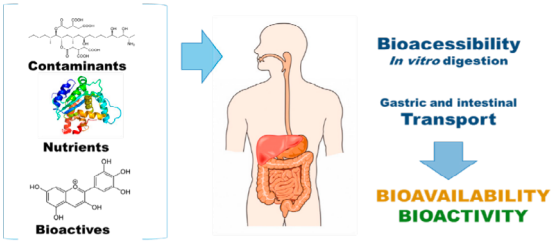
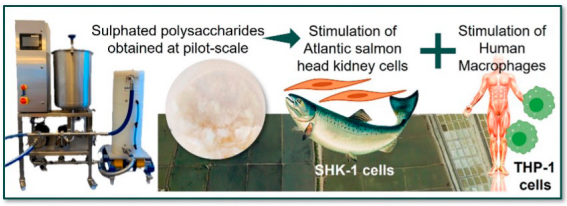
RESEARCH THEMES/ FOOD AND HEALTH

BIOAVAILABILITY AND FUNCTIONAL MECHANISMS

- Digestion, absorption, metabolism and activity of nutrients/ bioactive compounds assessed through in vitro methods using human cell lines and tissue models;
- Molecular, cellular, and functional mechanisms that underlie protective/therapeutic effects of nutrients and bioactive compounds against oxidative damage, hypertensive and vascular dysfunction, inflammation, angiogenesis, and cancer;
- Role of nutrition in the prevention of chronic diseases and overall health improvement (e.g. immunomodulatory and anti inflammatory activity; hypocholesterolemic ingredients);
- Bioactive properties of novel foods (e.g. insects);
- Find scientific evidence that supports or refutes the impact of harmful compounds vs bioactives;



- Understand the impact of new raw materials, such as algae and insects on human health;
- Impact of malnutrition on the pathophysiology mechanisms of fetal programming of hypertension;
- Impact of molecular interactions between polyphenols and macromolecules (proteins, polysaccharides, and cell membrane lipids) in health state or disease;



- Impact of gastrointestinal digestion on bioactive organosulfur compounds from Brassicaceae
- Impact of gastrointestinal digestion and transport mechanisms on protein allergenicity;
- Use of polyphenols as modulators of immune reactions to food (celiac disease and food allergies to egg, peanut, and milk;
- Study of the role of dietary polyphenols in protein digestibility, bioavailability, and further immunogenicity;
- Study of the prebiotic behavior of polyphenols. Gut microbiotapolyphenol interactions and health;
- Synthesis of bluish flavylium and pyranoflavylium compounds towards topical photodynamic therapy (PDT);
- Phenolic compounds as Natural Allies for Skin Health Maintenance and Protection.

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128 171. F.C.O Silva, et al., Carbohydr. Polym., 2025, 363, 123738. doi: 10.1016/j.carbpol.2025.123738

RESEARCH THEMES/ FOOD AND HEALTH

FOOD SUPPLEMENTS: FROM GALENIC DEVELOPMENT TO CONSUMPTION PATTERNS

- Design and functional optimisation of novel food supplement formulations;
- Implementation of advanced green extraction technologies and encapsulation systems to enhance the bioaccessibility and stability of food supplements;
- Assessment of food supplements labelling compliance and regulatory conformity, ensuring the accuracy of nutritional declarations such as health claims;
- Quality and Safety control of food supplements ingredients to detect undeclared pharmacological substances or contaminants;
- Epidemiological monitoring of food supplement consumption patterns and motivational drivers through validated instruments and population-based surveys;
- Evaluation of health literacy and clinical evidence-based knowledge among distinct cohorts, including healthcare professionals, to mitigate risks of food-drug interactions and promote safe supplementation;
- In vitro bioaccessibility and bioavailability studies using simulated gastrointestinal digestion models to predict the physiological impact of supplement ingestion.

SELECTED PUBLICATIONS

129 M.J. Campos, Nutrients, 2025, 17, 2802.
doi: 10.3390/nu17172802

130 M.J. Campos, Foods, 2025, 14, 84.
doi: 10.3390/foods14050884

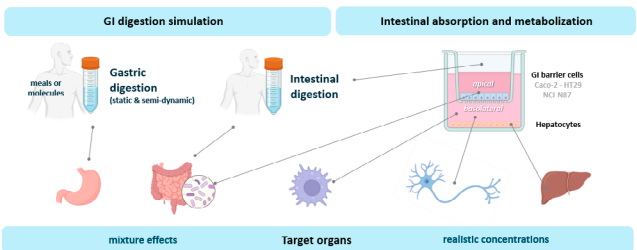
131 M. Di Martino, FAO, 2025.
doi: 10.4060/cd4280en

132 M. Lopes, Crit. Rev. Food Sci. Nutr., 2023, 19, 4106.
doi: 10.1080/10408398.2021.1997909

HIGHLIGHTS

OPTIMIZATION OF PHYSIOLOGICALLY RELEVANT MULTI-ORGAN HUMAN CELL-BASED MODELS TO EVALUATE THE IMPACT OF COMPLEX FOODS ON HEALTH

The optimization of physiologically relevant multi-organ in vitro cell-based assays to evaluate the impact of complex foods on human health is an important and rapidly evolving area in nutrition research and food toxicology. Assessing the health effects of a wide variety of food compounds — consumed as complex meals containing numerous active molecules—requires experimental systems that enable testing under physiomimetic conditions including mixtures effect evaluation.



Our research group has been actively developing and optimizing integrated experimental platforms that combine simulated gastrointestinal digestion to generate bioaccessible fractions, in vitro gastric and intestinal transport models to determine bioavailability, and the evaluation of biological activity—both beneficial and deleterious—in relevant target organs modeled using cultured human cell lines. This integrated approach allows for a more comprehensive and physiologically relevant assessment of food-derived compounds impact on health.

Assessing the differential responses in normal and inflamed in vitro intestinal models exposed to food contaminants complex mixtures.

Food Research International 2025, 205, 115907

A comprehensive study on the digestion, absorption, and metabolization of tropane alkaloids in human cell models.

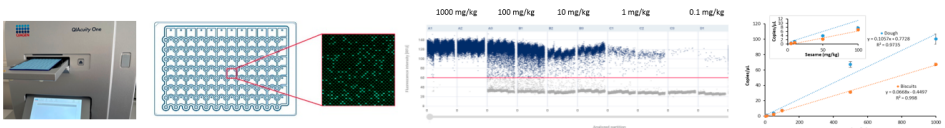
Journal of Hazardous Materials 2024, 480, 136192

In Vitro Digestion and Intestinal Absorption of Mycotoxins Due to Exposure from Breakfast Cereals: Implications for Children's Health.

Toxins 2024, 16 (5), 205

NANOPLATE DIGITAL PCR: A PROMISING STRATEGY FOR MONITORING FOOD ALLERGENS IN COMPLEX FOOD MATRICES

Digital PCR represents the third and most recent generation of PCR technology. Its defining feature is the partitioning of a reaction mixture into thousands of individual compartments, within which amplification occurs independently. Microfluidic nanoplate digital PCR (ndPCR) uses fixed partitions embedded in a nanoplate, enabling a more reproducible determination of positive versus negative partitions compared with earlier droplet-based digital PCR systems. This architecture simplifies workflow and reduces analysis time while maintaining high quantitative accuracy. The successful transfer of real-time PCR to ndPCR was first demonstrated for the quantification of food allergens, using sesame as case study. Sensitivity was 10-fold decreased in ndPCR, with assay performance remaining unaffected by food processing and matrix. ndPCR showed high potential for the detection of food allergens at trace levels, offering high robustness and reliable quantification across complex food matrices.



First nanoplate digital PCR method to trace allergenic foods: improved sensitivity for the detection of sesame.

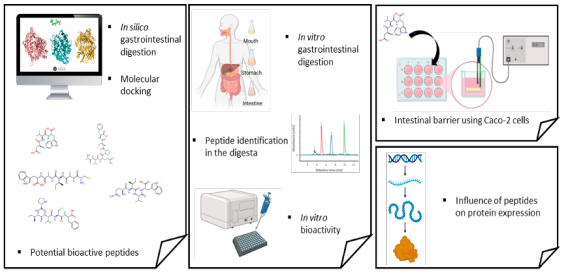
Food Chemistry, 2024, 444, 138650

HIGHLIGHTS

IDENTIFICATION AND CHARACTERIZATION OF BIOACTIVE PEPTIDES DERIVED FROM NOVEL FOOD SOURCES

Climate change and global population growth are increasing the demand for sustainable alternative protein sources. Edible insects are promising candidates due to their high nutritional value and environmental sustainability. Besides supplying essential amino acids, protein digestion can release small bioactive peptides (2–20 amino acids) with potential health benefits, including antihypertensive activity through inhibition of the somatic angiotensin-converting enzyme (sACE).

In silico gastrointestinal digestion of insect proteins, followed by the evaluation of enzyme-peptide interactions using molecular docking, allowed the identification of peptides with potential sACE-inhibitory activity. LC-MS/MS analysis confirmed the presence of these peptides in insect digesta, and enzymatic assays demonstrated sACE inhibition by both the peptides and the digesta. The peptides were further evaluated in Caco-2 cells to assess intestinal absorption, cytotoxicity, barrier integrity, and modulation of gene expression markers related to diabetes and hypertension. Two peptides downregulated sodium-glucose cotransporter 1 (SGLT1)) expression suggesting potential antidiabetic effects through reduced glucose absorption. Overall, the results highlight the potential of edible insects as multifunctional ingredients for promoting cardiometabolic health..



Exploiting Locusta migratoria as a source of bioactive peptides with anti-fibrosis properties using an in silico approach.

Food & Function 2024, 22;15(2):493-502

An in silico approach to unveil peptides from Acheta domesticus with potential bioactivity against hypertension, diabetes, cardiac and pulmonary fibrosis

Food Research International, 2023, 169, 112847

Uncovering the potential somatic angiotensin-converting enzyme (sACE) inhibitory capacity of peptides from Acheta domesticus: Insights from in vitro gastrointestinal digestion.

Foods, 2024, 13, 3462

GREEN DEEP EUTECTIC SOLVENTS FOR SUSTAINABLE DETECTION OF EMERGING CONTAMINANTS IN FOOD

The team develops innovative analytical methods to detect emerging contaminants in food samples. Their work emphasizes green chemistry principles, particularly using deep eutectic solvents (DESs) as sustainable alternatives to traditional organic solvents. They design advanced microextraction techniques to enhance sensitivity and selectivity, applying them to compounds such as endocrine-disrupting chemicals, pesticides, and polycyclic musks in complex matrices (e.g., food products). A key strength is integrating sample preparation strategies like QuEChERS, membrane-based extraction, and DLLME. The researchers employ experimental design and optimization tools to improve performance, coupling methods with GC-MS for accurate identification and quantification.

Green Approaches for Preparation of Natural Deep Eutectic Solvents for Determination of As, Cd, and Pb in Plant Samples by ICP-MS.

ACS Omega 2025 10 (24), 26118-26128

Deep eutectic solvents for microextraction of endocrine disruptor contaminants from water and food: Review.

Trends in Analytical Chemistry, 171, 2024, 117495

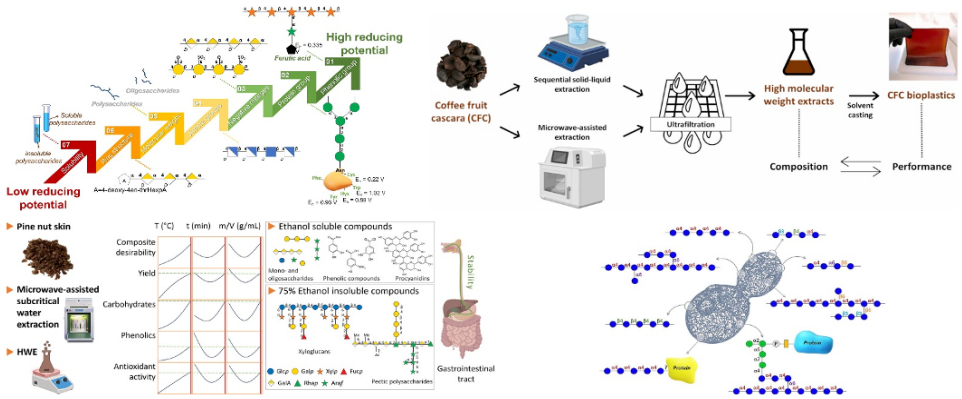
Determination of pesticide residues in soybeans using QuEChERS followed by deep eutectic solvent-based DLLME preconcentration prior to gas chromatography-mass spectrometry analysis.

Journal of Chromatography A, 1727, 2024, 464999

HIGHLIGHTS

VALUATION OF FOOD BY-PRODUCTS TARGETING POLYSACCHARIDES AND THEIR PROPERTIES

Over the last years, polysaccharides have been linked to antioxidant effects using both in vitro chemical and biological models. Polysaccharides' antioxidant action is highly dependent on their solubility, sugar ring structure, molecular weight, occurrence of positive or negatively charged groups, protein moieties and covalently linked phenolic compounds.
Targeting an organic solvent-free approach, pectic polysaccharides were recovered from coffee fruit cascara (CFC) by microwave-assisted extraction (MAE) and purified by ultrafiltration. This was a fast and organic solvent-free methodology to obtain pectic polysaccharides with film-forming ability suitable for developing bioplastics for application as active food packaging.



Pine nut skin (PNS) can be extracted subcritical (SWE) and hot water (HWE) extraction, producing extracts rich in soluble fiber and phenolic compounds. The oligo- and polysaccharides structures proved to be stable during the gastrointestinal digestion process, being able to reach the colon intact, where they can be selectively metabolized by healthy gut microbiota, promoting a prebiotic effect on the host.
Yeast cell walls undergo modifications during the brewing process, leading to a remodeling of their architecture. One significant change is the increased insolubility of the cell wall glycogen pool, likely due to the formation of covalent bonds between glycogen and cell wall polysaccharides. The combination of multiple enzymatic approaches and NMR methods shed light into the role of yeast cell wall glycogen as a structural core covalently linked to other cell wall components during the brewing process, allowing their application in mayonnaise formulations.

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The antioxidant activity of polysaccharides: A structure-function relationship overview.
Carbohydrate Polymers, 2023, 314, 120965

Antioxidant and flexible bioplastics based on microwave-assisted extracted coffee fruit cascara pectic polysaccharides.
Journal of Cleaner Production, 2024, 453, 142264

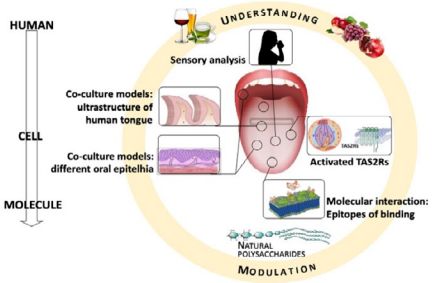
Structural role of yeast cell wall glycogen upon brewing revealed by enzymatic approaches and advanced NMR.
Carbohydrate Polymers, 2024, 324, 121475

Industrial byproduct pine nut skin factorial design optimization for production of subcritical water extracts rich in pectic polysaccharides, xyloglucans, and phenolic compounds by microwave extraction.
Carbohydrate Polymer Technologies and Applications, 2024, 7, 100508

HIGHLIGHTS

PLANT-BASED BIOACTIVE COMPOUNDS IN TASTE AND MOUTHFEEL PROPERTIES: LINKING HEALTHY AND FLAVOURFUL COMPOUNDS

Plant-based foods promote health, especially when rich in polyphenols, yet these compounds can induce astringency and bitterness that curb intake. New models combining salivary proteins, oral mucosal pellicle, oral cells, bitter receptors and oral microbiota are being developed to probe the onset of these tastes directly in food matrices, including oral microbiota-driven effects. This knowledge unravels mechanisms and enables screening of food/byproduct extracts to identify natural or biotechnological modulators (e.g., polysaccharides, microorganisms) that enhance acceptance. A key goal is to decipher inter-individual traits that drive personal perception and to progress toward precision nutrition and tailored flavour experiences. This research line adopts an integrative and comprehensive approach spanning sensory evaluation, cell-based assays, and molecular analyses.



Development of a New Cell-Based Oral Model To Study the Interaction of Oral Constituents with Food Polyphenols

Journal of Agricultural and Food Chemistry 2019, 67, 12833-12843

Development of a cell-based quaternary system to unveil the effect of pectic polysaccharides on oral astringency.

Carbohydrates Polymers, 2024, 323, 121378

A look upon the adsorption of different astringent agents to oral models: Understanding the contribution of alternative mechanisms in astringency

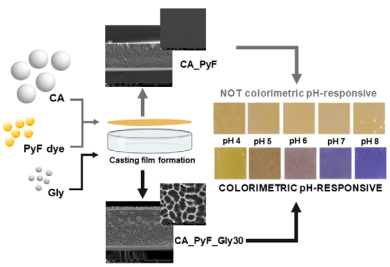
Food Chemistry 2024, 448,139153

Deciphering the potential of orange peel polysaccharides for modulating black tea astringency

Food Hydrocolloids, 2026, 174, 112428

DEVELOPMENT OF PH-RESPONSIVE SENSORS FOR FOOD INTELLIGENT PACKAGING

A pyranoflavylium salt was incorporated into cellulose acetate-based films to build up a colorimetric pH-indicator as a smart label for monitoring food freshness. The chromatic responsive properties of the films were tested in solutions at different pH values (pH 4 to 8) and in the headspace of biogenic amines and ammonia-containing solutions at different concentrations. The results showed that the films without glycerol are not color-responsive to different pH values. On the other hand, the incorporation of glycerol above 20% (w/w) demonstrated effective pH responsiveness after 20 min of immersion and after exposition to an amine-rich environment. The glycerol-containing films showed relevant and remarkable color change at the pH range of food spoilage indicating a great potential for application as a food freshness indicator. The label's performance was evaluated using real samples (fish and meat) at controlled conditions (3 ˚C and modified atmosphere packaging). The label demonstrated high efficacy in detecting spoilage of Atlantic horse mackerel (Trachurus trachurus). After 5 days of storage, freshness parameters exceeded the limit defined by EU regulations, indicating that the fish was unfit for consumption. Simultaneously, the yellow label started to turn purple, effectively indicating the beginning of the spoilage process. Regarding pigment migration and photostability, the label showed to be suitable for application in fresh meat and fish packaging



Pyranoflavylium-cellulose acetate films and the glycerol effect towards the development of pH-freshness smart label for food packaging

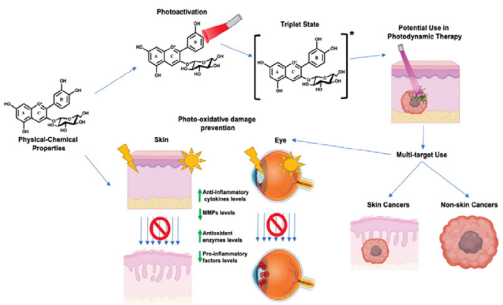
Food Hydrocolloids, 2022, 127, 107501

FoodSmarTag: An innovative dynamic labeling system based on pyranoflavylium-based colorimetric films for real-time monitoring of food freshness.

Food Hydrocolloids, 2023, 143, 108914

HIGHLIGHTS

ANTHOCYANINS AS PHOTOPROTECTIVES AGENTS IN DIFFERENT BIOLOGICAL SYSTEMS

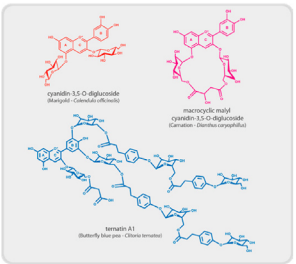


Due to their physical and chemical characteristics, anthocyanins are amongst the most versatile groups of natural compounds. Such unique signature makes these compounds a focus in several dierent areas of research. Anthocyanins have well been reported as bioactive compounds in a myriad of health disorders such as cardiovascular diseases, cancer, and obesity, among others, due to their anti inflammatory, antioxidant, anti-diabetic, anti-bacterial, and anti proliferative capacities.
Such a vast number of action mechanisms may be also due to the number of structurally dierent anthocyanins plus their related derivatives. We focus the efforts to develop recent advances on the potential use of anthocyanins in biological systems with particular focus on their photoprotective properties. Topics such as skin aging and eye degenerative diseases, highly influenced by light and the action of anthocyanins against such damages are the main research approaches as well as Photodynamic Therapy and the potential role of anthocyanins as novel photosensitizers.

Exploring the Applications of the Photoprotective Properties of Anthocyanins in Biological Systems.
International Journal of Molecular Sciences, 2020, 21, 7464

Photoactivated cell-killing amino-based flavylium compounds.
Scientific Reports, 2021, 11, 22005

EDIBLE FLOWERS AS AN EMERGING DIETARY SOURCE OF BIOACTIVE COMPOUNDS



Anthocyanins have become a key group of natural compounds during the last years due to their broad applications in different areas. From a nutritional and health perspective, these compounds have been showing potential roles against different pathologies. The excellent aroma, taste and appearance of anthocyanin-rich edible flowers turns meals more appealing to consumers. Moreover, their nutritional profile, bioactive properties, and health benefits, encourages the development of functional foods with nutraceutical purposes, thus promoting the consumption of these type of edible flowers worldwide
Further knowledge in food processing methods is a key factor on the comeback and the addition of anthocyanin-rich edible flowers to our dietary habits. In our recent developments we assessed the bioaccessibility of the bioactives of different edible flowers rich in anthocyanins, their absorption behaviour at the gastrointestinal level, their incorporation into food products, and their bioactivity, showing that understanding how these compounds behave under different food processing and digestion conditions is crucial to evaluate their potential as food sources.

Viola Tricolor L. *Centaurea cyanus* *Cosmos bipinnatus* *Clitoria ternatea*

Anthocyanin-rich edible flowers, current understanding of a potential new trend in dietary patterns.
Trends in Food Science & Technology, 2023, 138, 708-725.

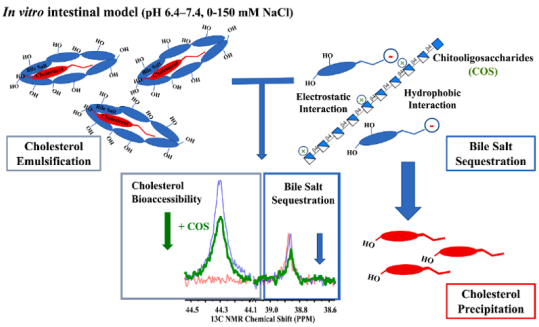
Phytochemical composition, antioxidant activity, and sensory evaluation of edible flower-enriched vinegars.
Food Chemistry, 2025, 496 (Part 3), 146897.

Anthocyanin-rich edible flowers – Impact of food matrix on anthocyanin stability, digestion and absorption: the case of wild pansy, cosmos and cornflower.
Food Chemistry, 2026 (Part B), 148137.

HIGHLIGHTS

FROM EXTRACTION TO FUNCTION: DECODING THE STRUCTURE-BIOACTIVITY RELATIONSHIP OF POLYSACCHARIDES

While polysaccharides are linked to various health advantages, the relationship between their structure and biological function is not yet fully understood. Current research emphasizes the precise extraction and characterization of compounds like chitosan, fucoidans, arabinogalactans, within others, to better define their roles. Establishing these structures is essential for validating their effects as dietary fibers, prebiotics, immunostimulatory and cholesterol-lowering agents.



Contribution of non-ionic interactions on bile salt sequestration by chitooligosaccharides: Potential hypocholesterolemic activity.
Journal of Colloid and Interface Science, 2023, 646, 775

Seaweed polysaccharides and their potential health effects via gut microbiota modulation.
Carbohydrate Polymers, 2026, 373, 124621.

In vitro human colonic fermentation of coffee arabinogalactan and melanoidin-rich fractions.
International Journal of Biological Macromolecules, 2024, 275, 133740

MOLECULAR-LEVEL INSIGHTS INTO THE CHEMISTRY AND BIOCHEMISTRY BEHIND THE PREVENTIVE POTENTIAL OF FOOD BIOACTIVES AGAINST ADVERSE FOOD REACTIONS TO WHEAT, MILK, EGG AND PEANUT PROTEINS

Across the globe, bioactive-functionalized foods are nowadays a remarkably growing market. As the COVID-19 pandemic fades, people are becoming more serious about decreasing the health risks connected to unhealthy eating, and more likely to adopt mindful or intuitive eating, paying more attention to what they consume and how it makes them feel protected against chronic disease conditions. Despite this major advance in people's consciousness, there is one big issue that cannot be disregarded when conceiving novel functional food products i.e. the rapid spread of food allergies and food intolerances to wheat, milk, egg and peanut proteins which, although as not life-threatening as other non-communicable diseases, can be as distressing as those. This poses, of course, a major drawback in functional food development, not eased by the still lack of knowledge regarding the biological significance and mechanisms of action of natural bioactives in these disease conditions. For this reasons our research has been focused on: (1) proteomic and metabolomic profiling of immunoreactive food antigens and bioactive-induced changes in their gastrointestinal processing; (2) development of top-notch NMR-based approaches and disruptive cell model technologies focused on understanding the structural, dynamic and biochemical implications of food bioactives within biological relevant systems; (3) metabolic-level insights into the immunomodulatory role of polyphenol compounds and their effect on gut microbiota ecology and function.

Recent advances on dietary polyphenol's potential roles in Celiac Disease.
Trends in Food Science & Technology, 2020

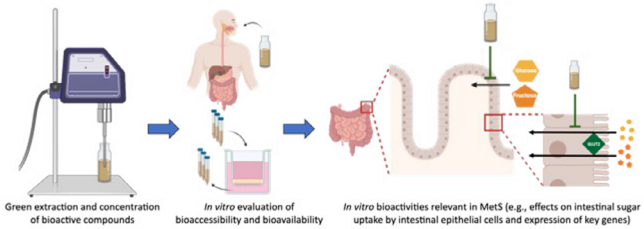
Unravelling the immunomodulatory role of apple phenolic rich extracts on human THP-1-derived macrophages using multiplatform metabolomics.
Food Research International, 2022, 155, 111037

New-Level Insights into the Effects of Grape Seed Polyphenols on the Intestinal Processing and Transport of a Celiac Disease Immunodominant Peptide.
Journal of Agricultural and Food Chemistry, 69(45), 2021, 13474-13486

HIGHLIGHTS

VALORIZATION OF COFFEE AND ITS BY-PRODUCTS: THE APPROACH FOR METABOLIC SYNDROME PREVENTION

Olive pomace is the major by-product generated in olive oil processing, being a source of added-value bioactive compounds with recognized benefits for human health. Our research has been focused on olive pomace valorization, by (i) exploiting its chemical composition and beneficial health properties; (ii) developing green processes to increase the recovery of olive pomace bioactive compounds; (iii) applying green methods to evaluate olive pomace authenticity; and (iii) developing olive pomace-based functional ingredients for innovative food products (e.g. olive oil-based spread functionalized with olive pomace extracts, enriched-pasta, toppings…), thus, addressing key-challenges as food security and environmental sustainability.



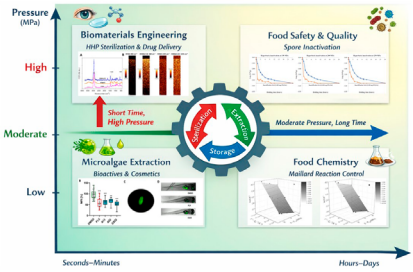
Can coffee silverskin be a useful tool to fight metabolic syndrome?
Frontiers in Nutrition, 2022, 9:966734.

Green/Roasted Coffee and Silverskin Extracts Inhibit Sugar Absorption by Human Intestinal Epithelial (Caco-2) Cells by Decreasing GLUT2 Gene Expression.
Foods, 2022, 11, 3902.

Decoding coffee cardiometabolic potential: Chemical composition, nutritional, and health relationships.
Comprehensive Reviews Food Science Food Safety, 2024, 13, 13414.

ENGINEERING WITH HIGH PRESSURE: APPLICATIONS ACROSS FOOD, BIOMATERIALS, AND MICROALGAL SYSTEMS, FOR MICROBIAL INACTIVATION, CONTROL MAILLARD REACTIONS, MOLECULAR COMPLEXATION, AND BIOACTIVES EXTRACTION

High hydrostatic pressure is a versatile engineering variable capable of modulating biological, chemical, and physicochemical processes across food, biomaterials, and microalgal systems. By finetuning pressure, time and temperature combinations, different technological objectives can be achieved within a unified processing concept. In food systems, hyperbaric storage at room temperature or below, promotes the inactivation of heat-resistant Alicyclobacillus acidoterrestris spores (described by nonlinear inactivation models) and simultaneously reduces the rate of Maillard reaction development (described through combined Arrhenius–Eyring kinetic modelling). These findings demonstrate that pressure can enhance microbial safety while preserving chemical quality. In biomaterials engineering, short high-pressure sterilization treatments improve cyclodextrin–drug molecular complexation within hydrogel eye contact lenses, increasing triamcinolone acetonide loading capacity and enabling controlled release without compromising optical or mechanical properties that are usually lost during traditional sterilization. In microalgal systems, nonthermal high-pressure extraction allows the recovery of proteins, pigments, and phenolic compounds, while bioactivity screening identifies functional metabolites, such as unsaturated fatty acids and nucleosides, capable of modulating appetite in zebrafish models. Together, these studies position high pressure as a multidisciplinary process engineering parameter for sustainable innovation in microbial control, reaction management, material functionality, and cold bioactive compounds extraction.



Hyperbaric inactivation at 150–250 MPa of Alicyclobacillus acidoterrestris spores at room temperature and effect of innovative technologies pre-treatments.
Innovative Food Science and Emerging Technologies, 2024, 98, 103861.

Improved triamcinolone acetonide-eluting contact lenses based on cyclodextrins and high hydrostatic pressure assisted complexation.
Foods, 2022, 11, 3902.

Microalgae extracts reduce appetite in zebrafish larvae linked to long-chain fatty acids and 5-methylthioadenosine.
Algal Research, 2025, 88, 104003.

HIGHLIGHTS

HUMAN BIOMONITORING STUDIES

Currently, it is known that there is continuous and increasing exposure to these chemical contaminants, which can accumulate in the human body, with lifelong consequences related to the increase of non-chronic transmissible diseases. Human biomonitoring provides an important scientific basis for human exposure to risk assessment, with the primary objective of protecting public health. There is still limited information on human exposure to mycotoxins and pesticides. The main objective of these biomonitoring studies was to assess exposure and risk to these contaminants, particularly in more vulnerable populations (pregnant women, infants, and children).

Mycotoxins Exposure in Cabinda, Angola—A Pilot Biomonitoring Survey of Breastmilk.

Toxins, 2022, 14, 204

Urine biomonitoring of glyphosate in children: Exposure and risk assessment.

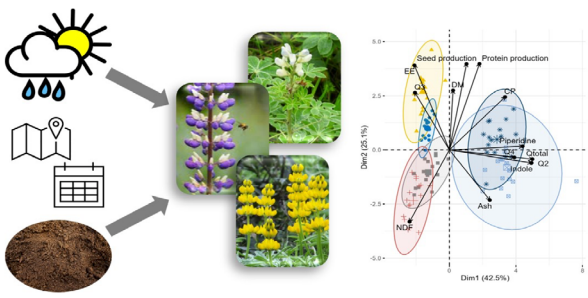
Environmental Research, 2021, 198, 111294

Ochratoxin A and Portuguese children: Urine biomonitoring, intake estimation and risk assessment.

Food and Chemical Toxicology, 2020, 135, 110883

LUPINS AS A VALUABLE PROTEIN SOURCE IN CLIMATE CHANGE SCENARIO: PROSPECTS ON NUTRITIONAL, ANTINUTRITIONAL, AND AGRONOMIC TRAITS

Lupins (Lupinus spp.) are plants with high nutritional, agronomic and environmental importance worldwide. Their reduced cost of production and high adaptability to different climate and soil conditions attract producers and consumers worldwide. Besides, the cultivation of lupin is of utmost importance for agricultural sustainable practices as being responsible for the improvement of the soil quality, namely through the fixation of atmospheric nitrogen. White lupin (L. albus L.), narrow-leafed lupin (L. angustifolius L.), and yellow lupin (L. luteus L.) species studied in our research have a wide range of adaptations to support adverse edaphoclimatic conditions, such as soil acidity, nutrient-poor soils and water deficit. The high protein content in lupin seeds is considered valuable for their use as food and feed, but their consumption may present risks due to the presence of alkaloids with toxic effects. Although lupins are best studied for their seeds for human consumption, the potential value of their co-products cannot be despised. Our research focused on an integrative study of productivity, nutritional factors and alkaloids content of seeds and the main co-products (straws, and pod shells) of the production of white, narrow-leafed and yellow cultivars adapted to the Mediterranean region climate. The production of seeds, nutritional traits, and alkaloid content showed a high variability among species and with edaphoclimatic conditions. The high protein content and low alkaloid content of some cultivars showed their suitability for both human and animal consumption, while co-products showed high-potential for ruminants feeding.



Insights from the yield, protein production, and detailed alkaloid composition of white (Lupinus albus), narrow-leafed (Lupinus angustifolius), and yellow (Lupinus luteus) lupin cultivars in the Mediterranean region.

Frontiers in Plant Science, 2023, 14, 1231777.

Agronomic, Nutritional Traits, and Alkaloids of Lupinus albus, Lupinus angustifolius and Lupinus luteus Genotypes: Effect of Sowing Dates and Locations.

ACS Agricultural Science & Technology, 2024, 4, 450.

Environmental conditions affect the nutritive value and alkaloid profiles of Lupinus forage: Opportunities and threats for sustainable ruminant systems.

Heliyon, 2024, 10, e28790.

HIGHLIGHTS

MICROENCAPSULATION FOR FUNCTIONAL FOOD INGREDIENTS

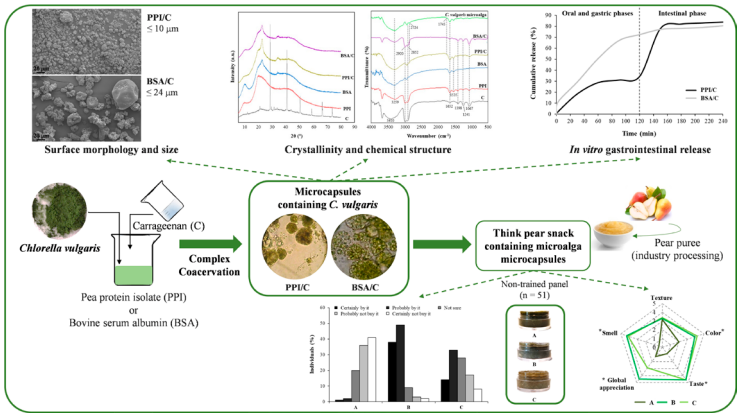
Microencapsulation has become a key strategy to stabilize sensitive bioactive compounds and enable their incorporation into food matrices. Through the formation of protective microstructures, often based on protein–polysaccharide interactions, encapsulation improves oxidative stability, masks undesirable flavors, enhances dispersibility, and may contribute for controlled release during processing, storage, and/or digestion. In line with this, complex coacervation offers high encapsulation efficiency and is well suited for hydrophobic or volatile compounds protection. Chlorella vulgaris was successfully microencapsulated by complex coacervation and incorporated into pear snacks as a feasible functional ingredient. The coacervate system improved the sensory acceptability of the snacks by masking the characteristic off-flavors and color of this green microalga, while preserving its nutritional and bioactive potential. The work demonstrated that tailored wall materials and process conditions can reconcile technological performance (encapsulation efficiency, stability) with consumer-oriented attributes in real food applications. Citrus limon essential oil was microencapsulated by complex coacervation to stabilize its highly volatile compounds and to modulate their release. The microcapsules showed high encapsulation efficiency and provided protection against volatiles loss and oxidation, relevant to food processing and consumption. This approach highlights how coacervation-based systems can be engineered to fine-tune aroma delivery and shelf-life in citrus-flavored foods.

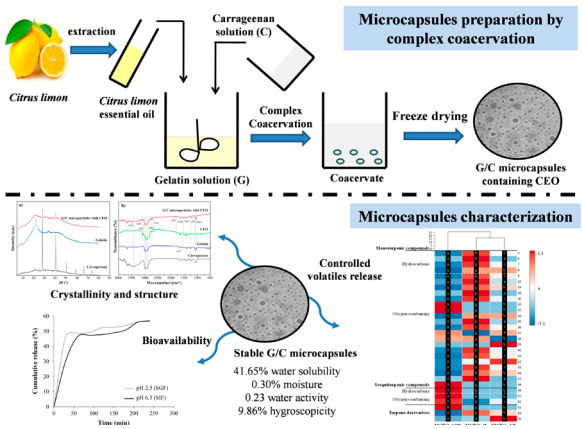
Microencapsulation of a green microalga (Chlorella vulgaris) by complex coacervation for its valuation as a feasible ingredient in pear snacks

Algal Research, 2024, 83, 103727.

Microencapsulation of Citrus limon essential oil by complex coacervation and release behavior of terpenic and derived volatile compounds.

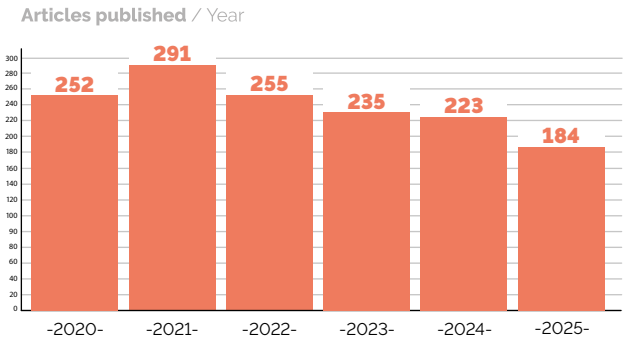
Food Hydrocolloids, 2024, 152, 109830.





GROUP IN NUMBERS

SCIENTIFIC PRODUCTION



H-index: **71**

1440 articles*
40031 citations

*01/2020-12/2025
From WOS core collection

FUNDED PROJECTS *(Representative projects)*

- **US2Coffee - Cápsulas de cafeína**
  POCI/01/0247/FEDER/033351, Beatriz Oliveira (PI).
  Total funding: € 773,806.14
- **IBERPHENOL - Research cooperative within the scope of polyphenols and its industrial applications**
  377_IBERPHENOL_6_E, European Fund for Regional Development – INTERREG Spain-Portugal, Nuno Mateus (PI).
  Total funding: € 208,592.97
- **NanoProMilk - Leite nanoestruturado para a prevenção da hipertensão**
  PTDC/BAA-AGR/4923/2021. Salette Reis (PI).
  Total funding: € 249,972.87
- **RoastPro - Modelação do perfil aromático do café através da torra: melhoramento de cafés de baixa qualidade e excelência para cafés de elevada qualidade**
  FEDER (COMPETE 2030) and FCT/MECI, operation n. 14972, reference COMPETE2030-FEDER-00859000. João Rodrigo Santos (PI).
  Total funding: € 249,480.00
- **DIETxPOSOME - Explore the impact of DIETary-eXPOSOME on chronic inflammation assessed through in vitro assays and mathematical modelling**
  PTDC/SAU-NUT/6061/2020, Isabel Ferreira,
  Total funding: 249.625,27 €
- **AlgaValor – Microalgas: produção integrada e valorização da biomassa e das suas diversas aplicações** POCI-01-0247-FEDER-035234
  Total funding: 10.481.791,21 €
- **COBY4HEALTH - Can coffee by-products decrease the risk of metabolic syndrome? A comprehensive approach to reduce waste and valorize health benefits.**
  PTDC/SAU-NUT/2165/2021. Rita Alves (PI).
  Total funding: € 242,048.70
- **Food4DIAB - Valorisation of fruit by-products as multifunctional food ingredients and functional foods for diabetics**
  EXPL/BAA-AGR/1382/2021, Tânia Albuquerque (PI).
  Total funding: € 49,850.56
- **AnthoE.Flos - Anthocyanin-Rich Edible Flowers: towards an emerging, more sustainable and healthier diet.**
  2022.01014.PTDC, Hélder Oliveira (PI).
  Total funding: € 50,000.00
- **FERMEN.TO: FERmented foods to struggle MEtabolic syNdrome. An inTegrated in vitro dynamic apprOach**
  2023.00164.RESTART. Iva Fernandes (PI), Total Funding - 50000€,
- **FLORA.MED - Exploring the Therapeutic Potential of Edible Flowers Rich in Anthocyanins in Metabolic Disease.**
  2023.11612.PEX. Hélder Oliveira (PI).
  Total funding: € 50,000.00
- **WHEATBIOME - Research and Innovation Action**
  HORIZON-CL6-2022-FARM2FORK-01, Susana Soares (PI).
  Total funding: € 5,060,547.50€
- **BeTASTy - New molecular and cell-based approaches to assess Food Astringency and Bitterness**
  European Research Council Starting Grant
  101040462, Susana Soares (PI).
  Total funding: € 1,500,000.00
- **SALIVA+ Novel tools for exposure assessment of food contaminants by saliva multiple biomarker monitoring**
  2022.08978.PTDC, Isabel Ferreira (PI)
  Total funding: € 249 721.32
- **Hypoallergen – Improving strategies to unveil, predict and modulate/mitigate the allergenicity of foods towards the development of new HYPOALLERGENic formulations**
  PTDC/BAA-AGR/4005/2021, Isabel Mafra (PI)
  Total funding: € 249 977,00
- **CleanH2O - Sustainable support liquid membranes based on deep eutectic solvents for the removal of contaminants of emerging concern from WWTPs effluents and surface waters**
  2022.03009.PTDC.
  Total funding: € 49 824,00
- **PORTOBIOCIDE - Assessment and mitigation of biocides in urban waters: Porto city as a case study**
  (COMPETE2030-FEDER-00835600, 2023.17544.ICDT. José Fernandes (PI)
  Total funding: € 249,955.20
- **ALLEVIATE - Strategies to mitigate the ALLErgenic potential of novel food ingredients: inVestIgAting the poTEntialities of (bio)chemical treatments**
  2023.12193.PEX. Caterina Villa (PI).
  Total funding: € 49,905.71
- **IMMUNOGATE - IMMUNOmodulation of allergenic Gut barrier to exploit the interactions of food processing, digestibility, Absorption, and Transport phEnomena towards protein allergenicity mitigation**
  COMPETE2030-FEDER-00848700. Joana Costa (PI).
  Total funding: € 248,529.60

GROUP IN NUMBERS

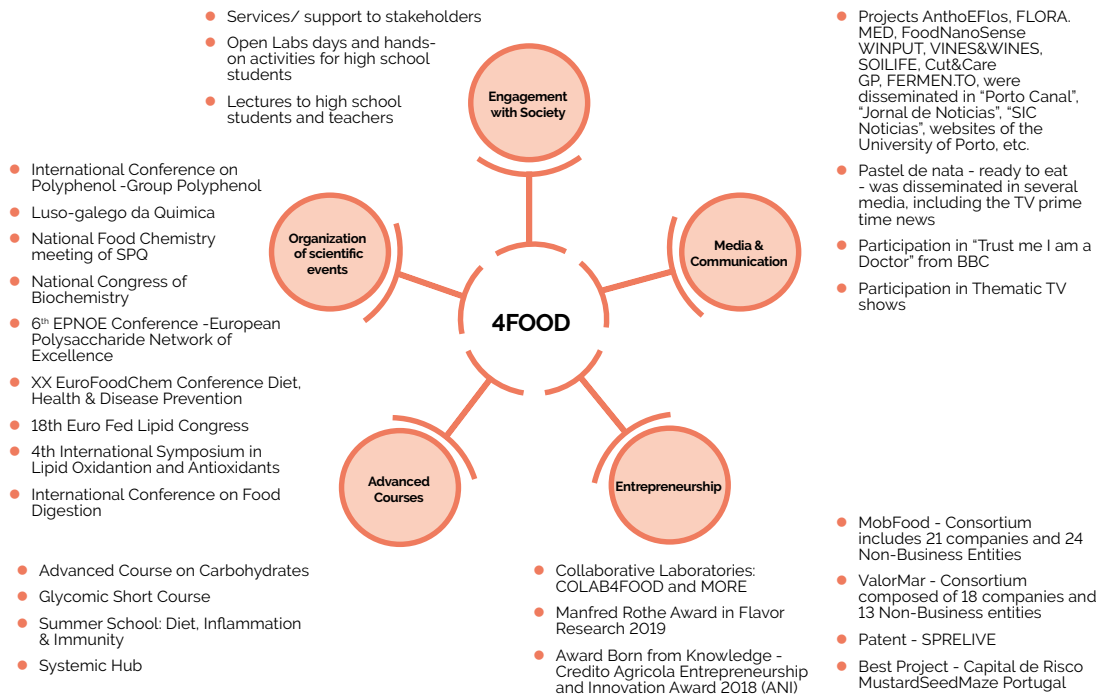
FUNDED PROJECTS *(continuation)*

- GENESIS - GENESIS-next-GEN biosEnsing: tailoring preciSion ImmunotherapieS for LTP allergies
  2024.17022.PEX. Joana Costa (PI)
  Total funding: € 59,964.51
- INSPIRE-Insects - Insects for Future: Sustainable Protein and Innovative Food Sources
  2024.14868.PEX. Carla Silvia Teixeira (PI)
  Total funding: € 59,993.38
- FODMAPS - Food Optimization for Dietary Management and Advanced Product Solutions
  COMPETE2030-FEDER-00901300, Susana Casal (PI).
  Total funding: € 249,739.20
- neuroNAMix - New Approach Methodologies for Assessing Neurodegeneration Risk from Food Contaminant Mixtures
  COMPETE2030-FEDER-00714200. Miguel Faria (PI)
  Total funding: € 230,515.20
- 3Rs - Regenerar, Reformular e Reinventar: culturas esquecidas para alimentos saudáveis e sustentáveis
  PD24-00012
  Total funding: € 107.470.00
- Waste2Taste - Sustainable approaches for transforming Agri-Food Waste into Flavourful Experiences
  COMPETE2030-FEDER-00914400, Elsa Brandão (PI)
  Total funding: € 246 110,40
- Food System of The Future (IDfoods) .
  Victor Freitas (PI).
  Total Funding: € 9.776.196,990
- Cut&Care GP - Green graphene-based antimicrobials for the control of phytopathogenic agents in Quercus suber L.
  COMPETE2030-FEDER-00799900, Raquel Nunes da Silva (PI)
  Total funding: € 233 582,40.
- MoodFood - Desenvolvimento de produtos alimentares enriquecidos em fibras como promotores de psicobióticos para a saúde cerebral.
  COMPETE2030-FEDER-00744200,MPr-2023-12, Elisabete Coelho (PI)
  Total funding: € 199,324.80
- StarchMod4BioPlas: Desvendando materiais à base de amido tolerantes à água rumo a uma indústria de plásticos circular descarbonizada
  COMPETE2030-FEDER-00764300,MPr-2023-12. Silvia Petronilho (PI)
  Total funding: € 212 278,32,
- BySweetTech- Development of sweet-tasting oligosaccharides with sugar-reducing potential in foods.
  COMPETE2030-FEDER-00840600, MPr-2023-12. Pedro Fernandes, (PI)
  Total funding: € 184 701,60.
- ProAqua+: Desenvolvimento de materiais multifuncionais para biofiltros em aquacultura: estabelecendo novos padrões de qualidade e sustentabilidade
  CENTRO2030-FEDER-02594500, Manuel A. Coimbra (co-PI)
  Total funding: €791,857.26
- PrOSFig: Dried fruits as a source of Prebiotic Oligosaccharides and Soluble dietary fiber: The case study of fig.
  HORIZON-TMA-MSCA-PF-EF - HORIZON TMA MSCA, Ramla Khiari (PI)
  Total funding: € 156 778,56
- AD4PurePort - Nova Gama de Vinhos do Porto, com base num inovador método de seleção de aguardentes vínicas.
  POCI-01-0247-FEDER-039956
  Total funding: € 908 114,25
- Cristal Eco Premium - Desenvolvimento de linha de vidro cristal sustentável (Sustainable crystal glass line development)
  POCI-01-0247-FEDER-047101
  Total Funding: € 2.184.428,72
- Espumante de Portugal, L.A. 9.5
  PRR-C05-i03-I-000194.
  Total funding: € 934.365,46
- PORTOBIOCIDE - Assessment and mitigation of biocides in urban waters: Porto city as a case study
  (COMPETE2030-FEDER-00835600, 2023.17544.ICDT. José Fernandes (PI)
  Total funding: € 249,955.20
- HoneySafe
  COMPETE2030-FEDER-00812000, Andreia Freiras (PI).
  Total funding: € 235 763,20

INTERNATIONAL COOPERATION AND NETWORKING

- INFOGEST - international network gathers more than 380 research scientists from 40 countries.
- COST Actions (Participant/Member): CA18227, CA18127, CA18111, CA20128, CA21149, CA17103, CA19124, CA18229, CA22134, CA24111, CA18125, CA24145
- COST Actions (Coordinator):
  CA18101, "SOURDOMICS - SOURDOugh biotechnology network towards novel, healthier and sustainable food and bloproCesseS", 2019-2023
  COST Action CA22161, "Flavoursome: Future of plant-based food: Bridging the gap of new proteins and Flavoursome", 2023-2027
- BIOFOODPACK – Biocomposite Packaging for Active Preservation of Food (M-ERA-NET2/0021/2016). The Consortium has 7 partners from University and Industry (Portugal, Cyprus and Poland), 2017-2020
- SYSTEMIC – Knowledge hub on Nutrition and Food Security (systemic-hub.eu)
- OENOVITI international network: >55 partners worldwide: academics, R&D and industrial partners
- HORIZON-CL6-2022-FARM2FORK-01 WHEATBIOME, Unraveling the potentialof the wheat microbiomefor the development of healthier, more sustainable and resilient wheat-derived food and feed products.
- Red CYTED AlProSos - Red de Alimentos ricos en Proteínas regionales Sostenibles (125RT0165), 2025-2028. Network of 47 research groups from 11 iberoamerican countries.

DISSEMINATION & OUTREACH



LABORATÓRIO ASSOCIADO
PARA A QUÍMICA VERDE

Computing

HIGH PERFORMANCE COMPUTING IN MOLECULAR MODELLING

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

Group Coordinator:

Pedro Fernandes

The High Performance Computing in Molecular Modelling uses advanced supercomputing resources to simulate chemical and biochemical systems of great interest with atomic and sub-atomic detail. These systems include proteins, enzymes, DNA, RNA, biological membranes, small biomolecules such as medicinal drugs, and novel functional materials, typically in aqueous physiological or application-relevant environments. We aim to understand how their physicochemical properties can be fine-tuned for specific applications, including the interaction of materials, such as nanotubes and graphene, with biomolecules.

We study reaction mechanisms in heterogeneous and homogeneous catalysis, involving enzymes and novel catalytic materials. Our work also addresses the formation and properties of nanostructured materials (NSMs), including molecularly imprinted and grafted polymers, carbon-based materials, deep eutectic solvents (DESs), ionic liquids (ILs), and self-assembled monolayers. These studies provide insights for applications in catalysis, sensors, drug-delivery systems, and biomedical devices. We also develop quantitative structure-activity relationship (QSAR) models to assess biological activity and potential toxicity.

Protein structure, protein-protein interactions, and structure-based drug discovery are also central to our research. Our simulations and modelling approaches are mostly grounded in classical and quantum mechanics (QM), allowing us to simulate, understand, and predict the behaviour of (bio) chemical systems with accuracy and reliability. The methods most frequently used include classical molecular dynamics (MD), hybrid quantum mechanics/molecular mechanics (QM/MM), electronic structure calculations, molecular docking, virtual screening, homology modelling, and computer-aided drug design. In addition, we increasingly integrate machine learning (ML) into molecular modelling workflows. These approaches include neural-network-based molecular descriptors and encoding schemes, models for predicting physicochemical properties, biological activity, toxicity, spectra, photoreactivity, and molecular origin, as well as tools to support drug discovery, drug repurposing, and the design of greener compounds and technologies.

RESEARCH OBJECTIVES [2025-2029]

One of the main objectives of the High Performance Computing in Molecular Modelling is to understand the chemical machinery of living systems. Within this vast chemical universe, our major goals are: (i) to understand the reaction mechanisms of important enzymes with atomic detail; (ii) to engineer enzymes for biotechnology processes, such as crude oil refining, biofuel production and plastic recycling; (iii) to understand and predict small-molecule diffusion across cell membranes, increasing the success rate of drug delivery; (iv) to discover small-molecule inhibitors for unmet clinical needs, including competitive inhibitors of therapeutic enzymes and covalent inhibitors against major snake-venom toxins, while also exploring the repurposing of venom components for therapeutic applications; and (v) to construct supramolecular biosystems coupling engineered enzymes to new-material solid surfaces, as greener and more efficient alternatives to industrial catalysts.

Our group also focuses on the rational design of advanced functional materials within the green chemistry paradigm. These materials are optimised for high performance during application and easy degradability at later stages of their life cycle, enabling a broader life cycle assessment. For this purpose, macromolecular systems are modelled using complementary approaches. Density Functional Theory (DFT) is used to study catalytic reaction mechanisms, while molecular simulations provide crucial information on the structural organisation and dynamics of complex systems at the microscopic level. These studies contribute to the design of effective solutions for frontier fields and to the identification of waste products formed during the life cycle of materials. In parallel, QSAR and ML models are used to assess the potential ecotoxicity of original materials and degradation products. We will also further integrate DFT, molecular dynamics and ML approaches into workflows addressing stereochemical assignment, selective nutrient capture by molecularly imprinted polymers, natural product characterisation, drug discovery and drug repurposing. Time-dependent DFT calculations will also support the elucidation of phototoxicity mechanisms, while curated datasets and AI-assisted strategies will help explore new small-molecule therapeutics, including compounds targeting immuno-oncology and glyco-immune checkpoints.

RESEARCH TEAM

SENIOR RESEARCHERS

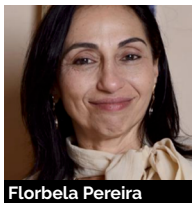
Alexandre Magalhães

Ana Rita Silva

André Melo

António Ribeiro

Carla Teixeira

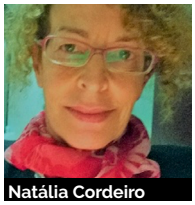

Florbela Pereira

Iulia Voroshylova

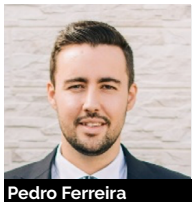
João Aires de Sousa

João Coimbra

Maria João Ramos


Natália Cordeiro

Pedro Fernandes


Pedro Ferreira

Pedro Paiva

Rui Neves

Sérgio Sousa

OTHER DOCTORATE RESEARCHERS

Alexandre Pinto
Amit Halder
Elisabete Ferreira
João Sousa
José Caetano
Natércia Brás
Nuno Cerqueira

PhD STUDENTS

Airam Silva
Ana Almeida
Duangnapa Kiriwan
Edgar Santos
Fábio Martins
Joana Silva
João Boazinha
Johander Azuaje
Jorge Oliveira
Juliana Amorim
Luís Teixeira
Mariana Sousa
Nádia Figueiredo
Patrícia Sobral
Rodolfo Caeiro
Samah Nassir
Sofia Sousa

RESEARCH GRANTEES

Inês Quintelas
Raúl Dias

 Group coordinator

RESEARCH THEMES/

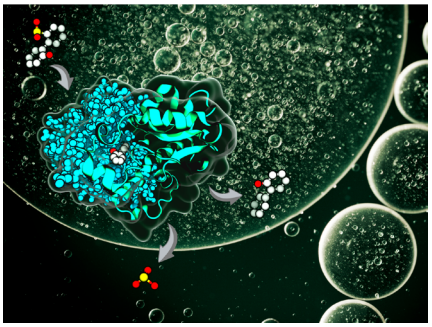
COMPUTATIONAL ENZYME DESIGN FOR SUSTAINABLE CATALYSIS: PLASTIC RECYCLING AND MITIGATION OF POLLUTANT EMISSIONS

Our computational biochemistry group develops integrated methodologies to engineer enzymes for **environmental sustainability**. By combining hybrid quantum mechanics/molecular mechanics (QM/MM) calculations and molecular dynamics (MD) simulations, we are focused on mapping enzyme catalysis with atomistic and thermodynamic resolution, enabling **rational design of biocatalysts** addressing pressing industrial challenges.

We currently integrate the **En'Zync** (Center for Enzymatic Deconstruction of Thermoset Plastics for a sustainable society) consortium, in the search for novel enzymes targeting polyurethane, polyester, and epoxy matrices jointly with experimental partners. This initiative aligns with our major research on the investigation of enzyme-polymer binding modes and **enzyme-based degradation of PET and thermoset plastics**.

Our research also addresses the exploration of the **bacterial sulphur metabolism** to address sulphur pollution downstream and upstream. Downstream, we characterized bacterial pathways for **crude oil desulphurization**, supporting cleaner oil refining. Upstream, we are assessing the efficiency and thermostability of H_2S-oxidases and SO_2-reductases in extremophilic bacteria to capture sulphur pollutants and retrieve sulphur, a feedstock for agricultural and energy sectors.

We also develop pipelines for **mutation strategy optimization** by evaluating electrostatic contributions to catalysis, and software to **automate mechanistic analysis** by systematically exploring reaction pathways, calculating structures and free energies of reactants, transition states, and intermediates. With these, we aim for more efficient and systematic approaches to support studies of enzyme evolution and inform enzyme design efforts."



The enzyme DszB, shown at the centre, is a key component of the '4S pathway' in Rhodococcus erythropolis, a metabolic route that removes recalcitrant organosulphur compounds from crude oil. The bacterium resides in microscopic water droplets within the oil, capturing pollutants at the water-oil interface. While traditional desulphurization relies on polluting chemical methods, our computational group utilizes this natural system as a template. Through QM/MM simulations and rational design, we aim to engineer DszB and the broader pathway to accelerate sulphur removal, offering a greener alternative to prevent acid rain.

Our **bioinformatics tools and databases** unify mechanistic insights across projects, creating predictive models for enzyme evolution and design. By bridging computation with experimental validation, we transform computational predictions into scalable biotechnological solutions for circular economy applications.

SELECTED PUBLICATIONS

1 A. J. M. Ribeiro, et al., J. Chem. Phys. 2025, 163, 134102. **doi: 10.1063/5.0288283**

2 A. J. M. Ribeiro, et al., FEBS J. 2025, 292, 4200-4210. **doi: 10.1111/febs.70106**

3 L. M. C. Teixeira, et al., ACS Catal. 2025, 15, 17, 14728-14740. **doi: 10.1021/acscatal.5c03228**

4 L. M. C. Teixeira, et al., ACS Catal. 2025, 15, 11, 9171-9180. **doi: 10.1021/acscatal.5c01146**

5 Z. Li, et al., Adv. Sci. 2025, 12, 2416019. **doi: 10.1002/advs.202416019**

6 L. Rotilio, Angew. Chem. Int. Ed. 2025, 64, e202419535. **doi: 10.1002/anie.202419535**

7 S. Das, et al., ACS Catal. 2025, 15, 11, 9785-9792. **doi: 10.1021/acscatal.5c02431**

8 P. Paiva, et al., Chem. Sci. 2025, 16, 2437-2452. **doi: 10.1039/D4SC06688J**

9 P. Paiva, et al., Phys. Chem. Chem. Phys. 2025, 27, 2139-2150. **doi: 10.1039/D4CP03488K**

10 P. Ferreira, et al., J. Chem. Inf. Model. 2024, 64, 10, 4218-4230. **doi: 10.1021/acs.jcim.4c00301**

11 R. P. P. Neves, et al., J. Chem. Inf. Model. 2023, 63, 1, 20-26. **doi: 10.1021/acs.jcim.2c01337**

12 R. P. Magalhães, et al., Catal. Sci. Technol. 2022, 11, 3474-3483. **doi: 10.1039/D1CY02271G**

13 P. Ferreira, et al., Coord. Chem. Rev. 2022, 455, 214358. **doi: 10.1016/j.ccr.2021.214358**

14 P. Ferreira, et al., Chem. Catalysis 2022, 2, 2481-2498. **doi: 10.1016/j.checat.2022.09.036**

15 C. Jerves, et al., ACS Catal. 2021, 11, 18, 11626-11638. **doi: 10.1021/acscatal.1c03700**

16 A. V. Pinto, et al., ACS Catal. 2021, 11, 16, 10416-10428. **doi: 10.1021/acscatal.1c02444**

17 J. P. M. Sousa, et al., ACS Catal. 2020, 10, 16, 9545-9554. **doi: 10.1021/acscatal.0c03122**

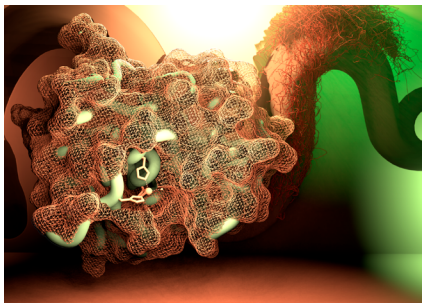
18 J. P. M. Sousa, et al., Green Chem. 2020, 22, 7604-7621. **doi: 10.1039/D0GC02055A**

RESEARCH THEMES/
COMPUTATIONAL DISCOVERY & SAFETY: FROM BIODIVERSITY TO CLINICAL SOLUTIONS

Our group leverages advanced computational chemistry to bridge natural biodiversity and clinical therapeutics, addressing global health crises through physics-based simulations and machine learning (ML). Central to this effort is **Biodiversity2Drug**s, a global collaboration where we combine ML predictions with rigorous physics-based simulations to mine natural sources – from plants to marine organisms – for novel peptide drugs targeting G-Protein Coupled Receptor (GPCRs) for chronic pain and autoimmune diseases.

Beyond natural peptides, we deploy **structure-based drug design** to combat infectious diseases and resistance. For **Flaviviruses** (Zika, Dengue, Yellow Fever), we employ molecular dynamics, QM/MM, and docking to map the dynamics of viral enzymes, identifying inhibitors for both catalytic and allosteric sites. Similarly, to tackle the **antimicrobial resistance** crisis, we elucidate bacterial entry mechanisms and resistance pathways (porin-mediated resistance, antibiotic-degrading enzymes), guiding the design of next-generation antimicrobials and metalloantibiotics that can bypass traditional resistance. Our scope further includes computational strategies to disrupt **biofilms**, a major barrier to effective antimicrobial therapy.

Addressing another critical gap in global health, we aim to identify broad-spectrum inhibitors for **snakebite envenoming**, the deadliest neglected tropical disease according to the WHO. Current antivenom treatments are expensive, require cold-chain logistics, and must be administered in hospital settings. To address this, we investigate the mechanisms by which snake venom toxins exert their toxicity and conduct computer-aided drug discovery campaigns to identify small molecules targeting the main toxic components, particularly neurotoxic three-finger toxins and phospholipase A2 enzymes. This work is carried out in collaboration with multidisciplinary teams to ensure that computationally identified molecules can be synthesized and experimentally tested.



Snake venoms are complex cocktails of toxins that induce rapid, often fatal physiological collapse in prey. Among these, metalloproteinases play a critical role by degrading collagen in blood vessel walls, causing haemorrhage, while synergizing with other toxins to render blood incoagulable. This multi-pronged attack leads to uncontrollable bleeding and death. Current treatments relying on animal-derived antivenoms face significant logistical and safety challenges. Our research employs computer-aided drug discovery to identify small-molecule inhibitors capable of neutralizing these diverse toxic components, aiming to develop a universal, stable, and accessible therapy to replace traditional antivenoms.

Unified by a **computational-first strategy**, our workflow spans from high-throughput virtual screening and mechanistic QM/MM studies to the rational optimization of leads. By translating atomic-level insights into tangible drug candidates, we accelerate the discovery of sustainable, effective therapies for neglected tropical diseases, pandemics, and chronic conditions.

SELECTED PUBLICATIONS

19 A. R. Calixto, et al., Biochimie 2026, 242, 108-117. **doi: 10.1016/j.biochi.2025.12.003**

20 D. Malafaia, et al., ACS Chem. Neurosci. 2025, 16, 16, 3184-3203. **doi: 10.1021/acschemneuro.5c00425**

21 C. W. Gruber, et al., Br. J. Pharmacol. 2025, 182, 3691-3694. **doi: 10.1111/bph.70072**

22 J. R. da Silva, et al., Expert Opin. Drug Discov., 20, 317–335. **doi:10.1080/17460441.2025.2465364**

23 J. Castro-Amorim, et al., Chem. Sci. 2025, 16, 1974-1985. **doi: 10.1039/D4SC06511E**

24 J. T. S. Coimbra, et al., JACS Au 2024, 4, 11, 4295-4306. **doi: 10.1021/jacsau.4c00646**

25 A. V. Pinto, et al., Chem. Sci. 2024, 15, 9793-9805. **doi: 10.1039/D4SC02315C**

26 T. F. Vieira, et al., J. Appl. Microbiol. 2024, 135, lxae088. **doi: 10.1093/jambio/lxae088**

27 J. T. S. Coimbra, et al., J. Chem. Inf. Model. 2023, 63, 20, 6354-6365. **doi: 10.1021/acs.jcim.3c00962**

28 J. Castro-Amorim, et al., J. Chem. Inf. Model. 2023, 63, 13, 4056-4069. **doi: 10.1021/acs.jcim.2c01156**

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30 L. M. C. Teixeira, et al., J. Chem. Inf. Model. 2022, 62, 10, 2510-2521. **doi: 10.1021/acs.jcim.1c01561**

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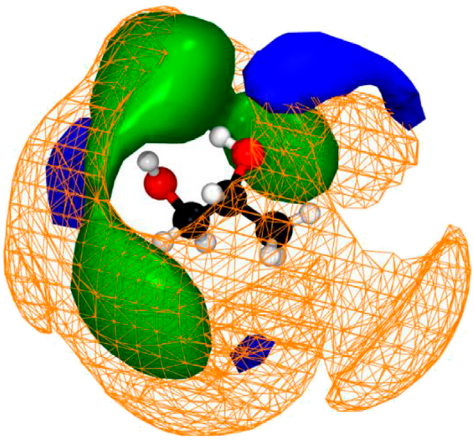
RESEARCH THEMES/
COMPUTATIONAL MODELLING OF CONFINEMENT, NEOTERIC SOLVENTS, AND NANOSTRUCTURED MATERIALS

Our research focuses on the theoretical modelling of chemical species under spatial and chemical confinement, where dramatic changes in physical and chemical properties emerge compared to gas phase conditions. We employ a diverse suite of computational methods to study single molecules, metal complexes, and small aggregates trapped within media such as **zeolites, porous dipeptide crystals, and carbon nanotubes**. This approach yields enhanced molecular-level insights into catalysis, bioinorganic chemistry, and gas storage, exemplified by our analysis of SN2 reaction mechanisms inside pristine nanotubes and the simulation of O2 diffusion through nanopores.

Parallel to these confinement studies, we address the critical challenge of reconciling industrial development with environmental sustainability through the atomistic simulation of **neoteric solvents**. While conventional solvents generate vast toxic waste, alternatives like i**onic liquids (ILs), deep eutectic solvents (DESs), and dipolar aprotic solvents (DASs)** offer low volatility and non-flammability. However, issues with biodegradability persist. Our simulations aim to fine-tune the structure and properties of these systems to create truly green solvents, balancing performance with environmental safety.

Furthermore, we leverage high-level theoretical methods to unlock the extraordinary properties of **nanostructured materials (NSMs)** for applications ranging from water desalination and drug delivery to gas adsorption and molecular imprinting sensing. By combining quantum calculations with molecular simulations, we investigate carbon nanotubes, graphene-based materials, and electrochemical molecularly imprinted polymers. Together, these efforts form a cohesive strategy: using computational power to predict and optimize the behaviour of matter under confinement, in novel solvents, and within engineered nanostructures, driving innovation in catalysis, green chemistry, and nanotechnology.



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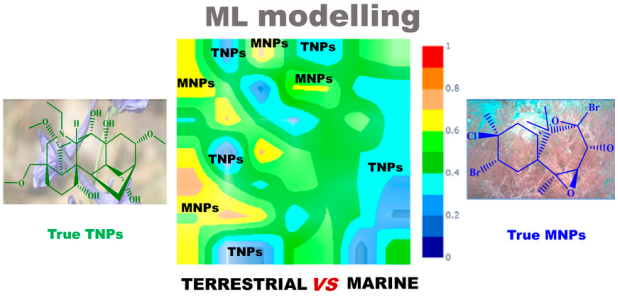
RESEARCH THEMES/
QSAR-DRIVEN SAFETY ASSESSMENT AND ACCELERATED DRUG DISCOVERY

Our research leverages advanced **Quantitative Structure-Activity Relationship (QSAR)** modelling and **machine learning (ML)** to address critical challenges in material safety and therapeutic development. Facing the rising risks of novel functional materials (NFMs), we develop robust in silico models to predict biological activity and toxicity, overcoming the cost and speed limitations of experimental assays. By implementing Quantitative Structure-Property Relationship (QSPR) frameworks, we simultaneously optimize conflicting properties, ensuring that new modelled materials balance effectiveness with environmental and human safety.

This data-driven approach extends to **computer-aided drug repurposing**, where we integrate large-scale QSAR modelling with virtual screening to rapidly identify therapeutics. For instance, utilizing Random Forest, SVM, and CNN classifiers trained on over 10,000 molecules, we screened FDA-approved libraries to identify dihydroergocristine as a cytotoxic candidate for p53-expressing colorectal cancer. Similarly, a second QSAR framework trained on nearly 30,000 molecules predicted PD-1/PD-L1 inhibition, successfully validating sonidegib as an immune checkpoint modulator. These pipelines demonstrate how validated QSAR classifiers can accelerate the discovery of agents targeting tumour-suppressor pathways and immune checkpoints.

Furthermore, we are decoding the **chemical diversity of natural products (NPs)** to accelerate drug discovery. We developed a pioneering machine-learning framework to classify marine, terrestrial, and dual-origin NPs, defining the applicability domains for QSAR models in these complex chemical spaces. By integrating docking-based estimations with LightGBM models using NMR-derived spectral descriptors, we successfully identified NP scaffolds with high potential for PD-1/PD-L1 modulation. This integrated strategy – combining spectral information, ML, and QSAR prediction – provides a powerful engine for prioritizing bioactive compounds and accelerating the transition from chemical diversity to clinical candidates.



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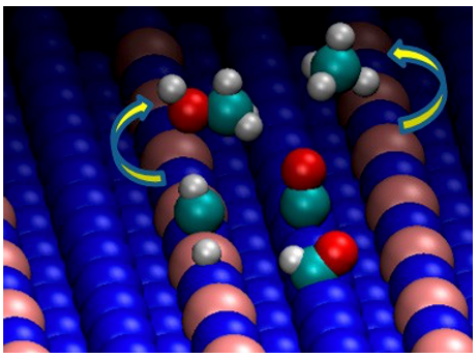
RESEARCH THEMES/
HETEROGENEOUS-CATALYSED REACTIONS

The development of new catalysts for a specific reaction is a complex and demanding task, usually done by a trial-and-error procedure. Computational methods, however, are particularly suited for shedding light on the active sites of the catalyst, the reaction mechanism, the role of coverage effects, and even the prediction of the catalyst activity. We perform theoretical studies on heterogeneous-catalysed reactions, with the aim of elucidating their mechanisms and predict the catalytic activity of new materials. Both periodic plane-wave Density Functional Theory (DFT) methods and first-principles-based kinetic Monte Carlo simulations are used in these studies. Different metallic surfaces are used in our research. This includes (Au and Ag) monometallic, (Ag/Au and Ni/Cu) bimetallic and (Al/Zn/Cu) trimetallic surfaces. The mechanisms of different heterogeneous-catalysed reactions are studied. This includes: the nitrous oxide hydrogenation, the methanol steam reforming to produce hydrogen, the carbon oxide oxidation and the water gas shift reaction.



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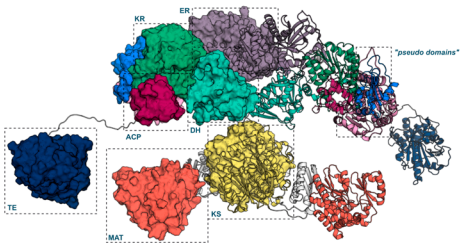
HIGHLIGHTS

ANIMAL FATTY ACID SYNTHASE: AN AMAZING CHEMICAL NANOFACTORY

Fatty acids are vital, conserved molecules for energy storage, membranes, and signalling. Their de novo synthesis can be achieved either by a metabolic pathway composed of a sequence of individual enzymes, as in most bacteria, or by a single large multienzyme, as in animals, fungi, and some bacteria.



In our review, "Animal Fatty Acid Synthase: A Chemical Nanofactory" (Chem Rev, 2021), we overview this field and describe animal FAS's architecture: a homodimeric multienzyme with seven different active sites per dimer and a transport domain shuttling intermediates from one active site to the next. The review critically discusses the atomic-detail chemical mechanisms for synthesizing a single fatty acid. Additionally, the review addresses open questions regarding FAS architecture, such as its substrate-shuttling arm, and explores possible reasons for the emergence of large megasynthases during evolution.

This work sets the stage for our investigations. More recently, we published studies on the potential applications of FAS in biotechnology, including carbon-carbon bond formation kinetics and the engineering of homologous polyketide synthases.

Animal Fatty Acid Synthase: A Chemical Nanofactory

Chemical Reviews 2021, 121 (15), 9502

The Kinetics of Carbon-Carbon Bond Formation in Metazoan Fatty Acid Synthase and Its Impact on Product Fidelity

Angewandte Chemie International Edition 2024, 64, e202412195

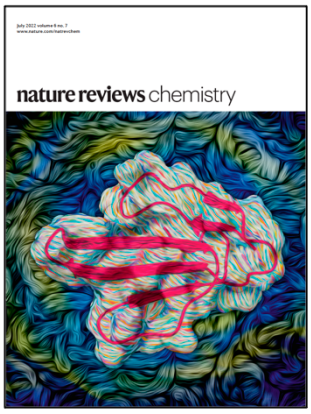
Engineering of PKS Megaenzymes – A Promising Way to Biosynthesize High-Value Active Molecules

Topics in Catalysis 2022, 65, 544-562

THE CHEMISTRY OF SNAKE VENOM AND ITS MEDICINAL POTENTIAL

The fascination and fear of snakes dates to time immemorial. Their lethality has often been associated with images of perfidy, treachery, and death. However, snakes did not always have such negative connotations. The curative capacity of venom has been known since antiquity, also making the snake a symbol of pharmacy and medicine.

Today, there is renewed interest in pursuing snake-venom-based therapies. Our project focuses on the chemistry of snake venom and its potential to be exploited for medicinal purposes, developing drugs and covalent small-molecule inhibitors against major venom components like three-finger toxins and phospholipase A2 enzymes. In our recent review, "The Chemistry of Snake Venom and its Medicinal Potential" (Nat Rev Chem, 2022), the mixture of toxins is examined, focusing on molecular structure, chemical reactivity, and target recognition of bioactive toxins to develop drugs or antidotes. We also discuss the design and working mechanisms of snake-venom-derived drugs, and strategies for transforming toxins into therapeutics.



This review served as a foundation for our ongoing work, exemplified by studies on zinc metalloproteinases, PLA2 enzymes, and toxin databases.

The Chemistry of Snake Venom and its Medicinal Potential

Nature Reviews Chemistry, 2022, 6, 451

Beyond Fang's fury: a computational study of the enzyme–membrane interaction and catalytic pathway of the snake venom phospholipase A2 toxin

Chemical Science, 2025, 16, 1974-1985

Viper Venom Phospholipase A2 Database: The Structural and Functional Anatomy of a Primary Toxin in Envenomation

Toxins, 2024, 16, 71

Unraveling the Reaction Mechanism of Russell's Viper Venom Factor X Activator: A Paradigm for the Reactivity of Zinc Metalloproteinases?

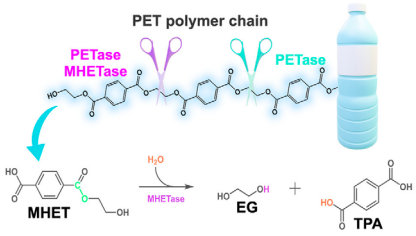
Journal of Chemical Information and Modeling, 2023, 63, 13, 4056-4069

Catalytically Active Snake Venom PLA2 Enzymes: An Overview of Its Elusive Mechanisms of Reaction

Journal of Medicinal Chemistry, 2023, 66, 5364-5376

HIGHLIGHTS

NEW STRATEGY TO RECYCLE PLASTIC PET



Over the last half century, the massive production of plastics has created a global environmental problem, making sustainable recycling technologies urgently needed. PETase and MHETase, produced by Ideonella sakaiensis 201-F6, act sequentially in the degradation of polyethylene terephthalate (PET), one of the most widely used plastics. Through our previous QM/MM MD studies, we established a computational pipeline to characterize the catalytic mechanisms of these enzymes, confirming their ability to fully depolymerize PET back into its monomeric precursors: ethylene glycol and terephthalic acid.

Building on this work, we are now extending our research to polyurethane (PUR), a chemically diverse and recalcitrant plastic for which efficient biocatalysts are still scarce. As a key partner in the En'Zync consortium, we aim to identify enzymes with PUR-degrading potential, characterize their catalytic mechanisms, and propose mutations to enhance activity and substrate scope. This work contributes to the rational design of improved biocatalysts for plastic biodegradation and circular recycling, leveraging our established computational pipeline to tackle the next generation of plastic waste.

Reaction Mechanism of MHETase, a PET Degrading Enzyme.
ACS Catalysis 2021, 11, 16, 10416−10428

Reaction Mechanism of the PET Degrading Enzyme PETase Studied with DFT/MM Molecular Dynamics Simulations.
ACS Catalysis 2021, 11, 18, 11626−11638

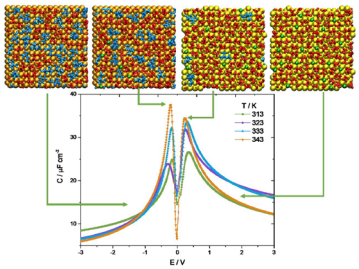
Rate-enhancing PETase mutations determined through DFT/MM molecular dynamics simulations.
New Journal of Chemistry, 2024, 48, 45-54

Hydrolysis of the Urethane Bond Catalyzed by Pseudomonas sp. MIS38 Lipase: A QM/MM Mechanistic Insight.
ACS Catalysis, 2025, 15, 17, 14728-14740

Unveiling the enzymatic pathway of UMG-SP2 urethanase: insights into polyurethane degradation at the atomic level.
Chemical Science, 2025, 16, 2437-2452

INSIGHTS INTO IONIC LIQUID AND DEEP EUTECTIC SOLVENTS | ELECTRODE INTERFACES

The complex interfaces between solid electrodes and ionic liquids (ILs) or deep eutectic solvents (DESs) are of significant interest due to their multifaceted properties, spanning actuating ability, gating and charge capacity, catalytic activity, electrochemical stability, super lubricity, and sustainable energy storage applications. Understanding the origins of differential capacitance peaks at the molecular level is key for taking full advantage of IL|electrode and DES|electrode interfaces, fostering further progress in the development of supercapacitors, capacitive sensors, thin-film transistors, actuators, and other innovative electrochemical devices. We provide a molecular dynamics (MD) perspective on this subject by investigating the interfaces of 1-butyl-3-methylimidazolium hexafluorophosphate and ethaline (1:2 choline chloride:ethylene glycol) with single-crystalline Au(100), Au(110), and Au(111) surfaces over a range of temperatures and applied surface charges. Our MD results, combined with semi-quantitative approaches within the bilayer model of the electric double layer, reveal that the differential capacitance behaviour is governed by ions' and hydrogen-bond donor molecules' structural reorganization within the first interfacial layers, including charge-dependent layering, molecular orientation, and counterion accumulation at the electrified interface.



Hysteresis in the MD Simulations of Differential Capacitance at the Ionic Liquid–Au Interface.
J. Phys. Chem. Lett. 2020, 11, 24, 10408−10413

Ionic Liquid–Metal Interface: The Origins of Capacitance Peaks.
Electrochim. Acta 2021, 379, 138148

Double layer in ionic liquids: Temperature effect and bilayer model
Journal of Molecular Liquids, 2022, 363, 119747

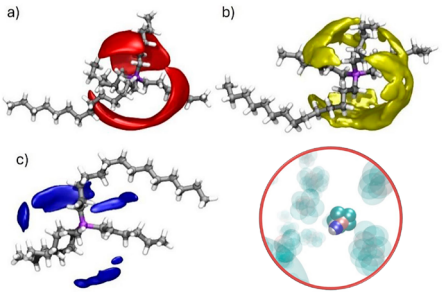
Probing the Local Structures of Choline-Glycine Electrolytes: Insights from Ab Initio Simulations.
J. Mol. Liq. 2023, 390, Part A, 122946

Ionic Liquid-Metal Interface: The Origins of Capacitance Peaks
Electrochimica Acta, 2021, 379, 138148

HIGHLIGHTS

MAGNETIC IONIC LIQUIDS FOR GAS CAPTURE AND SEPARATION

Magnetic ionic liquids (MILs) have emerged as promising materials for gas capture and separation due to their unique combination of ionic liquid properties and magnetic responsiveness. Understanding the molecular mechanisms governing gas solvation, transport, and selectivity in MILs is essential for advancing environmentally sustainable separation technologies. We provide a molecular-level perspective on this subject through molecular dynamics (MD) simulations and density functional theory (DFT) calculations on imidazolium- and phosphonium-based MILs containing transition-metal and rare-earth anions. Our results reveal how the nature of the paramagnetic species controls gas adsorption, mobility, and local solvation structure, highlighting the key role of multivalent magnetic anions in enhancing selective CO2 and SO2 capture and guiding the rational design of advanced gas separation materials.



Magnetic Ionic Liquids: Current Achievements and Future Perspectives with a Focus on Computational Approaches

Chemical Reviews, 2024, 124, 6, 3392-3415

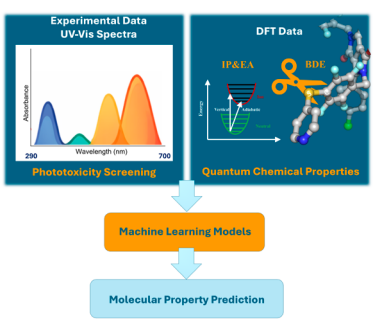
Properties and interactions of magnetic ionic Liquids: Focus on greenhouse gas capture from MD simulations

Separation and Purification Technology, 2025, 364, Part 1, 132329

INTEGRATING EXPERIMENTAL AND QUANTUM CHEMICAL DATA THROUGH MACHINE LEARNING

Machine learning models offer a powerful approach to integrate experimental and density functional theory (DFT) data for predicting molecular properties vital to pharmaceuticals and materials science. For phototoxicity prediction, Random Forest models trained on over 74,000 experimental UV–Vis spectra successfully classify molecules based on absorption in the 290–700 nm range, achieving 0.89 accuracy and validating the use of mined experimental data for high-throughput safety screening.

Where experimental data is scarce, we turn to quantum chemistry. Consensus ML models trained with over 9,600 DFT-calculated structures now predict ionization potential and electron affinity with mean absolute errors as low as 0.23 eV, serving as a rapid alternative to new calculations for organic electronics applications. Furthermore, a hybrid approach for bond dissociation energies was developed with Random Forest models trained on DFT data with a correction layer based on experimental bond memories. This strategy improved accuracy significantly, reducing errors from 5.36 to 1.52 kcal/mol against experimental values.



Together, this integrated approach leverages ML to extract knowledge from both experimental databases and DFT calculations, creating fast, accurate predictors that accelerate the design of safer, high-performance molecules

Machine learning prediction of UV–Vis spectra features of organic compounds related to photoreactive potential.

Scientific Reports 2021, 11, 23720.

Machine learning prediction of ionization potential and electron affinity from DFT-calculated data

ChemistrySelect 2023, 8, e202300036

Random Forest QSPR models for bond dissociation energies combining DFT and experimental data

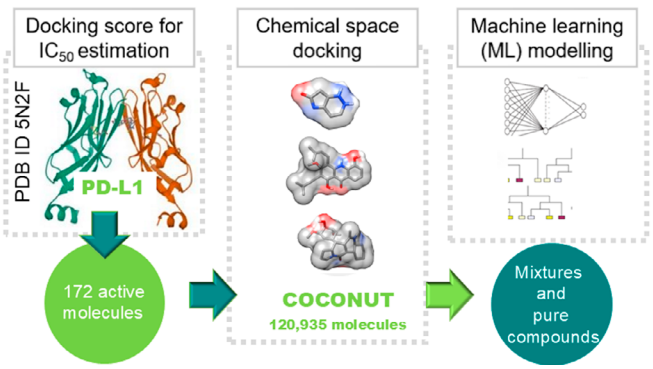
Molecular Informatics 2022, 42, 2200193

HIGHLIGHTS

DECODING NATURAL PRODUCTS TO ACCELERATE DRUG DISCOVERY

Understanding the chemical diversity of natural products (NPs) is essential for unlocking new therapeutic opportunities. To explore how terrestrial and marine environments shape molecular space, a machine-learning framework was developed to classify NPs into marine, terrestrial, and dual-origin categories. This represents, to our knowledge, the first approach designed to distinguish these overlapping chemical domains, offering new insights into NP chemical space and supporting virtual screening by defining the applicability domain of QSAR models.

Building on this foundation, we investigated the immuno-oncological potential of natural products targeting the PD-1/PD-L1 immune checkpoint. By integrating docking-based IC_{50} estimation with machine-learning prediction, we identified promising NP scaffolds capable of modulating this pathway. Among the tested models, LightGBM delivered the best performance, particularly when utilizing 570 NMR-derived SPINUS spectral descriptors. The resulting QSAR classifier achieved strong external validation metrics (sensitivity 0.74, specificity 0.81, accuracy 0.78, MCC 0.55), demonstrating that combining spectral information with ML can effectively prioritize bioactive natural products. This integrated strategy shows considerable promise for accelerating the discovery of active pure compounds.



Machine Learning Methods to Predict the Terrestrial and Marine Origin of Natural Products

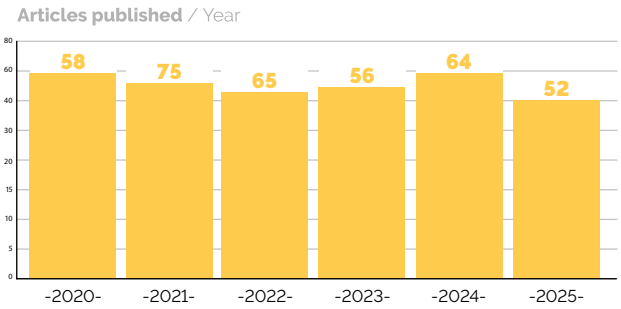
Molecular Informatics 2021, 40, 2060034

A Chemoinformatics Investigation of Spectral and Quantum Chemistry Patterns for Discovering New Drug Leads from Natural Products Targeting the PD-1/PD-L1 Immune Checkpoint, with a Particular Focus on Naturally Occurring Marine Products

Marine Drugs 2025, 23, 247

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION



H-index: **35**

370 articles*
5601 citations

*01/2020-12/2025
From WOS core collection

FUNDED PROJECTS *(Representative projects)*

- **Biodiversity2Drugs – Nature-based solutions for biodiversity, human well-being and transformative change**
  Funded by BIODIVERSA+, Call 2023-24 (BiodivNBS/0009/2023) | 2025-2028 | Pedro Fernandes (local PI), António Ribeiro (local co-PI) | Total Funding: € 106,250.00
- **En'Zync – Center for Enzymatic Deconstruction of Thermoset Plastics for a Sustainable Society**
  Funded by NOVO NORDISK FONDEN's Challenge Programme 2022 (0072891) | 2022-2028 | Maria João Ramos (local PI), Pedro Fernandes (local co-PI) | Total Funding: € 753,403.47
- **SUPercapacitor performance through Rational Electrolyte and Electrode design: Modular computational Approach**
  Funded by Fundação para a Ciência e a Tecnologia – Call for Exploratory Research Projects in all Scientific Domains 2024 (2024.18148.PEX) | 2026-2027 | Iuliia Voroshylova (PI) | Total Funding: € 59,375.00
- **Murderous Venom – Towards a Universal Antidote Against Snakebite**
  Funded by Fundação para a Ciência e a Tecnologia – Projects in all scientific fields 2020 (PTDC/QUI-OUT/1401/2020) | 2021-2024 | Pedro Fernandes (PI), Maria João Ramos (co-PI) | Total Funding: € 249,750.00
- **Machine Learning-Driven Virtual Screening of Nature-derived Peptides towards G-Protein Coupled Receptors**
  Funded by Fundação para a Ciência e a Tecnologia – FCT/CPCA/2025/01 (2025.11147.CPCA.A3) | 2025-2026 | João Sousa (PI), Pedro Ferreira (co-PI) | Total Funding: € 316,052.00
- **Exploring Alternative Enzyme Mechanisms: Parallel DFTB/MM Characterization of Mechanistic Networks Using EzMechanismQM**
  Funded by Fundação para a Ciência e a Tecnologia – FCT/CPCA/2025/01 (2025.11800.CPCA.A1) | 2025-2026 | António Ribeiro (PI) | Total Funding: € 33,944.00
- **Venomous Relief: Harnessing Snake and Spider Toxins to Inhibit the ASIC1a ion channel for Pain Suppression and Cardioprotection**
  Funded by Fundação para a Ciência e a Tecnologia – FCT/CPCA/2024/01 (2025.00046.CPCA.A3) | 2025-2026 | Pedro Fernandes (PI), Pedro Ferreira (co-PI) | Total Funding: € 69,173.00
- **Establishing the mechanism for plastic degrading newly-discovered enzymes**
  Funded by Fundação para a Ciência e a Tecnologia – FCT/CPCA/2024/01 (2025.00056.CPCA.A3) | 2025-2026 | Maria João Ramos (PI), Pedro Paiva (co-PI) | Total Funding: € 79,673.00
- **Development of an enzymatic technology for green biomining,**
  Funded by Fundação para a Ciência e a Tecnologia – FCT/CPCA/2024/01 (2025.00176.CPCA.A3) | 2025-2026 | Pedro Ferreira (PI), João Sousa (co-PI) | Total Funding: € 31,277.00
- **Unraveling the role of NS2 cofactor in flavivirus NS2B-NS3 protease activity**
  Funded by Fundação para a Ciência e a Tecnologia – FCT/CPCA/2024/01 (2024.07911.CPCA.A2) | 2025-2026 | Ana Rita Silva (PI) | Total Funding: € 6,173.50
- **Atomistic and thermodynamic characterization of the capabilities of bacterial sulfide:quinone reductase on the conversion of pollutant sulfide to elemental sulfur**
  Funded by Fundação para a Ciência e a Tecnologia – FCT/CPCA/2023/01 (2023.10904.CPCA.A2) | 2024-2025 | Rui Neves (PI), João Coimbra (co-PI) | Total Funding: € 31,260.00
- **Solvent-in-salt electrolytes for safe and efficient energy storage: Multiscale Theoretical Approach**
  Funded by Fundação para a Ciência e a Tecnologia – FCT/CPCA/2023/01 (2023.10811.CPCA.A2) | 2024-2025 | Iuliia Voroshylova (PI) | Total Funding: € 6,972.00

- **Solvent-in-salt electrolytes for safe and efficient energy storage: Multiscale Theoretical Approach**
  Funded by Fundação para a Ciência e a Tecnologia – FCT/CPCA/2023/01 (2023.10811.CPCA.A2) | 2024-2025 | Iuliia Voroshylova (PI) | Total Funding: € 6,972.00

GROUP IN NUMBERS

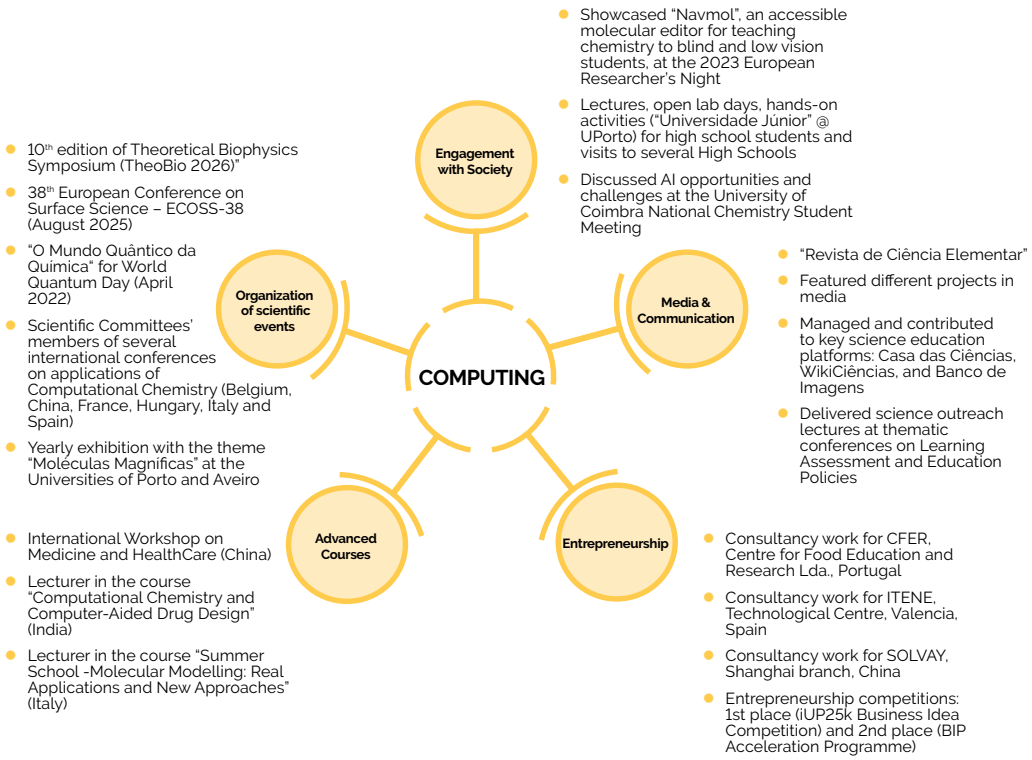
FUNDED PROJECTS *(Representative projects)*

- **Biodegrading unsaturated polyesters**
  Funded by EuroHPC Joint Undertaking (EHPC-REG-2023R03-163) | 2024-2025 | Maria João Ramos (PI), Pedro Fernandes (co-PI) | Total Funding: est. € 145,000.00 (~16 million core-hours @ € 0.009 cost/core-hour)
- **Optimization of Validated SARS-CoV-2 Antivirals against the New Emerging Variants**
  Funded by Fundação para a Ciência e a Tecnologia – FCT/CPCA/2021/01 (2021.09752.CPCA) | 2022-2023 | Sérgio Sousa (PI) | Total Funding: € 14,812.00
- **Drug discovery targeting Covid-19**
  Funded by XSEDE, Covid-19 Consortium, USA (Project ASC200029) | 2020 | Maria João Ramos (PI) | Total Funding: est. € 135,000.00 (15 million core-hours @ € 0.009 cost/core-hour)

INTERNATIONAL COOPERATION AND NETWORKING

- Global Initiative for Academic Networks (GIAN), funded by the Indian government, 2019.
- International collaboration with several universities in Valencia (Spain), Basque Country (Spain), Autonoma de Madrid (Spain), Autonoma de Barcelona (Spain), Tartu (Estonia), Gdansk (Poland), Calabria (Italy), Antwerp (Belgium), Stockholm (Sweden), Rio Grande do Sul (Brazil), Quito (Ecuador), Cuenca (Ecuador), Andres Bello (Chile), Bangalore (India), Kolkata (India), Yantai (China), Academia Sinica (Taiwan), Nanyang (Singapore), Frostburg (USA), Minneapolis (USA), and Lethbridge (Canada).
- Maintained active research ties with institutions in: USA (Oak Ridge National Laboratory; Frostburg; Minneapolis), Canada (Lethbridge), Brazil (Rio Grande do Sul; Goiás; São Paulo), Chile (Andrés Bello), Costa Rica, Ecuador (Quito, Cuenca), China (Yantai), Taiwan (Academia Sinica), Singapore (Nanyang; Singapore National University), India (Bangalore; Kolkata; IASST Guwahati), Morocco (Mohammed VI Polytechnic University), and South Africa (Stellenbosch).
- Collaborations with over 30 international partners spanning Europe, Asia, the Americas, and Africa to advance computational chemistry and AI.

DISSEMINATION & OUTREACH



LABORATÓRIO ASSOCIADO
PARA A QUÍMICA VERDE

MolSyn
MOLECULAR SYNTHESIS

CHEMBIO
NATURAL PRODUCTS CHEMISTRY AND BIOACTIVITY

OAD
OMICS & ANALYTICAL DEVELOPMENT

EnvChem
ENVIRONMENTAL CHEMISTRY

BCPE
(BIO)CHEMICAL PROCESS ENGINEERING

Charm
CULTURAL HERITAGE AND RESPONSIVE MATERIALS

MatSusWell
MATERIALS FOR SUSTAINABILITY AND WELLNESS

NanoPlat
NANOPLATFORMS

4FOOD
FOOD QUALITY AND TECHNOLOGY

Computing
HIGH PERFORMANCE COMPUTING IN MOLECULAR MODELLING

LAQV requimte
LABORATÓRIO ASSOCIADO PARA A QUÍMICA VERDE

2020-2025
ACTIVITY REPORT
& HIGHLIGHTS

04

Post-Graduation

MASTER PROGRAMS | MSC

Biochemistry
FCUP

DIRECTOR:
Paula Gameiro (LAQV)

Biochemistry
U.Aveiro

DIRECTOR:
Pedro Oliveira (LAQV)

Bioorganic Chemistry
FCT NOVA (Lisbon)

COORDINATOR:
Luísa Ferreira (LAQV)

Biotechnology
FCT NOVA (Lisbon)

COORDINATOR:
Ana Rita Duarte (LAQV)

Chemistry
U.Aveiro

DIRECTOR:
M. Amparo Faustino (LAQV)

Conservation and Restoration
FCT NOVA (Lisbon)

DIRECTOR:
Joana Lia Ferreira (LAQV)

Food Science and Technology
FCUP

DIRECTOR:
Nuno Mateus (LAQV)

Gastronomic Sciences
FCT NOVA (Lisbon)

LOCAL COORDINATOR:
Bruno Leite (LAQV)

Quality Control
FFUP

DIRECTOR:
Beatriz Oliveira (LAQV)

Integrated Master in Pharmaceutical Sciences
FFUP

LOCAL COORDINATOR:
Isabel Ferreira (LAQV)

Health Products of Natural Origin
FFUP

COORDINATOR:
Salette Reis (LAQV)

Applications in Biotechnology and Synthetic Biology
FCUP

COORDINATOR:
Paula Gomes (LAQV)

Bioresources
IPP

COORDINATOR:
Simone Morais (LAQV)

Pharmacy
IPP

COORDINATOR:
Marlene Lima (LAQV)

Biomaterials and Nanomedicine
FCT Nova (Lisbon)

COORDINATOR:
Luís Branco (LAQV)

Food Technology and Safety
FCT NOVA (Lisbon)

DIRECTOR:
Ana Luísa Fernando (LAQV)

DOCTORAL PROGRAMS | PHD

Sustainable Chemistry

DIRECTOR:
Ana Aguiar Ricardo (LAQV),

CO-DIRECTORS:
Artur Silva (LAQV),
Victor de Freitas (LAQV)

Conservation and Restoration of Cultural Heritage

DIRECTOR:
Maria João Melo (LAQV)

Molecular and Cellular Biotechnology Applied to Health Sciences

BiotechHealth

CO-DIRECTOR:
Salette Reis (LAQV)

Refining, Petrochemical and Chemical Engineering

EngIQ

DIRECTOR:
Fernando Gomes Martins (FEUP)

LOCAL COORDINATOR:
João Crespo (LAQV)

Animal Science

SANFEED

DIRECTOR:
António Mira da Fonseca (LAQV)

Biochemistry

U.Aveiro

COORDINATOR:
Maria do Rosário Domingues (LAQV)

Chemical and Biological Engineering

PDEQB

COORDINATOR:
José Paulo Mota (LAQV)

Chemistry

U.Aveiro

COORDINATOR:
Augusto Tomé (LAQV)

Chemistry

FCT NOVA (Lisbon)

COORDINATOR:
Marco Gomes da Silva (LAQV)

Food Sciences

FCT NOVA (Lisbon)

COORDINATOR:
Marco Gomes da Silva (LAQV)

Pharmaceutical Sciences

FFUP

DIRECTOR:
Alberto Araújo (LAQV)

Food Science and Technology and Nutrition

PDCTAN

DIRECTORS:
Victor Freitas (LAQV)
Silvia Rocha (LAQV)

Analytical Chemistry and Engineering for Environmental Sustainability

IPP

DIRECTOR:
Simone Morais (LAQV)

Bioenergy

FCT NOVA (Lisbon)

DIRECTOR:
Ana Luísa Fernando (LAQV)

requimte
LABORATÓRIO ASSOCIADO PARA A QUÍMICA VERDE

2020-2025
ACTIVITY REPORT
& HIGHLIGHTS

05

Scientific Platforms

BIOCHEMICAL AND BIOPHYSICAL ANALYSIS

This facility is devoted to the comprehension of cellular and molecular mechanisms, including the in vitro characterization of molecular interactions. This facility provides a unique set of state-of-the-art biophysical and biological technologies.

EQUIPMENT – FCT NOVA

- Circular Dichroism - Applied Photophysics Chirascan™ qCD
- Multi Parametric Surface Plasmon Resonance - Bionavis™ SPR Navi 200
- Differential Scanning Calorimetry - TA™ Nano DSC; Setaram, DSC 131
- Isothermal Titration Calorimetry - TA™ Nano ITC
- MicroScale Thermophoresis - Nano Temper Technologies™ Monolith NT.115
- Flow Cytometry - Attune™ Acoustic Focusing Cytometer

For more information:
https://sites.fct.unl.pt/biolab/

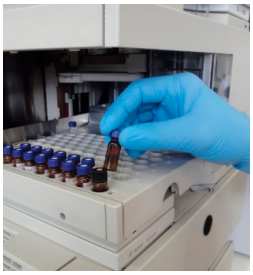
EQUIPMENT – U. PORTO

- Langmuir Trough with Brewster Angle Microscopy - KSV-NIMA KN1006 trough with Nanofilm_Ultrabam (Accurion GmbH)
- Langmuir Trough with Polarizationmodulation infrared reflectionabsorption spectroscopy (PM-IRRAS) - KSV-NIMA KN-1002 trough with KSVNIMA PM-IRRAS spectrophotometer
- Isothermal Titration Calorimetry - MicroCalTM iTC200
- Differential Scanning Calorimetry - MicroCalTM VP-DSC

EQUIPMENT – U. AVEIRO

- Optical contact angle measuring and contour analysis system – Dataphysics OCA20
- Shear rheometer – Netzsch Kinexus
- Texture analyser – TA HDi Stable Micro Systems & TA.XTplusC
- OxySense® GEN III 5000 Analyzer
- ChemiDoc, BioRad

CHEMICAL ANALYSIS



The analytical laboratories aim to provide quality services to researchers at LAQV, guaranteeing them scientific and technical support in their areas of competence and also providing qualified service to public and private entities.

EQUIPMENT – FCT NOVA

Elemental Analysis:

- CHNS Analyzer – Thermo Finnigan CE Instruments Flash EA 1112 CHNS
- Atomic Absorption Spectrometry – Analytik Jena AG AAS ZEEnit 650 | Thermo Scientific Solaar S Series AA
- Inductively Coupled Plasma – Atomic Emission Spectroscopy - Horiba Jobin-Yvon Ultima

Chromatography:

- HPLC: Dionex ICS-3000 | Thermo Scientific Surveyor | Waters 600 | Merck-Hitachi
- Size Exclusion Chromatography – Knauer Smartline/Polymer laboratories PL-ELS1000
- GC: FID – Agilent 6890; TCD – Thermo Scientific Trace GC Ultra

Materials Characterization:

- Fourier Transform Infrared Spectroscopy – Perkin-Elmer Spectrum Two
- Gas Porosimeter – Micromeritics, ASAP2010
- Mercury Intrusion Porosimeter – Micromeritics, Autopore IV
- Thermogravimetric Analizer – Setaram Labsys EVO

Mass Spectrometry:

- LC/MS - Agilent 6130B Single Quadrupole with an ESI source and coupled with an HPLC Agilent 1200 Series with Binary pump
- GC/MS - DSQ (Thermo) with an EI source and coupled with an GC Agilent 6890N

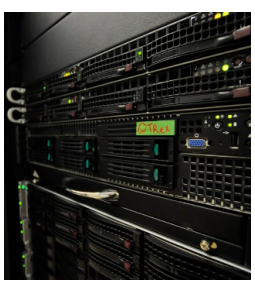
For more information:
https://sites.fct.unl.pt/labanalises

EQUIPMENT – U.AVEIRO

- Inductively Coupled Plasma: ICP-MS Thermo X Series | ICP-OES
- Cold Vapour Atomic Fluorescence Spectroscopy (CV-AFS), PSA 10.023 & PSA 10.025 Millennium Merlin
- Thermal decomposition AAS - LECO 254 Advanced Mercury Analyzer
- Ultrafiltration System – LABSCALE TFF SYSTEM Millipore
- Supercritical Fluid extraction equipment – Applied Separations
- Ionic Chromatograph - Thermo Scientific Dionex ICS-6000 HPIC system
- GC×GC–ToFMS Pegasus 4D: comprising an GC Agilent GC 7890, with a Zoex dual stage jet cryogenic modulator and mass spectrometer equipped with a ToF analyzer
- Spectrofluorimeters: Fluoromax 3; Fluoromax® Plus (range 180-980 nm) Horiba Jobin-Yvon
- HPLC: DAD Ultimate 3000 Thermo Scientific; UV detector Gilson; IR detector Gilson
- GC-MS: QP 2010 Shimadzu; 6890N+MS Agilent
- GC: FID: CP-3800 Varian; Scion 436-GC Bruker
- Multi-Mode Microplate Reader Synergy HTX Biotek
- Digital Polarimeter POLAX-2L ATAGO
- Microwave synthesizers: Microsynt Milestone | Discover SP CEM
- Microwave Extraction Systems – NEOS (Milestone)
- Elemental analyses apparatus truSpec CHNS Micro 630-200-200 LECO.

COMPUTER CLUSTER

The current configuration of the computational system has a total of 1568 CPU cores and little more than 83k GPU cores, spread across a platform with ultrafast infiniband network and 10 Gbit/s links between master and slave nodes. Having more than 300 TB in total storage space, 3248 GB in memory available and a total of 59270 kWh for the all year energy consumption, this system had an average occupancy rate above 112% in the last year, minimum and maximum "wait time" around 1.45 h and 8.76 days respectively and accumulated total offline time of 11 days for the slave nodes and 4 h for the master nodes. Users have access to the master nodes only, from there, they can submit whatever calculation they need for their work to the slave nodes using the queuing system implemented in the cluster. This system will select, from the several types of slave nodes, the ones suitable for the submitted job according to the demand of resources of the job, the availability of the slave nodes and the user total usage. No reservation is active, all online slave nodes are available for all the users and the priority is set by the following rule 0.1 (FIFO) + 0.5 (academic degree) + 0.4 (least usage/user usage).



EQUIPMENT – UPORTO

Master nodes

- Intel Server Xeon E5620 8 cores; 16 GB RAM; 6TB HDD RAID; Dual Infiniband FDR 56Gbit/s; Quad 10Gbit/s Ethernet
- Supermicro Storage Xeon E5-2609v2 4 cores; 16GB RAM; 72TB HDD RAID; 3TB SSD RAID; Dual Infiniband FDR 56Gbit/s; Quad 10Gbit/s Ethernet
- Tyan Storage Xeon E5405 2 cores; 4GB RAM; 26TB HDD RAID - Supermicro Storage Xeon E5335 4 cores; 6GB RAM; 12TB HDD RAID

Network

- 3x Dell Powerswitch 48p 1Gbit/s; 2p 10Gbit/s v 2x SMC 8748L2 50p 1Gbit/s
- 2x EdgeCore ECS4610-50T 48p 1Gbit/s; 128Gbit/s stacking
- 3Com 3824 24p 1Gbit/s - Voltaire 36p Infiniband QDR 40Gbit/s

Slave nodes

- 36x Supermicro Server Xeon E5420 8 cores; 8GB RAM; 1TB HDD RAID
- 10x Tyan server Xeon E5430 8 cores; 8GB RAM; 1TB HDD RAID
- 24x Intel Server Xeon E5620 8cores; 8GB RAM; 1TB HDD RAID; Infiniband QDR 40Gbit/s
- 4x Supermicro Server Xeon E5645 12 cores; 32GB RAM; 1TB v 28x Intel Server Xeon E5-2609 8cores; 8GB RAM; 1TB HDD RAID
- 28x Supermicro Server Xeon E5-2640 12 cores; 32GB RAM; 1TB
- 4x Supermicro Server Xeon E5-2630v2 12 cores; 32GB RAM; 1TB
- 8x Supermicro Server Xeon E5-2620v3 12 cores; 32GB RAM; 1TB
- 8x Supermicro Server Xeon E5-2650 16 cores; 64GB RAM; 2TB HDD RAID; 256GB SSD; 3x NVIDIA Tesla K20
- 4x Supermicro Server Xeon E5-2630v3 16 cores; 64GB RAM; 256GB SSD; 2x NVIDIA Tesla K40
- 4x Supermicro Server Xeon E5-2640v3 16 cores; 128GB RAM; 8TB HDD RAID; 512GB SSD

Energy

- APC Symmetra 160K UPS - 64KVA Installed

Chillers

- 2x YORK 20kW Chillers
- 2x APC InRow RD20
- CLIVET 14kW - Mitsubishi PUHZ140

COMPUTER CLUSTER (CONT.)

EQUIPMENT – FCT NOVA

Masters:

- PowerEdge SC1435; Dual-Core AMD Opteron(tm) Processor 2220; 4 Cores; 8GB RAM; 2x500GB HDD
- Supermicro SSG-6029P-E1CR12T; Intel(R) Xeon(R) Silver 4110 CPU @ 2.10GHz;16 Cores; 96GB RAM; 36TB RAID

Nodes:

- 20x PowerEdge SC1435; Dual-Core AMD Opteron(tm) Processor 2220; 4 Cores; 4GB RAM; 250GB HDD
- 16x PowerEdge SC1435; Dual-Core AMD Opteron(tm) Processor 2220; 4 Cores; 8GB RAM; 250GB HDD
- 8x PowerEdge SC1435; Dual-Core AMD Opteron(tm) Processor 2220; 4 Cores; 16GB RAM; 250GB HDD
- 14x Dell C6100; Intel(R) Xeon(R) CPU E5649 @ 2.53GHz; 12 Cores; 36GB RAM; 3x1TB HDD
- 3x Supermicro SYS-1028GQ-TR; Intel(R) Xeon(R) CPU E5-2630 v3 @ 2.40GHz; 16 Cores; 64GB RAM;2x240GB SSD; 4xNVIDIA GeForce GTX TITAN X
- 4x Supermicro SYS-2029TP-HTR; Intel(R) Xeon(R) Silver 4216 CPU @ 2.10GHz; 16 Cores; 96GB RAM; 960GB SSD;

Network:

- 2x Supermicro Switches, 48 ports, 1Gbit/s

Energy:

- APC UPS Smart-UPS VT 40 kVA

Cooling:

- 2x Emerson Network Power, Model S23UA0000300012PO

MAGNETIC RESONANCE

The NMR Facility at LAQV (FCT NOVA, University of Aveiro, and UPORTO) is integrated in the Portuguese Nuclear Magnetic Resonance Network (PTNMR). PTNMR is a distributed National Research Infrastructure that integrates the Portuguese Roadmap of Research Infrastructures. PTNMR provides coordinated access to a national platform of equipment, resources, services, and skills in NMR for participating institutions and the scientific community, from both national and international R&D industry and academia. The main goal is the maintenance of a single platform that supports the technical integration, sharing of resources and a combined management of the national NMR infrastructure, enabling access to modern and fully operational NMR spectrometers and support of R&D initiatives.

EQUIPMENT – FCT NOVA (LISBON)

- Magnet: Bruker Avance II+ 600 14.1 T, narrow bore 1H frequency: 600 MHz
- Console: 4-channel digital AQS/2 Bruker Avance II+ Gradient: GREAT Z-Gradient Temperature controlled BCU-05
- NMR probes: Cryoprobe TCI (1 H, 13C, 15N); 5 mm QNP (1 H, 19F, 13C, 31P)
- Magnet: Bruker Avance II+ 400 9.4 T, narrow bore 1H frequency: 400 MHz
- Console: 3-channel digital AQS/2 Bruker Avance II+ Gradient: GREAT Z-Gradient HRMAS control unit Temperature controlled BCU-xtreme
- NMR probes: 5 mm TXI (1 H, 13C, 15N); 4 mm HR-MAS (1 H, 13C, 15N)
- Magnet: Bruker AvanceIII 400 9.4 T, narrow bore 1H frequency: 400 MHz
- Console: Nanobay, 2-channel digital Automatic sampler NMR case
- NMR probes: 5 mm QNP (1H, 19F, 13C, 31P)

For more information:
https://www.dq.fct.unl.pt/en/external-services/nuclear-magnetic-resonance-nmr

MAGNETIC RESONANCE (CONT.)

EQUIPMENT – U.PORTO

- Magnet: Bruker Ascend 600 14.1 T, narrow bore 1H frequency: 600 MHz
- Console: 3-channel digital AQS/2 Bruker Avance III Gradient: GREAT Z-Gradient, Temperature controlled BCU-Xtreme, with automatic sampler Sample Express
- NMR probes: 5 mm TCI Prodigy BBO; 5 mm TXI (1 H, 13C, 15N)
- Magnet: Bruker AvanceIII 400 9.4 T, Ultrashielded 1H frequency: 400 MHz
- Console: Avance III 3-channel digital Gradient: GRASP IIP Temperature controlled BCU-Xtreme
- Magnet: Bruker Ascend II+ 400 9.4 T, narrow bore 1H frequency: 400 MHz
- Console: 3-channel digital AQS/2 Bruker Avance II+ Gradient: GREAT Z-Gradient HRMAS control unit Temperature controlled BCU-xtreme
- NMR probes: 5 mm broad band BB-1H-D 5 mm inverse detected triple resonance 1H-BB-D 5 mm dual DUAL
- EPR spectrometer BRUKER ELEXYS III E580
- EPR cavities X band (9.5 GHz) and Q band (35 GHz)
- Temperature control unit (4 to 400 K)

EQUIPMENT – U.AVEIRO

- Magnet: BRUKER AVANCE III - 300 MHz, Liquid-state NMR spectrometer (narrow-bore), 7.1 T magnetic field
- Liquid state probes: 5 mm QNP (1H; 13C, 19F, 31P); 5 mm TBI inverse detection (triple tuned probe; X = broadband; Y = 31P); 10 mm broadband (31P - 103Rb)
- Magnet: BRUKER AVANCE III - 400 MHz, Solid-state NMR spectrometer (widebore), 9.4 T magnetic field (ultrashield)
- Solid state probes: CP/MAS 2.5 mm broadband, 2xCP/MAS 4 mm broadband, CP/MAS 4 mm for low gnuclei, 7 mm 1H CRAMPS, 2xCP/MAS 7 mm broadband, wide-line multi-nuclei, HXY triple resonance 4 mm MAS equipped with a short circuit, shunt capacitor X-channel and four exchangeable XY inserts providing 31P/27Al, 13C/15N2H, 27Al/15N-29Si and 13C/29Si XY combinations
- Magnet: BRUKER AVANCE III TM HD - 500 MHz, Liquid/solid-state NMR spectrometer (narrow-bore), 11.75 T magnetic field (ultrashield)
- Liquid state probes: 5 mm QNP (1H, 13C, 19F, 31P), 5 mm BBI inverse detection (broadband); 5 mm TBI, 10 mm BBO, 3 mm LCSEI, 5mm TXI 500 MHz Z-gradient high resolution; HRMAS probe
- Magnet: BRUKER AVANCE III TM HD - 500 MHz, Liquid-state NMR spectrometer (narrow-bore), 11.75 T magnetic field (ultrashield ascend)
- Liquid state probes: BBO prodigy cryoprobe, double resonance 5 mm broadband observe probe with inverse capabilities, N2-cryocontrol unit for prodigy probe
- Magnet: BRUKER AVANCE III TM HD - 700 MHz., Liquid/solid-state NMR spectrometer (narrow-bore), 16.44 T magnetic field (ultrashield ascend)
- Solid state probes: CP/MAS triple resonance 1.3 mm, CP/MAS TriGamma 2.5 mm, CP/MAS triple resonance 4 mm
- Liquid state probe: 5 mm TBI 700MHz Z-gradient high resolution

MASS SPECTROMETRY

The MS Facility at LAQV-U.Aveiro is integrated into the Portuguese Mass Spectrometry Network (RNEM). RNEM is a distributed National Research Infrastructure that integrates the Portuguese Roadmap of Research Infrastructures. Currently, we develop many research projects mainly focused on omics (Proteomics, Lipidomics, and Glycomics) applications to biochemistry and health sciences. The facility is also strongly committed in providing MS services to support external and in-house biochemistry, biology, chemistry, and bioengineering research groups. The MS facility of LAQV-UPORTO is part of the Structural Analysis Laboratory of the University of Porto Materials Center (CEMUP). The available spectrometers provide routine services to support in-house researchers, graduate, and postgraduate students as well as external users.

EQUIPMENT – FCT NOVA

- Bruker GC 456 coupled with a Bruker MSD Scion TQ (triple Quadrupole)
- Pegasus® BT GC-TOFMS coupled to Agilent GC 6890
- GL Science PHASER CG Olfactory (GC-O) coupled to Agilent GC 6890
- 5975C MSD GC/MS Agilent
- Dionex® Ultimate 3000 System UHPLC+ focused system coupled to a TSQ QuantisTM triple-stage quadrupole mass spectrometer (Thermo Scientific,)

EQUIPMENT – U.PORTO

- LTQ-Orbitrap XL (Thermo) with an ESI source coupled to an ACCELA 600 HPLC system
- Orbitrap Exploris 120 coupled to a Vanquish HPLC system
- Thermo Scientific EasyNanospray Ion Source coupled with a nano LC Thermo Scientific™ UltiMate™ 3000
- BRUKER UltrafleXtreme MALDI-TOF/TOFMS
- Shimadzu Nexera UHPLC coupled to LCMS-8040 ESI-QqQ-MS

EQUIPMENT – U.AVEIRO

- Q-EXACTIVE (Thermo) with a Thermo Scientific Nanospray Flex Ion Source coupled with a nano LC Thermo Scientific™ UltiMate™ 3000
- Q-EXACTIVE (Thermo) equipped with an ESI source and coupled with a microLC Thermo Scientific™ UltiMate™ 3000
- Q-Tof II (Micromass) with electrospray and APCI sources
- LXQ (Thermo) equipped with an ESI source and coupled with an HPLC Dionex 3000 Ultimate nano LC

MICROSCOPY

The electron microscopy network laboratory is a focal point of the Portuguese Electron Microscopy Network. It is hosted at the Universities of Aveiro and Porto and is available to be used by students, faculty, and staff members of LAQV. At the University of Porto, it is also possible to have access to high-resolution Atomic Force Microscopes and to Fluorescence Lifetime Imaging (FLIM) on a Confocal Microscopy.

EQUIPMENT – FCT NOVA

- AFM Workshop TT-AFM

EQUIPMENT – U.PORTO

- XPS Kratos Axis Ultra HSA
- FEI Quanta 400FEG ESEM / EDAX Genesis X4M
- AFM Workshop TT2-AFM
- Prototype high-resolution AFM
- AFM | Veeco Metrology Multimode / Nanoscope IVA
- Confocal Microscopy - Fluorescence Lifetime Imaging (FLIM), Leica - STELLARIS 8 FALCON

EQUIPMENT – U.AVEIRO

- Two SEM/EDS/ microscopes, of which additionally has EBDSD Electron lithography
- Two HRTEM/STEM (200, 300 kV) microscopes, and a cold field emission STEM with SEM image mode of atomic resolution.

PILOT PLANT

FCT NOVA

The Pilot Platform has a total area of 350 m² and comprises educational and research equipment of multi-stage extraction, supercritical extraction and membrane processing. The LAQV pilot plant is used for training and education of Master and graduate students in the fields of Chemical Engineering/ Biochemical Engineering. It is also used to provide samples at the kg scale in collaborative projects with industry, allowing scale-up of processes developed at the laboratory scale. LAQV researchers use it mainly for the design of clean separation methods.

Supercritical Fluid Extraction (SFE) Pilot Equipment

The SFE pilot units are used for the design and optimization of separation processes. The facility enables to produce samples up to the kg-scale, in collaborative projects with the industry, providing the scale-up of processes developed at the laboratory scale

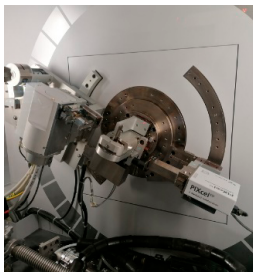
- 5 AISI 316 Extractors (up to 500 bar and 80 °C; Volume capacity: 4 with 1800 cm^3+ 1 with 3800 cm^3)
- 2 AISI 316 Cyclones (up to 450 bar; Volume capacity: ca. 200 cm^3)
- Countercurrent packed column (4 m high; 4 cm of internal diameter; Sulzer structured gauze packing; up to 300 bar and 100 °C; Gas flow up to 20 kg/h)

Membrane Pilot Equipment

The membrane pilot units were conceived to be operated in place or to be installed and operated in industrial sites under contract or in the frame of joint projects.

- Membrane micro/ultrafiltration unit with polymeric capillary membranes
- Membrane micro/ultrafiltration unit with ceramic SiC membranes
- Membrane nanofiltration unit
- Reverse Osmosis unit
- Pervaporation unit
- Electrodialysis unit

X-RAY DIFFRACTION



The X-ray Diffraction facility provides the screening, testing, and complete data collection from X-ray diffraction of single crystals, either from protein or small molecule compounds. Data is obtained in the in-house X-ray diffractometer or through access to synchrotron macromolecular crystallography beamlines (ESRF, DIAMOND, SLS, SOLEIL, DESY, ALBA). Diffraction is performed using an X-ray diffractometer, and complete data are collected according to experimental requirements. A microspectrophotometer is available and can be coupled to the goniometer. Dedicated software permits indexing, integration, scaling of data, and 3D structure solution. Small-Angle X-ray Scattering (SAXS) experiments can be performed through access to synchrotron facilities. A service for Single Crystal X-ray Structure Determination of small molecules is available.

EQUIPMENT – FCT NOVA

- Bruker D8 Venture,Single-crystal X-ray Diffractometer with IμS 3.0 microfocus Mo-K and Cu-K X-ray sources, KAPPA four-circle goniometer, Photon 100 CMOS detector, Oxford Cryostream 600 series for low temperature data collections (down to 100 K)
- Benchtop X-Ray Diffractometer RIGAKU, model MiniFlex II with: Cu X-ray tube (30KV/15 mA) Scanning range: 3~ +145°; Scanning speed: 0,01~ +100°/min; Minimum step width: 0,01°.

EQUIPMENT – U.AVEIRO

Single-Crystal X-Ray Diffractometers

- Kappa APEX, Single-crystal X-ray Diffractometer with Mo radiation, 4-circle Nonius Kappa Goniometer, APEX II CCD detector, Oxford Cryostream 700 series for low temperature data collections (up to 100 K)
- D8 Quest, Single-crystal X-ray Diffractometer with Mo radiation, TRIUMPH Monochromator, 4-circle Bruker Kappa Goniometer, PHOTON II CMOS detector, Oxford Cryostream 700 series for low temperature data collections (up to 100 K)

Powder X-Ray Diffractometers

- PANalytical Empyrean powder X-ray Diffractometer with Cu radiation, Highperformance PIXcel-1D detector, reflection/transmission geometry with rotating sample and "beam knife", K1 monochromator - Johansson Monochromator, spinning capillary, Bragg–Brentano optics and focusing geometry, parallel beam geometry with Göbel mirror
- X'Pert Powder X-ray Diffractometer with Cu radiation, High-performance PIXcel1D detector, Reflection/transmission geometry with rotating sample and "beam knife", multi-purpose support for large samples, Bragg–Brentano optics and focusing geometry, 15-Slot automatic sample changer, Anton Paar HTK16 High temperature furnace, high vacuum system with a turbomolecular pump
- X'Pert Pro MRD, High-resolution X-ray Diffractometer with Cu radiation a 4-circle goniometer, Göbel mirror for parallel incident beam, 4-Crystal asymmetrical (2 2 0) Ge monochromator for the incident radiation, Open 1/2 circle Eulerian cradle with motorized XYZ sample stage.

NONTHERMAL FOOD PROCESSING TECHNOLOGIES

High pressure processing (HPP) is a nonthermal food pasteurization technology that makes use of elevated hydrostatic pressures (commercially up to 600 MPa) to eliminate vegetative pathogenic microorganisms of foods, allowing enhancing food safety and considerably extend the shelf-life, especially for heat-sensible food products. The fact that no heat is applied allows to better preserve the fresh(er)-like attributes of foods. HPP is also being used to create clean-label food products, wherein the use of chemical additives can be significantly reduced/avoided, promoting the consumption of healthier foods, or even to obtain new foods with improved texture characteristics (cold texturization).

Pulsed electric fields and ultrasounds are other two nonthermal food processing technologies, with applications within a large spectra of food matrices and processes, e.g., for fermentative and extraction processes.

EQUIPMENT – U.AVEIRO

High Pressure Processing Equipment

- Lab scale high pressure equipment up to 700 MPa and temperature between -20 to 90 °C
- Pilot scale high pressure equipment up to 700 MPa and temperature between -20 to 90 °C
- Industrial scale high pressure equipment up to 600 MPa

Pulsed electric fields

- Pilot scale PEF equipment (30 kV, continuous operation mode)

LAQV
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LABORATÓRIO ASSOCIADO
PARA A **QUÍMICA VERDE**

LAQV
2020-2025 ACTIVITY REPORT & HIGHLIGHTS

PORTO
Abril 2026