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LABORATÓRIO ASSOCIADO
PARA A **QUÍMICA VERDE**

2020 ACTIVITY REPORT & HIGHLIGHTS

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

LAQV
2020 ACTIVITY REPORT & HIGHLIGHTS

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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 2020-2023, 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.

GOVERNANCE

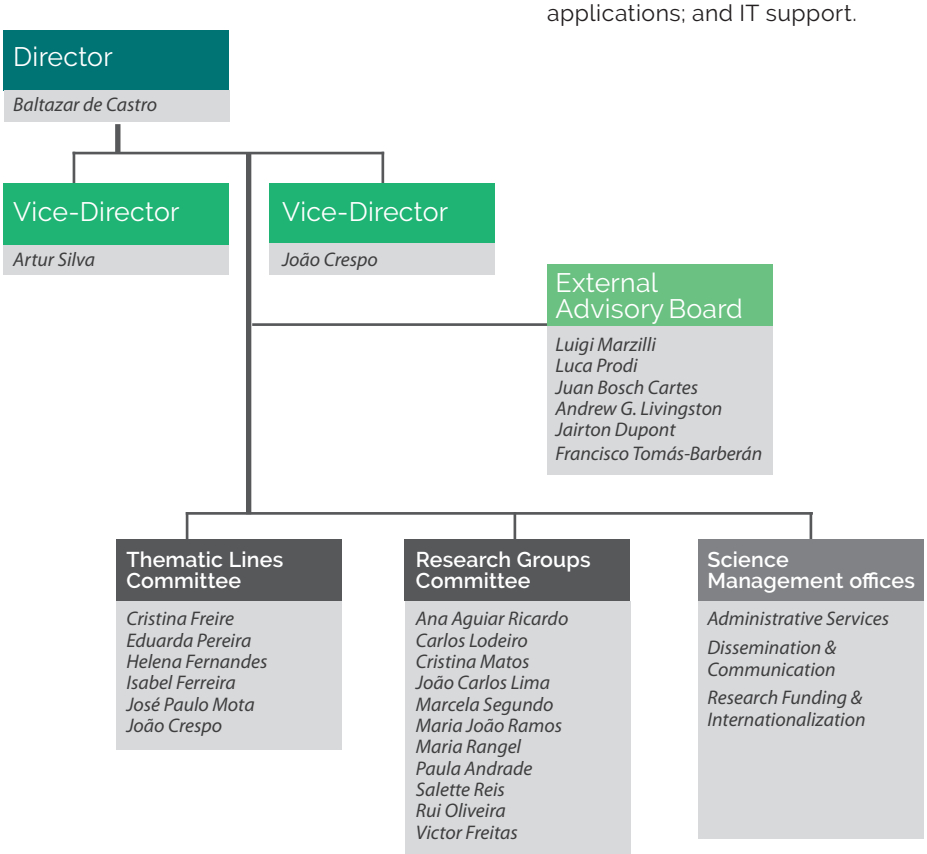
LAQV is managed through a simple and efficient governance structure, with well-defined responsibilities and clearly allocated tasks, which has ensured the smooth implementation and successful execution of its activities since 2001.

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.

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 six 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. Health & Wellbeing
B. Environment - Monitoring & Analysis
C. Energy - Clean & Renewable
D. Food & Nutrition
E. Resource Efficiency - Sustainable Processing
F. Functional Materials

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

1. Molecular synthesis
2. Natural products: chemistry and bioactivity
3. Analytical development
4. (Bio)Chemistry & omics
5. Environmental chemistry
6. (Bio)Chemical process engineering
7. Cultural heritage and responsive materials
8. Materials for sustainability and wellness
9. Nanoplatforms
10. Food quality and technology
11. High Performance Computing in Molecular Modelling

FACTS & FIGURES

→ Our community

453
Senior Researchers

22
Other doctorate Researchers

26
Post-doctoral fellows

356
PhD students

172
MSc students

117
Other researchers (research grantees and technicians

1146 members... From 31 different countries.

→ Our numbers in 2020

989
Indexed publications

24780
Citations*

360
Research Projects in execution

20 M€
Funding

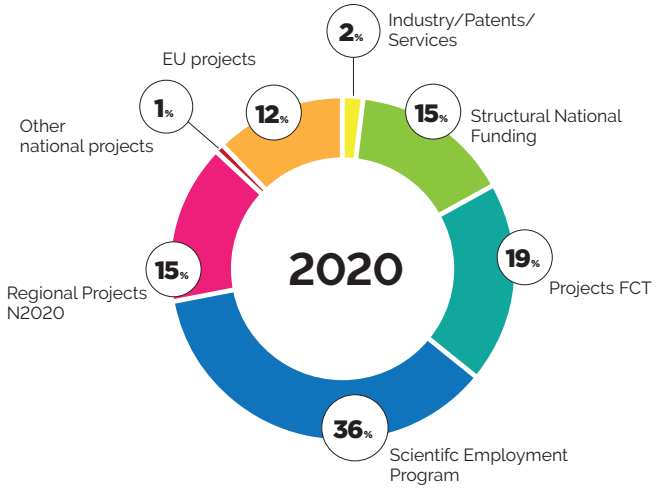
15
Patents

42%
International Coauthoring

31
PhD dissertations

154
MSc dissertations

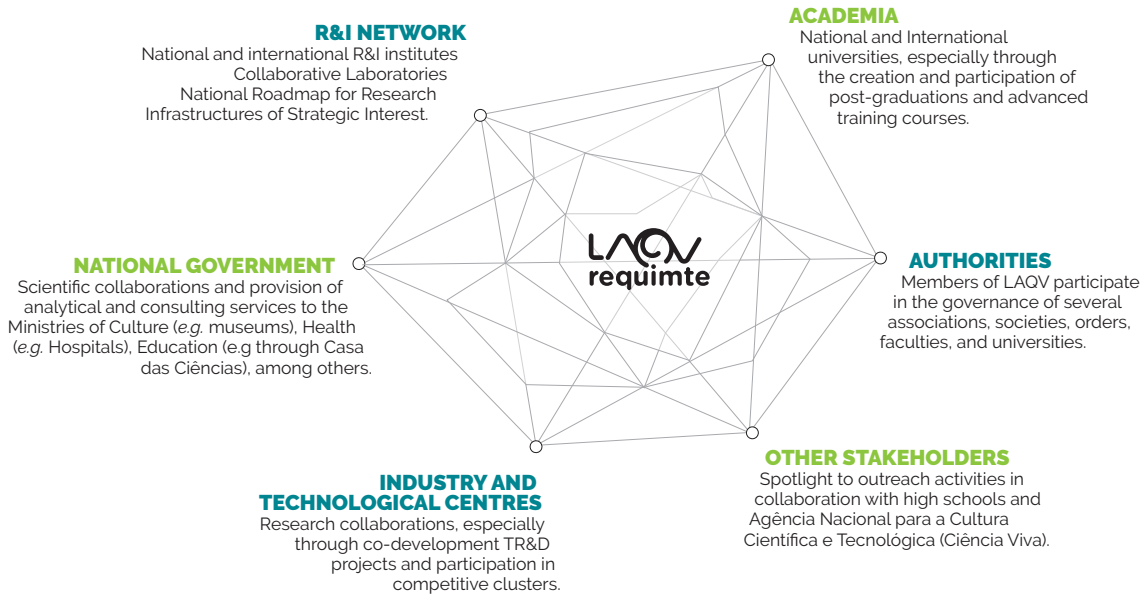
* total number of citations in 2020 for all the publications published since the beginning of LAQV



TOTAL

20 M€

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



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Thematic Lines

HEALTH & WELLBEING

Thematic Line Coordinator:
Maria Helena Raposo Fernandes

Research Groups that contribute to the Thematic Line:

- Molecular Synthesis
- Natural Products: Chemistry and Bioactivity
- Analytical Development
- Environmental Chemistry
- Nanoplatforms
- Cultural Heritage and Responsive Materials
- (Bio)Chemistry & OMICS
- Food Quality and Technology
- (Bio)Chemical Process Engineering
- Materials for Sustainability and Wellness

The Health and Wellbeing thematic line sets the ground on the 21st Century Grand Global Challenges by promoting a constructive guidance on the lives of individuals and societies. The focus is the translation of conceptual models and research into operative devices and practices that contribute effectively to improve healthy life expectancy, wellbeing, and enjoyment of life. Improving population's health and wellbeing - within a clinical, communal, and societal perspective, embraces other important benefits, including the economic, social, and environmental dimensions, as fundamental pillars for the sustainable development global strategy.

Multidisciplinary research groups put their efforts into creating strategic frameworks by embracing Sustainable & Green Chemistry design principles. Groundbreaking research and development is accomplished through a unity of approach, setting a global focus on:

- The design, advancement, and upscaling of efficient and sustainable ways to remove hazardous chemicals from the environment;
- The development of "nutrition-sensitive" food systems, aiming for improved food quality and safety for healthy eating;
- The creation of innovative analytical solutions for monitoring health status and for the diagnosis and prognosis of disease progression;
- The validation of the efficacy and biosafety of new bioactive compounds and medicines, targeting specific markers for communicable and noncommunicable diseases;
- The design of novel compounds with antimicrobial, anti-malarial, antioxidant, and anti-cancer properties and study of structure-activity relationships;
- The development and characterization of groundbreaking biomedical materials, implants and advanced strategies for drug delivery, heightened tissue healing and regeneration;
- Entrepreneurship & Business Development.

The team shares a common vision of excellence, which encompasses a a) valued breakthrough scientific knowledge in strict alignment with existing societal demands; b) unity in the interdisciplinary scientific background; and c) anticipation of new societal needs and challenges to foster ahead scientific knowledge. The ultimate goal is scientific knowledge transfer to generate scalable outcomes and solutions.

Regular activities include the dissemination of the research results in academic fora, presentations to targeted stakeholders, dynamic working out of the university-industry interface, and fostering commercialization activities, i.e. invention disclosures, patent application, and start-up creation. This strategy has been fruitful in acknowledged benefits for health care, scientific productivity, and economic development.

ENVIRONMENT – MONITORING & ANALYSIS

Thematic Line Coordinator:
Eduarda Pereira

Research Groups that contribute to the Thematic Line:
- Molecular Synthesis
- Natural Products: Chemistry and Bioactivity
- Analytical Development
- Environmental Chemistry
- Nanoplatforms
- (Bio)Chemistry & OMICS
- (Bio)Chemical Process Engineering
- Materials for Sustainability and Wellness

The main goal of this thematic line is to provide knowledge, technologies, methodologies, and products to assess the effects and possible threat of contaminants and other stressors on marine, freshwater, and terrestrial ecosystems, enabling their protection and the sustainable exploitation of the services they provide to the Society.

Priority research activities are:

- assessment of climate changes and human pressure on marine, freshwater, and terrestrial organisms and ecosystems;
- monitoring, modelling, and risk assessment of contaminants in ecosystems;
- analysis of environmental matrixes for contaminants of emerging concern, such as pharmaceuticals and personal care products, pesticides, disinfection by-products, wood preservatives, major, minor and trace elements namely Hg, Cd, As, and Pb, anions (cyanides, phosphates, carbonates, halydes), and metallic and non-metallic nanoparticles;
- monitoring plans of contaminants in waters, soils, sludges, sediments, plants, and fauna;
- assessment of drinking water quality;
- analysis of food matrices, food safety, and security;
- elaboration of mitigation strategies to decrease food, water, and soil contamination;
- development of membranes for water treatment and reuse;
- design and testing of sensors for a fast screening of contaminants;
- development of innovative products and low carbon technology;
- use of biotechnology and molecular tools to address the impact of contaminants on cell cascades signaling;
- evaluation of indoor and outdoor air contaminants with emphasis on the most health-relevant particulate and gaseous pollutants, including personal exposure studies with emphasis on susceptible populations;
- development of innovative approaches for sample treatment, including automation and miniaturization, to cope with intensive environmental sampling and extended data acquisition.

The co-existence of groups devoted to synthesis, analytical development, and environmental chemistry permits the design and evaluation of new products to monitor environmental contaminants. A special emphasis is also placed on waste prevention and reduction, reusing, and recycling since these strategies can help to save natural resources and energy and reduce pollution. These activities are included in the research and innovation strategy of LAQV and aim to support, among others, the Water Framework Directive and the Integrated Coastal Management. The Line is also developed in close cooperation with the economic sector, environmental policy-making authorities at regional, national, and international level, and with other stakeholders. Furthermore, it also contributes to LAQV Science and Society program through outreach activities with schools, children, families and the general public, and by participating in advanced training courses in the frame of PhD, Master, Integrated Master, and BSc programs.

ENERGY – CLEAN & RENEWABLE

Thematic Line Coordinator:
José Paulo Mota

Research Groups that contribute to the Thematic Line:
- Molecular Synthesis
- Environmental Chemistry
- Cultural Heritage and Responsive Materials
- (Bio)Chemistry & OMICS
- Food Quality and Technology
- Materials for Sustainability and Wellness

We are strongly committed over the next years to help find sustainable solutions for energy conversion, storage, distribution, and recycling, gathering the know-how of several LAQV Research Groups in Synthesis, Materials, Food, Environmental Chemistry, Process Engineering, and OMICS. The coordination of research efforts will proceed through the organization of short events, like mini-symposia and specialized workshops. The scientific program of this Thematic Line focus three research vectors:

1. Climate change mitigation and carbon dioxide

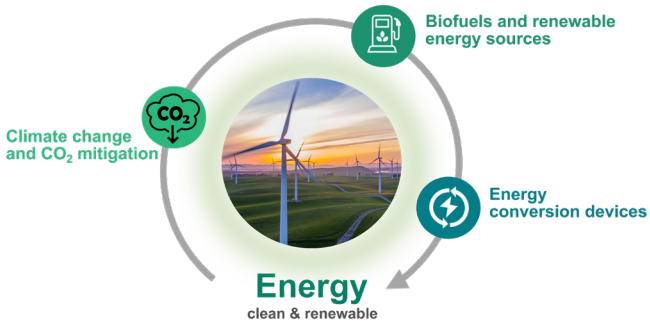
We shall pursue and expand our research on CO_2 capture and utilization, comprising capture with ionic liquids, eutectic solvents, membranes, and novel adsorption processes. Furthermore, we will focus on new membranes incorporating ionic liquids and metal-organic frameworks (MOFs), as well as novel cyclic adsorption processes for purification of industrial gaseous streams; and carbon dioxide (electro)chemical reduction to fuels and its hydrogenation into CH_4. Specific enzymes, such as formate dehydrogenase (biocatalyst for formate/CO_2 reversible interconversion), will be used in emission mitigation. They will be incorporated in enzymatic cascade bioreactors, aiming at the production of biofuels as secondary products. We shall continue studying new nanostructured materials, such as MOFs and clathrates, to evaluate their physicochemical properties in the context of storage/release of gases of pressing industrial relevance. CH_4/CO_2/CO clathrates are critical for a better design of oil pipelines and a clearer understanding of the Earth permafrost.

2. Energy conversion devices

Photovoltaic cells based on metallic chalcogenides are being developed to convert solar light into electricity, specifically, using CdTe technology. We are particularly interested in the conversion of thermal energy into electric energy (and vice-versa), using solid-state thermoelectric devices. In this context, we shall focus our efforts on the development of new nanochemical materials based on Tellurium for the production of bimetallic nanostructures (MxTey) with new optoelectronic properties. The nanomaterials projected are based on less toxic metals, such as Cu, Zn, Ag, Pd, or Pt. We will improve natural dye performance in DSSCs and up and down conversion emitting glasses to increase energy efficiency.

3. Biofuels

We shall pursue our research on enhancing biogas and methane yields for later upgrading to biomethane through anaerobic co-digestion and post-purification of the organic fraction of municipal solid wastes and other types of biomass.



FOOD & NUTRITION

Thematic Line Coordinator:
Isabel Ferreira

Research Groups that contribute to the Thematic Line:
- Molecular Synthesis
- Analytical Development
- Environmental Chemistry
- Nanoplatforms
- (Bio)Chemistry & OMICS
- Food Quality and Technology
- (Bio)Chemical Process Engineering

This thematic line is focused on improving the quality of food by ensuring its authenticity and controlling allergens, additives, and chemical contaminants. Moreover, it aims to enhance food nutritional and sensorial characteristics using optimized and advanced processing methods. Ultimately, this line ensures high levels of food safety and traceability and helps consumers to make informed choices. Our research activities are focused on conserving natural resources through the promotion of sustainable procedures/technologies that minimize food losses and waste and the implementation of circular economy principles across the whole food system, while reducing its environmental footprint. Thus, this line contributes to climate change mitigation and increases the quality of products by adding commercial value to them.

The Food & Nutrition thematic line is also focused on understanding the mechanisms that underlie the protective effects of nutrients and bioactive compounds and on reducing the incidence of non-communicable diet-related diseases. Therefore, this line is anchored to the work program of the Horizon Europe challenges and address the four key food and nutrition security priorities of FOOD2030 strategy, namely: Nutrition for sustainable and healthy diets; Climate smart and environmentally sustainable food systems; Circularity and resource efficiency of food systems; and Innovation and empowerment of communities.

This thematic line works on four main topics: a) innovative analytical methods for food compounds analyses; b) food composition and new technological processes that promote higher quality, nutritional properties, preservation/shelf-life, safety, and authenticity; c) understand the mechanisms of biologically active food components; d) recovery of high-value compounds from complex (bio)medium.

The main research vectors include, but are not limited to:

- multi-parametric chromatographic and spectroscopic methods for evaluation of nutrients, bioactive and aroma compounds;
- DNA-based methods for species identification and adulterants detection;
- electrochemical (bio)sensors for foodstuffs quality control that present high selectivity and sensitivity, while allowing portability and miniaturization;
- design of novel fertilizers;
- novel chemometric methods that provide real-time, non-destructive analysis in laboratory and industrial settings;
- testing the activity of beneficial and harmful food compounds by using *in vitro* human cells and tissues;
- use of non-invasive techniques to study animal metabolism and their environmental impact;
- extracting bioactive compounds from industrial wastes, including agro-industrial effluents and microalgae biomass, for novel technological applications;
- application of omics-based approaches to understand the patterns of expressed genes and proteins, to have new insights into complex regulatory networks and relevant genes to new biological processes.

RESOURCE EFFICIENCY – SUSTAINABLE PROCESSING

Thematic Line Coordinator:
João Crespo

Research Groups that contribute to the Thematic Line:
- Molecular Synthesis
- Analytical Development
- Environmental Chemistry
- Cultural Heritage and Responsive Materials
- (Bio)Chemistry & OMICS
- (Bio)Chemical Process Engineering
- Materials for Sustainability and Wellness

Development of clean (Bio)Chemical Processes and their application to the efficient use of resources represents a core activity of LAQV. This Thematic Line will bring together extensive expertise in membranes and adsorption, intensification of processes and use of green solvents, valorization of biomass and CO_2 utilization, design of new smart materials, and effective recovery of non-renewables sources. Contributions from several LAQV Research Groups, from Synthesis and Analytical Development to Cultural Heritage Conservation, Materials, and Process Engineering, will be required. Coordination of the scientific programme will act mainly by promoting networking activities, such as short meetings, workshops, and webconferences. It will also be highly committed to innovation fostered by collaboration with industry, taking advantage of an already existing record.

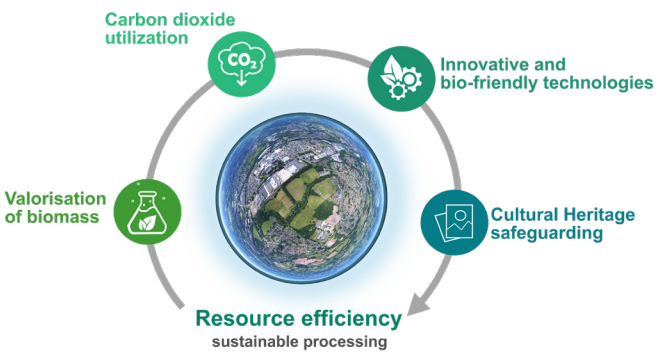
The main research efforts will focus on:

1. Valorization of biomass from local agroindustrial wastes (such as brewer spent grain and yeast, fruit peels and pomace, spent coffee, olive pomace, eggshell, and canned fish wastes). This will continue to be a key area, due to its potential to combine local industry-relevant projects with LAQV know-how in green processing, including clean production and separation processes, and green solvents. The use of systems biotechnology platforms and intensification of biotechnological processes will represent added value for some of these projects. The production of biodegradable microbial polymers will also use biomass feedstocks.

2. CO_2 utilization is another key development area, which will build on the extensive expertise on supercritical carbon dioxide as a solvent to venture into its chemical and electrochemical transformation. Apart from the power-to-gas and CO_2 capture schemes, carbon dioxide catalytic reaction with natural epoxides to produce polymers will be exploited, as well as reactions in heterogeneous media ionic liquid + carbon dioxide.

3. Cultural Heritage safeguarding, using cleaner and greener chemical methods will continue to be a "niche" application of LAQV expertise with a positive social impact, improving the image of Chemistry.

4. The use of innovative and bio-friendly technologies, namely involving supercritical fluid-based particle formation, micro-wave heating, plasma activation and imprinting methodologies, microfluidics, and layer-by-layer deposition, will envisage the synthesis and engineering of new (bio)materials for biomedical, pharmaceutical, and sensing applications. We shall pursue our research on membrane-based treatment of (agro)industrial and domestic effluents for water reuse; and integration of membranes with advanced oxidation processes.



FUNCTIONAL MATERIALS

Thematic Line Coordinator:
Cristina Freire

Research Groups that contribute to the Thematic Line:
- Molecular Synthesis
- Environmental Chemistry
- Nanoplatforms
- Cultural Heritage and Responsive Materials
- (Bio)Chemistry & OMICS
- Materials for Sustainability and Wellness

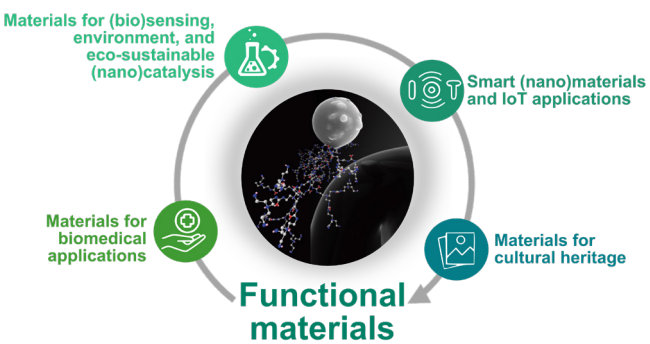
The design and fabrication of new advanced Functional Materials is a vital area of LAQV to address the 21st Century Grand Challenges.

We will be strongly committed to the development of new high-performance functional and smart (nano)(bio)materials through eco-sustainable, cost-effective, and scalable processes, to boost innovation in Biomedical, Catalytic, Environmental, Energy, and Textile Applications. This will be grounded on a strong cooperation between several LAQV Research Groups with expertise in Chemical Synthesis and Multifunctional and Responsive (Nano)Materials.

The coordination of R&D will proceed through networking activities, joint projects and will be highly committed with knowledge transfer/technological valorization in collaboration with Industry, with the goal of contributing to innovative products/technologies for Society.

The main research vectors will be.

- Materials for biomedical applications: we will pursue the design of innovative therapeutic solutions for drug loading and delivery systems, musculoskeletal reconstruction, tissue regeneration, and craniofacial applications. New functional nanomaterials will be developed and applied as cargo materials, fluorescent imaging nanodevices, and for monitoring biomedical/proteomic samples.
- Nanoplatforms for (bio)sensing and environment: we will continue integrating nanomaterials for wastewater treatment and (bio) sensors to achieve improved analytical performance for simultaneous detection and signaling of multiple analytes. The most efficient (bio)sensors will be included in portable devices and/or disposable devices, resulting in cost-effective point-of-care and/or *in situ* applications.
- Eco-sustainable (Nano)catalysts and Adsorbents: we shall pursue developing innovative catalytic technologies for wastewater remediation, fuels desulfurization, biomass valorization, energy-related reactions, selective catalysis, and gas adsorption, separation, and capture.
- Functional and smart (nano)materials and IoT applications: We shall continue the fabrication of (nano)materials with high-efficiency energy storage and/or responsive properties to be integrated into textiles/flexible substrates. These materials will be used to produce wearable technologies able to store energy, respond to external stimuli, and/or to power sensors and other electronic devices, aiming to address the needs of IoT applications. The electrochromic display technology developed by CHARM group & Ynvisible has been implemented in products with societal impact.
- Molecular building blocks with fine-tuned properties: to achieve all innovative (nano)(bio) materials with enhanced performance, we will continue pursuing their functionalization with molecular frameworks (chromic and antimicrobial molecules, peptides, carbohydrates, porphyrin, and dyes).
- In cultural heritage field: we will contribute to the history of plastics, to the preservation of historic photographic collections, and to the creation of an online access to Winsor & Newton artist materials supplier database.



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03

Research Groups

MolSyn
MOLECULAR SYNTHESIS

NATPRO
NATURAL PRODUCTS CHEMISTRY AND BIOACTIVITY

AnalytDev
ANALYTICAL DEVELOPMENT

BCO
(BIO)CHEMISTRY & OMICS

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, amino acids, alkylaminophenols, cyclitols, benzimidazoles, and peptides are functionalized with several chemical groups to produce molecules whose physicochemical properties are fine-tuned 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 dyes like coumarin and xanthene derivatives are preferential frameworks to produce innovative [Bio]materials with potential applications in Biomedical Engineering, [Bio] sensing, Catalysis, Separation, and Cleaner Energies.

RESEARCH OBJECTIVES [2020-2023]

The Molecular Synthesis group will continue to pursue work aiming for the preparation 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.

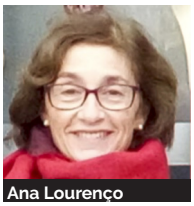
The development of innovative methods for chemical synthesis or computational design and study of relevant target molecules will be pursued. Additionally, we also intend to reinforce the development of new synthetic routes that use green chemistry procedures for the most common types of chemical reactions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

From 2018 the group has benefited from the incorporation of new members upcoming from the University of Aveiro. This circumstance reinforced the expertise in organic synthesis both in terms of new classes of molecules and materials and new methods of synthesis, including asymmetric synthesis. In particular, new molecules for chemo- and bio-sensing, photodynamic therapy of tumors, or the photodynamic inactivation of protozoa, bacteria, viruses, and fungi will be prepared.

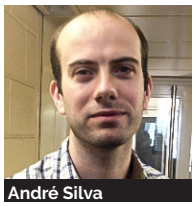
Regarding new methods, the use of Ohmic Heating (ΩH), which is an advanced thermal processing method that leads in most cases to better yields, better selectivity, and shorter reaction times, will be increasingly used in the synthetic routes under development.

RESEARCH TEAM

SENIOR RESEARCHERS


Ana Lourenço


Ana Margarida Silva


André Silva


Andreia Leite


Anthony Burke


António Santos


António Teixeira


Artur Silva


Augusto Tomé


Baltazar de Castro


Carla Queirós


Carlos Monteiro

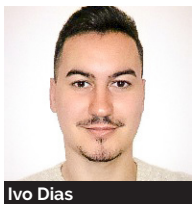

Carolina Marques

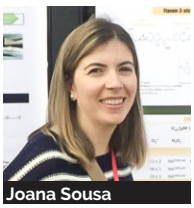

Catarina Ramos


Cátia Teixeira


Elisabete Carreiro


Florbela Pereira


Ivo Dias


Joana Sousa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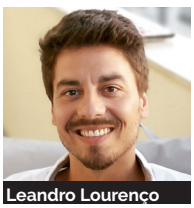
José Enrique Borges


Julían Martínez


Krasimira Petrova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Luísa Aguiar


Luísa Amaral


Luisa Ferreira

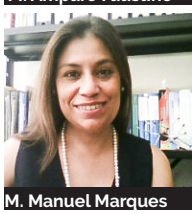

M. Amparo Faustino


Maria Rangel


M. Graça Neves


M. João Araújo


M. Luisa do Vale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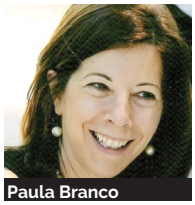
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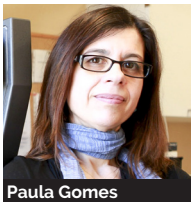
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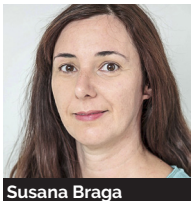
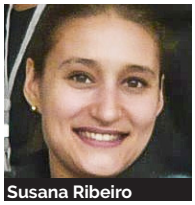

Susana Braga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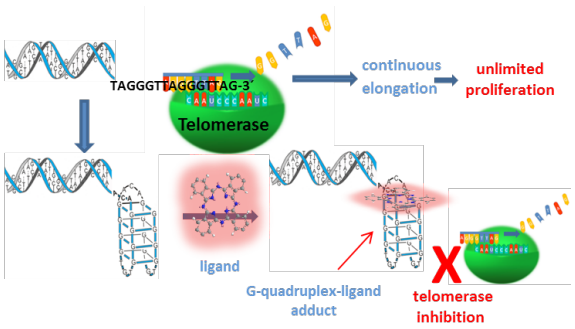
RESEARCH THEMES/ MOLECULES

Chemical synthesis of a wide diversity of molecules for:

BIOMEDICAL APPLICATIONS

- Biologial imaging, such as molecular probes for the detection of protein aggregates
- Oxygen heterocycles as potential antioxidant, anticancer and anti-diabetic agents
- Pyrazole-based compounds as potential antioxidant and anti-inflammatory agents
- Phthalocyanine–sulfonamide conjugates as potential antimicrobial agents
- Photosensitizers for photodynamic therapy of cancer (PDT) or photodynamic inactivation of microorganisms (PDI)
- Hybrids Based on Graphene Oxide, Porphyrin@GO, as Tools for Detection and Stabilization of DNA G-Quadruplexes
- Multicharged Phthalocyanines as Selective Ligands for G-Quadruplex DNA Structures
- Potentiation effect of potassium iodide on a PDT efficacy
- Synthesis of new functionalized nitroindazolylacetonitrile derivatives with higher antiproliferative effect against HeLa cancer cells
- ß-functionalized mono-charged porphyrinic derivatives as photosensitizers for photoinactivation of *Escherichia coli*
- Protonation of *meso*-tetraphenylporphyrin and its ß-functionalized derivatives by photogenerators of acidity in toluene and polymer film
- Cationic Porphyrin Formulation (FORM) and the tricationic porphyrin derivative [Tri-Py(+)-Me] are promising photosensitising candidates to photoinactivate *C. albicans* in blood plasma
- Synthesis of cationic corrole derivatives with antibacterial activity at micromolar concentrations against the Gram-negative bacterium *Allivibrio fischeri*



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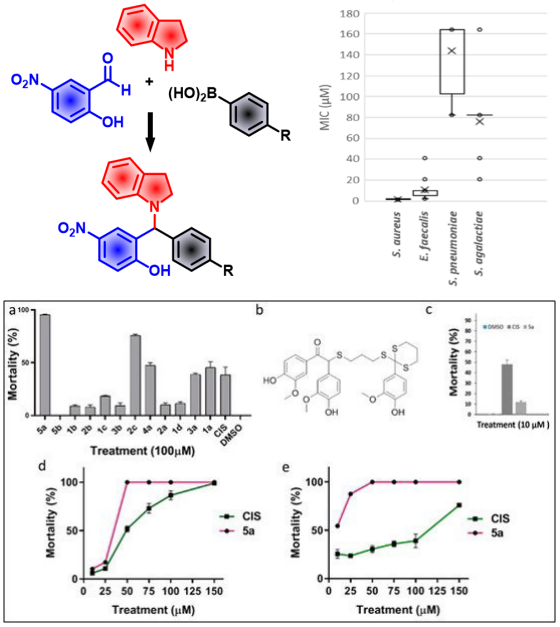
RESEARCH THEMES/ MOLECULES

Chemical synthesis of a wide diversity of molecules for:

BIOMEDICAL APPLICATIONS (CONT.)

- Effective photodynamic approach to control *S. aureus* infection in skin, with a tetra-cationic porphyrin, inactivating the bacterium to the detection limit after three successive cycles of treatment or after one cycle by using the combination the photodynamic treatment and the antibiotic ampicillin
- Chelates and chelators to address iron imbalance-related diseases and diabetes
- New hetero-arylidene-9(10H)-anthrone derivatives with antiproliferative and highest cytotoxic activities
- Nature-inspired molecules, from marine compounds and plants, to bacterial cell wall disaccharide components, and sugar-based compounds with antimicrobial and cytotoxic activities
- Phenol derivatives as potential antibacterial and cytotoxic agents for inhibition of glioblastoma and prostate cancers.
- Vicinal diols, boroxazolidones and orthothioesters as novel molecular scaffolds for treatment of glioblastoma multiforme
- Chemiluminescent photosensitizers for photodynamic therapy
- Peptidomimetics to address neurodegenerative disorders
- Dual-action antimicrobial and wound healing peptides for topical treatment of severe skin and soft tissue infections
- Ionic liquids derived from active pharmaceutical ingredients
- Amino acid-derived gemini surfactants for drug delivery



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RESEARCH THEMES/ MOLECULES

Chemical synthesis of a wide diversity of molecules for:

AGRICULTURAL, ENVIRONMENTAL AND FOOD APPLICATIONS

- *N*-confused porphyrin immobilized on solid supports for metal ions sensing
- An efficient hybrid adsorbent based on silica-supported amino pentacarboxylic acid for water purification
- New hybrid adsorbent based on porphyrin functionalized silica for heavy metals removal
- Supramolecular hybrid material based on engineering porphyrin hosts for an efficient elimination of lead(II) from water
- Control of *Pseudomonas syringae* pv. *Actinidiae* in kiwifruit plants, by antimicrobial Photodynamic Therapy (apdt) using cationic porphyrin and sunlight, without leaves damaging
- Highlighting shikimic acid pathway as a source of research topics for improving sustainability in chemistry
- Chelators for regulation of iron uptake and storage in plants
- Pyridinone chelators for iron speciation in waters
- Peptides and proteins of relevance in wine properties
- Ferrocene-based imine ligands as selective sensors for mercury(II)
- Organometallic molecules as catalysts for CO_2 functionalization and other chemical reactions
- Porphyrin derivatives as potential antimicrobial agents
- Porphyrin derivatives and analogues as chemosensors for anions and metal ions
- Cellulose-based polymer with wine stabilization properties – technology transfer process
- Imine ligands for mercury detection

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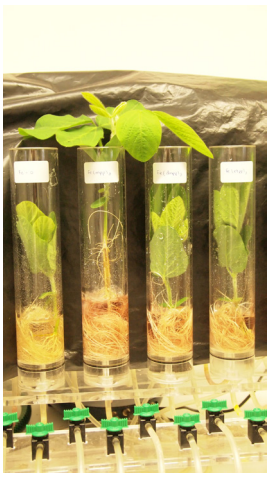
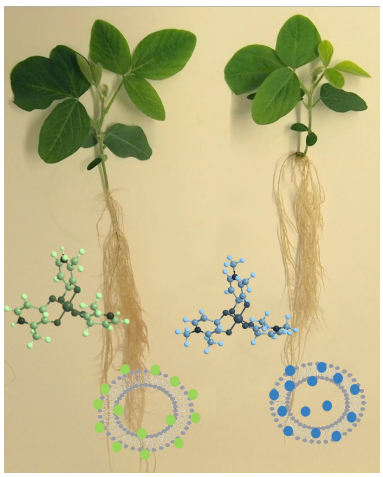
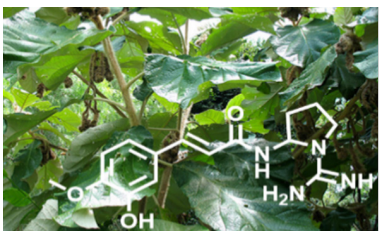


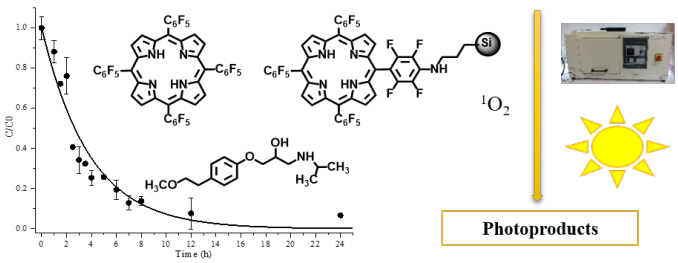




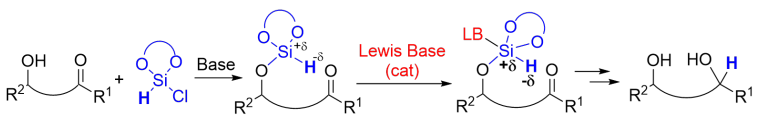
RESEARCH THEMES/ MOLECULES

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



- Homogeneous oxidation of indole to afford indigo dye
- *N*-Heterocyclic Olefin-based catalysts for lactam's synthesis and metal-catalyzed synthesis of *N*-heterocycles
- 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



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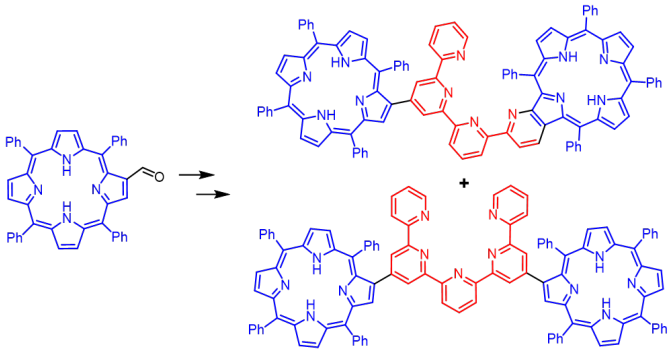
RESEARCH THEMES/ METHODS

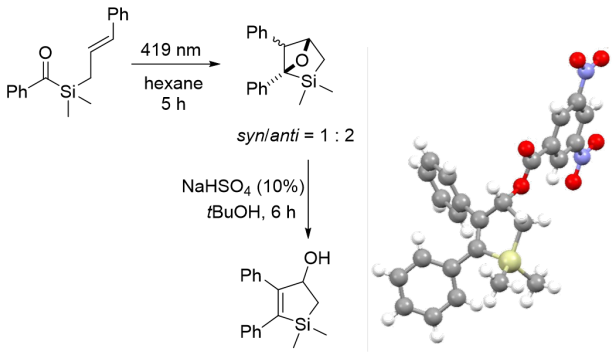
Development of innovative methods for the chemical synthesis or computational design and study of relevant target molecules

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



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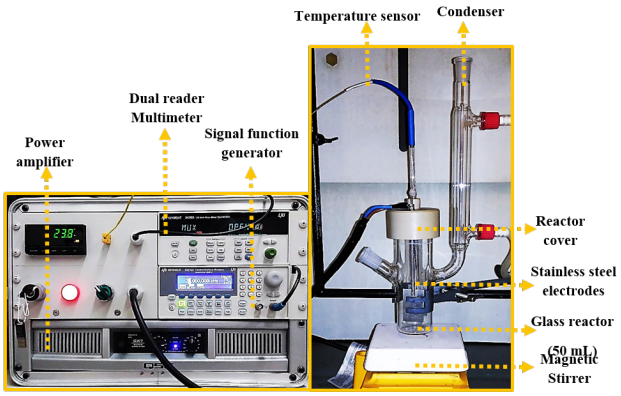
RESEARCH THEMES/ METHODS

SYNTHETIC APPROACHES (CONT.)

- One-pot synthesis of amides
- Chemoenzymatic synthesis of complex carbohydrates
- Innovative approach for an efficient solid-phase one-pot synthesis of a EGFR inhibitor
- 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

COMPUTATIONAL APPROACHES

- Density Functional Theory (DFT) studies for mechanism elucidation
- DFT and Time-Dependent DFT orbital analysis and vertical excitations of functional materials.
- Machine learning to enable prediction of the specific optical rotation[79,80] and of the molecular dipole moments
- Improved navmol molecular editor for blind users

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RESEARCH THEMES/ MATERIALS

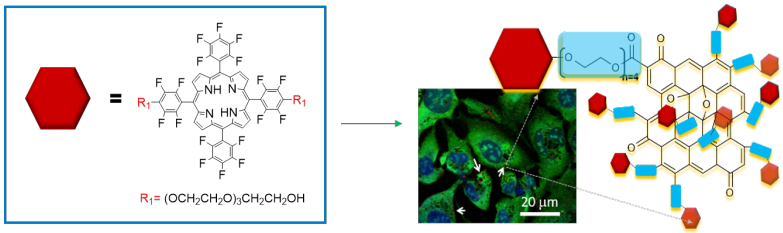
Use of molecular synthesis tools towards development of innovative [bio]materials with potential applications in Biomedical Engineering, Drug Delivery, Separation Techniques and Cleaner Energies

BIOMEDICAL ENGINEERING

- Hybrids based on graphene oxide and porphyrin as tools for detection and stabilization of DNA G-Quadruplexes.
- Synthesis and characterization of photoactive porphyrin and poly(2-hydroxyethyl methacrylate) based materials with bactericidal properties.
- Synthesis and characterization of photoactive porphyrin and poly(2-hydroxyethyl methacrylate) based materials with bactericidal properties.
- peptide-tethered antimicrobial coatings for bone implants.

IMAGING

- Novel hybrid materials based on graphene derivatives (graphene oxide, nanographene oxide, graphene quantum dots (GQD)) covalently linked to porphyrins.



SEPARATION AND CLEANER ENERGIES

- Hybrids of graphitic carbon nitride sensitized with free-base mesotetrakis(carboxyphenyl) porphyrins for efficient visible light photocatalytic.
- ß-Cyclodextrin as a precursor to holey C-Doped g-C_3N_4 nanosheets for photocatalytic hydrogen generation.
- Boranils, boron-diketonates, dibenzalazines, and other all-organic fluorophores, for applications in luminescent materials.
- Coumarin-based chromophores for dye-sensitized solar cells.

SELECTED PUBLICATIONS

77 D. Gago, et al., Membranes, 2020, 10: 13. doi: 10.3390/membranes10010013

78 R. Chagas, et al., Cellulose 2020, 27: 1965-1974. doi: 10.1007/s10570-019-02952-6

79 C. Martins, et al., Sep. Purif. Technol., 2020, 250, 1169832. doi: 10.1016/j.seppur.2020.116983

80 A. I. Rodrigues, et al., Dalton Transactions 2020, 49(29), 10185–10202. doi: 10.1039/d0dt01845g

81 C. Monteiro, et al., Molecules 2020, 25: 3046. doi: 10.3390/molecules25133046

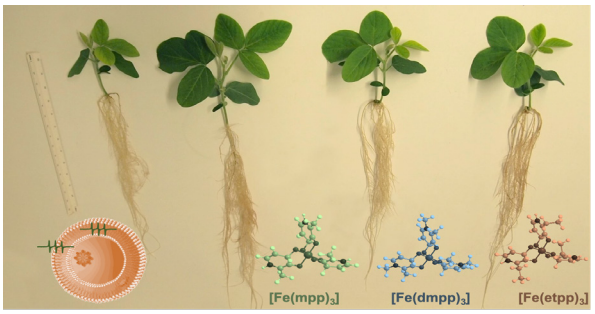
82 C. Monteiro, et al., Molecules 2020, 25: 3046. doi: 10.3390/molecules25133046

83 C. I. M. Santos et al., Carbon 2020, 166, 164-174. doi: 10.1016/j.carbon.2020.04.012

84 J. M. D. Calmeiro et al., Dyes and Pigments, 2020, 177, 108280. doi: 10.1016/j.dyepig.2020.108280

HIGHLIGHTS

DESIGN OF FE FERTILIZERS TO ADDRESS IRON DEFICIENCY CHLOROSIS



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

Plant Direct, 2020, 4(8), e00256

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.

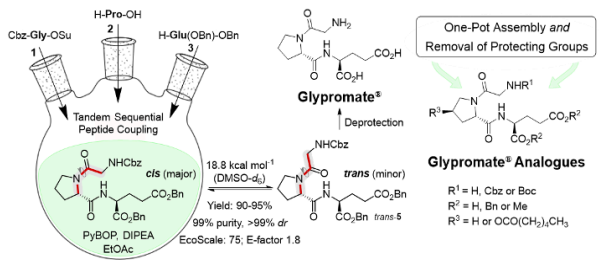
The results regarding the effectiveness of the [Fe(3,4-HPO)3] chelates to prevent IDC demonstrate that: (a) all three chelates are able to deliver Fe to plants and (b) their efficacy is dependent on the ligand following the order [Fe(mpp)3]> [Fe(dmpp)3]> [Fe(etpp)3].

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.

The studies performed for chelate [Fe(mpp)3] at variable concentration and pH values of the hydroponic culture medium demonstrate that the compound may be an efficient Fe fertilizer, even at lower dosages than those previously described and used for the commercially available fertilizers.

HIGHLIGHTS

STRATEGY FOR THE ASSEMBLY OF GLYPROMATE® AND ITS STRUCTURALLY-RELATED ANALOGUES



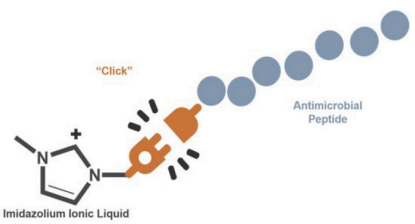
This work describes an improved and greener methodology of solution-phase synthesis for the preparation of Glypromate® (glycyl-L-prolyl-L-glutamic acid, GPE), a potent neuropeptide for applications in neurodegenerative conditions such as Huntington's, Parkinson's and Alzheimer's diseases. This protocol comprises the assembly of the perbenzylated form of Glypromate® [Cbz-Gly-Pro-Glu(OBn)-OBn (5)] from L-proline. Following a tandem sequential peptide coupling strategy, two chemoselective peptide bonds are formed without the need for purifying the intermediates ensuing a one-pot fashion synthesis. EcoScale score and E-factor were selected as the green metrics to assess the environmental impact of the preparation of tripeptide 5 using this protocol. After optimization and application of greener conditions, intermediate 5 was obtained with 95% global yield and 99% purity (NMR, HRMS, and rp-HPLC), with excellent final EcoScale score of 75 out of 100 and global E-factor of 1.8. Glypromate® is achieved by removing N- and C-protecting groups by hydrogenolysis using Pd/C as the catalyst in 98% yield, avoiding chromatographic techniques. Moreover, the protocol ensures stereochemical integrity (determined by VT-NMR and rp-HPLC) and was also successfully applied for the preparation of structurally-related Glypromate® analogues with higher degree of molecular complexity compatible with functionalized amino acids with different side chains. For the first time a one-pot protocol for the assembly of tripeptides with the removal of protecting groups in the same reaction vessel is reported.

A sustainable strategy for the assembly of Glypromate® and its structurally-related analogues by tandem sequential peptide coupling.

Green Chemistry 2020, 22, 3584-3596

"CLICKING" STRATEGY FOR ANTIMICROBIAL AGENTS

A covalent conjugate between an antibacterial ionic liquid and an antimicrobial peptide was produced via "click" chemistry, and found to retain the parent peptide's activity against multidrug-resistant clinical isolates of Gram-negative bacteria, and antibiofilm action on a resistant clinical isolate of Klebsiella pneumoniae, while exhibiting much improved stability towards tyrosinase-mediated modifications. This unprecedented communication is a prelude for the promise held by ionic liquids -based approaches as tools to improve the action of bioactive peptides



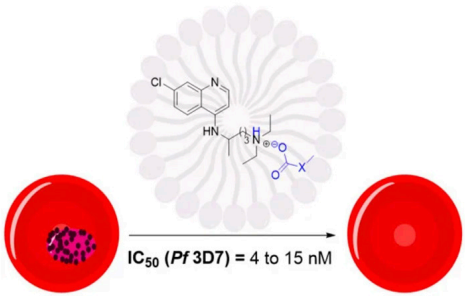
"Clicking" an Ionic Liquid to a Potent Antimicrobial Peptide: On the Route towards Improved Stability .

International Journal of Molecular Sciences 2020, 21:6174.

HIGHLIGHTS

ACTIVE IONIC LIQUIDS FOR THE RESCUING OF CHLOROQUINE

Ionic liquids derived from classical antimalarials are emerging as a new approach towards the cost-effective rescuing of those drugs. Herein, we disclose novel surface-active ionic liquids derived from chloroquine and natural fatty acids whose antimalarial activity in vitro was found to be superior to that of the parent drug. The observed parallelism between surface activity and antimalarial activity hardly seems coincidental, meaning that this activity, despite being due primarily to the bioactive cation, is also significantly influenced by the amphipathicity and surface activity conveyed by the fatty carboxylate. Furthermore, the ability of CQ-derived SAILs to co-assemble into colloidal nanostructures, strongly suggests that these systems could potentially act both as drugs and as enhanced drug delivery systems.

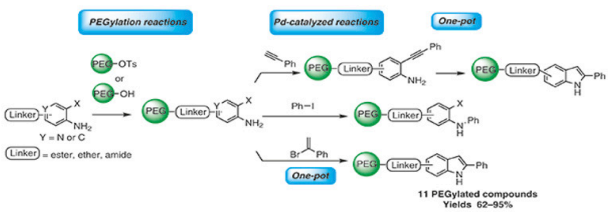


Building on Surface-Active Ionic Liquids for the Rescuing of the Antimalarial Drug Chloroquine.

International Journal of Molecular Sciences, 2020, 21:5334.

SUSTAINABLE METAL-CATALYSED SYNTHESIS AND FUNCTIONALIZATION OF N-HETEROCYCLES

A soluble polymer support - PEG2000 was applied on Pd-catalyzed reactions to improve the functionalization of aromatic amines and the synthesis of N-heterocycles. PEG-supported anilines were found to be suitable substrates for Pd-catalyzed N-arylation, Sonogashira and Heck reactions. PEGylated substrates were prepared in yields up to 94%. Indole core was attained in 82% and 62% yields, via two different routes.



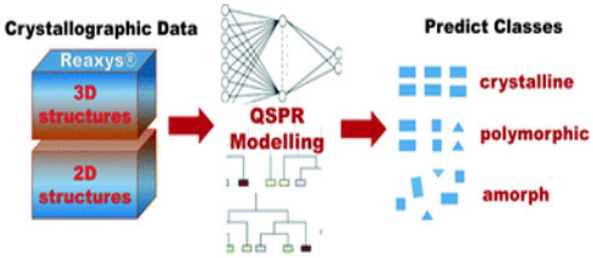
Sustainable metal-catalysed synthesis and functionalization of N-heterocycles.

Polymer Support, Synlett 2020, 31(20): 2027-2034

HIGHLIGHTS

MACHINE LEARNING METHODS TO PREDICT THE CRYSTALLIZATION PROPENSITY OF SMALL ORGANIC

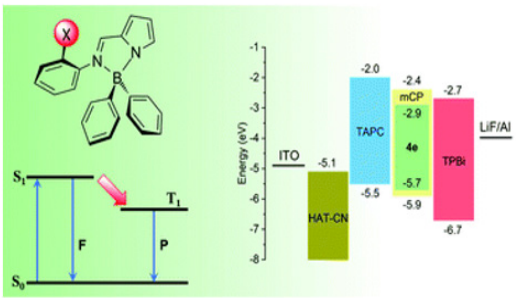
Machine learning (ML) algorithms were explored for the prediction of the crystallization propensity based on molecular descriptors and fingerprints generated from 2D chemical structures and 3D molecular descriptors from 3D chemical structures optimized with empirical methods. A training data set with 40 462 organic molecules was used to build the models, which were validated with an external test set comprising 17 353 organic molecules. Several ML algorithms such as random forest (RF), support vector machines (SVM), and deep learning multilayer perceptron networks (MLP) were screened. The best performance was achieved with a consensus classification model obtained by RF, SVM, and MLP models, which predicted the external test set with an overall predictive accuracy (Q) of up to 80%.



Machine learning methods to predict the crystallization propensity of small organic.

CrystEngComm, 2020, 22, 2817

LUMINESCENT HALOGEN-SUBSTITUTED 2-(N-ARYLIMINO)PYRROLYL BORON COMPLEXES: THE INTERNAL HEAVY-ATOM EFFECT



Luminescent halogen-substituted 2-(N-arylimino)pyrrolyl boron complexes: the internal heavy-atom effect

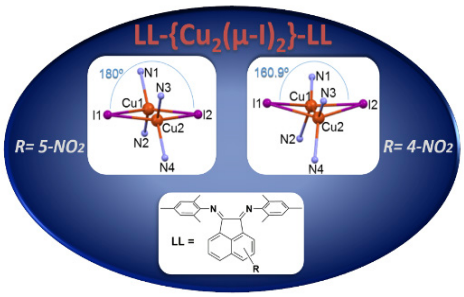
Dalton Transactions 2020, 49(29), 10185–10202

The internal heavy atom effect in luminescent boron complexes – In the production of luminescent emitters, there is already a variety of options based on fluorescent and/or phosphorescent chromophores, or in the newest thermally activated delayed fluorescent (TADF) molecules. Tetracoordinate iminopyrrolyl boron complexes are an example of such luminescent molecules. In this context, we recently synthesised and characterised a set of new boron complexes containing different halogens as substituents in the N-aryl ring. Their photophysical characteristics have been thoroughly studied, showing that these complexes exhibit an internal heavy atom effect strongly controlled by the position of the halogen atom in the N-aryl ring of the ligand moiety. Phosphorescence emission was found for some of the synthesized halogen-substituted boron molecules. Organic light-emitting diodes (OLEDs) based on these complexes, in the neat form or dispersed in a matrix, were also fabricated, the device displaying an EQE of ca. 1% along with a maximum luminance of 494 cd m−2

HIGHLIGHTS

THE DESIGN AND SYNTHESIS OF COPPER COMPLEXES AND THEIR APPLICATION IN A VARIETY OF METAL-MEDIATED TRANSFORMATIONS

d10 transition metal complexes have been extensively studied because of their unique photophysical and photochemical properties which led to applications for light emitting devices, sensing devices, solar cells, and artificial photosynthesis. Here we report the synthesis, structural characterization and DFT studies of two novel Ar-BIAN ligands bis(mes-imino-5-nitroacenaphthene), 1, and bis(mes-imino-4-nitroacenaphthene), 2 and their two new dimeric Cu(I) complexes 3 and 4 with a {Cu2(μ-I)2} core, which display a redshifted MLCT, characterized by TDDFT calculations, in comparison with the analogous complex 6 bearing the unsubstituted bis(mes-imino-acenaphthene) ligand.

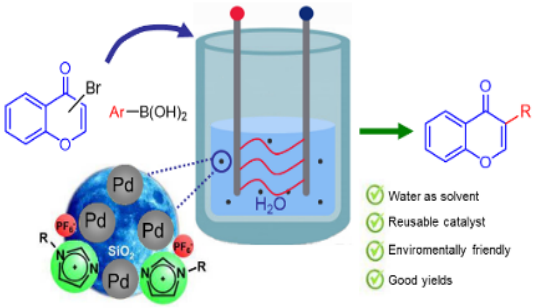


Synthesis, Crystal Structure, and DFT Study of Two New Dinuclear Copper(I) Complexes Bearing Ar-BIAN Ligands Functionalized with NO2 Groups

European Journal of Inorganic Chemistry 2020, 2900-2911

COMBINATION OF OHMIC HEATING AND SUPPORTED IONIC LIQUID PHASE CATALYSIS IN AQUEOUS MEDIA FOR THE SUSTAINABLE SYNTHESIS OF FLAVONOIDS

In order to meet the increasing demand for environmentally benign chemical processes, we developed a Suzuki–Miyaura reaction protocol based on the combination of ohmic heating and supported ionic liquid phase catalysis in aqueous media. This methodology was applied to the synthesis of a series of flavonoid derivatives, including isoflavones, styrylisoflavones, and diarylalkenylisoflavones. It offers significant improvements over existing procedures, as the absence of undesired side reactions, the short reaction times, the mild conditions required, the wide range of functionalities tolerated, the good yields, the environment-friendly reaction conditions, and the low catalyst loading. In addition, the supported catalyst can be recovered and maintains a good activity for at least three cycles. Thus, the combination of ohmic heating with supported ionic liquid phase catalysis in water not only is of considerable interest for cross-coupling reactions but also provides a convenient alternative to the existing methodologies for the synthesis of the above-mentioned flavonoid derivatives.

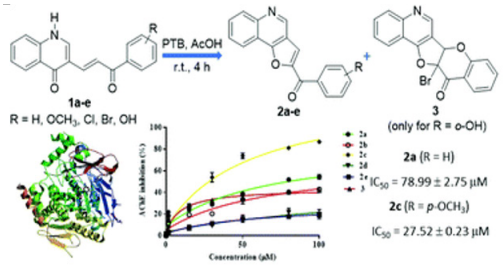


Combination of Ohmic Heating and Supported Ionic Liquid Phase Catalysis in Aqueous Media for the Sustainable Synthesis of Flavonoids .

Molecules 2020, 25, 1564

HIGHLIGHTS

2-AROYLFURO[3,2-C]QUINOLINES AS POTENTIAL ACETYLCHOLINESTERASE (ACHE) INHIBITORS



An elegant synthesis of 2-aroylfuro[3,2-c] quinolines (2) from quinolone-based chalcones 1 was achieved. The reaction involves bromination of the exocyclic double bond with pyridinium tribromide followed by furan ring formation. Interestingly, during bromination the tautomerization of the quinolin-4(1H)-one ring into the corresponding 4-hydroxyquinoline occurred followed by cyclization to give in a one-pot transformation, upon in situ oxidation, the 2-aroylfuro[3,2-c]quinolines. Two unexpected products were isolated and characterized, for the first time, in the bromination of the quinolone-based chalcone bearing a hydroxy group at the ortho-position of the aryl ring; the major compound was a 2-aroylfuro[3,2-c]quinoline dibrominated in the aryl ring, due to the activating effect of the hydroxy group, and the minor was identified as 12a-bromo-6b,12a-dihydro-12H-chromeno[2',3':4,5]furo[3,2-c]quinolin-12-one (3). Two possible mechanistic pathways were proposed to explain the formation of this last compound. Two of the synthesized 2-aroylfuro[3,2-c]quinolines 2a and 2c showed promising activity as acetylcholinesterase inhibitors (IC50 = 78.99 2.75 M and 27.520.23 M) being identified as templates for further development of more active inhibitors.

2-Aroylfuro[3,2-c]quinolines as potential acetylcholinesterase (AChE) inhibitors .

New J. Chem., 2020, 44, 6501

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. .

HIGHLIGHTS

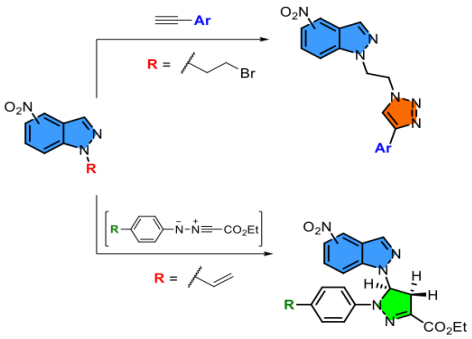
NITROINDAZOLE DERIVATIVES

The alkylation of a series of nitroindazole derivatives with 1,2-dibromoethane afforded the corresponding N-(2-bromoethyl)- and N-vinyl-nitro-1H-indazoles. The N-alkylated derivatives were used as scaffolds via 1,3-dipolar cycloaddition reactions.

Cu(I)-catalyzed azide-alkyne 1,3-dipolar cycloaddition was selected to substitute the nitroindazole core with 1,4-disubstituted triazole units after converting N-(2-bromoethyl) nitroindazoles into the corresponding azides.

The formation of the triazole ring was favored by the presence of electron-donating groups in the ethynylbenzene derivative, affording the expected nitroindazole-triazole derivatives in yields ranging from 71 to 87%.

1,3-Dipolar cycloaddition reactions with nitrile imines generated in situ from ethyl hydrazono--bromoglyoxylates was evaluated ed with nitroindazoles bearing a N-vinyl unit. This synthetic approach allows isolating selectively the corresponding nitroindazole-pyrazoline derivatives in yields ranging from 63 to 87%.

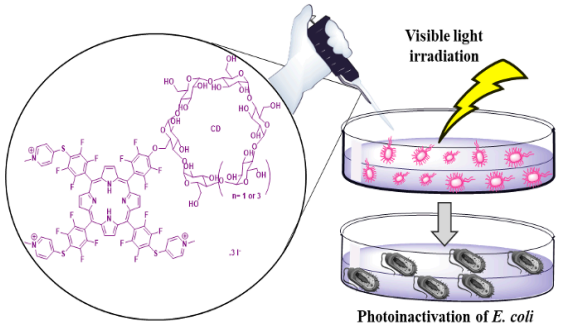


A suitable functionalization of nitroindazoles with triazolyl and pyrazolyl moieties via cycloaddition reactions.

Molecules 2020, 25, 126

PHOTOINACTIVATION OF *ESCHERICHIA COLI*

Photodynamic inactivation (PDI) of microorganisms have been used for the treatment of bacterial infections. PDI is based on the combination of three non-toxic elements: a photosensitizer (PS), light and molecular oxygen, which lead to the formation of reactive oxygen species (ROS) that cause lethal oxidative damage into the target pathogenic bacteria. For that, clinical approved tetrapyrrolic macrocycles, with particular emphasis on photoactive porphyrin (Por) dyes, which have been used as PS in PDI for different biomedical applications. Two novel unsymmetrical free-base thiopyridyl Pors conjugated with - or -CD units (Pors 2 and 3) were prepared and the corresponding cationic ones (Pors 2a and 3a) were assessed as water-soluble photosensitizer (PS) agents by photophysical, photochemical and E. coli photobiological studies. The presence of the CD unit and the positive charges on the Por periphery (2a and 3a) enhance their solubility in aqueous media. The photoactivity of the two cationic Pors 2a and 3a ensures their potential as PDI drugs against Gram-negative bacteria model, a bioluminescent E. coli, which the best PDI efficiency was determined for Por 3a that achieved the highest bacterial reduction of 4.0 log10 (ANOVA, $p < 0.0001$), reaching the detection limit of the method after 15 min.



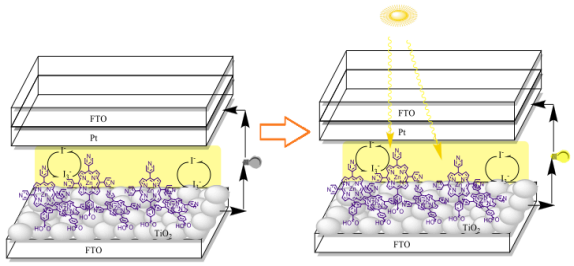
Unsymmetrical cationic porphyrin-cyclodextrin bioconjugates for photoinactivation of *Escherichia coli*.

Photodiagn. Photodyn. Ther., 2020, 31, 101788

HIGHLIGHTS

ZINC PORPHYRINS FOR DYE-SENSITIZED SOLAR CELLS

The sensitization activity of four zinc metalloporphyrin dyes: meso-tetrakis(4-pyridyl)porphyrinato Zn(II) (a), meso-triphenyl-(4-carboxyphenyl)porphyrinato Zn(II) (b), meso-tetrakis(4-carboxyphenyl) porphyrinato Zn(II) (c) and meso-tripyridyl(4-carboxyphenyl)porphyrinato Zn(II) (d), in terms of current-potential curve, open-circuit potential, fill factor, and overall solar energy conversion efficiency which have been evaluated under 100 mW/cm2 light intensity and their performances compared to the benchmark N719 (di-tetrabutylammonium cis-bis(isothiocyanato)bis(2,2-bipyridyl-4,4-dicarboxylato) ruthenium(II) was evaluated. The structural aspects of dyes with anchoring groups using TiO2-based dye sensitized solar cells (DSSCs), which includes pyridyl and carboxyphenyl acid groups and argue how the combination of both anchoring groups, in the same structure, may allow relevant optimization of DSSCs performance in the near future. Also, a noticeable improvement in the photovoltaic performance of all dyes, reaching a maximum increase from 25% to 69% in the overall DSSC efficiency under short periods of white light illumination was observed..

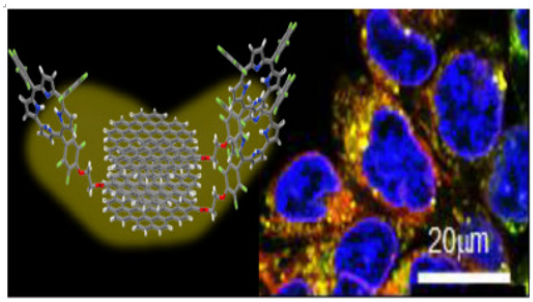


Influence of the meso-substituents of zinc porphyrins in dye-sensitized solar cell efficiency with improved performance under short periods of white light illumination

Dyes and Pigments, 2020, 177, 108280

GRAPHENE-CORROLE QUANTUM DOTS FOR MULTIPHOTON BIOIMAGING

The possibility of Graphene quantum dots (GQDs) to introduce a hydrophobic sensing unit inside animal cells and to add a nonlinear response to the sensing unit was evaluated by preparing novel hybrid based on GQDs covalently linked to corrole units bearing a glycol branch. Covalent functionalization was supported by X-ray photoelectron spectroscopy, Raman and Fourier transform infrared spectroscopy. Both the height and the diameter of the hybrid showed distributions peaking below 4 nm. The UV–vis absorption and emission spectra of the hybrids were additive with respect to that of the GQDs and the corrole. Insights about the most stable conformation of the corrole with respect to the GQDs core was provided by in silico studies using a model structure. The internalization and distribution of the hybrids in live animal cells was evaluated in human breast adenbocarcinoma cell line (MCF-7 cells) using confocal and multiphoton microscopy. Notably, multiphoton microscopy allowed for image collection using nonlinear excitation in the near-infrared and emission in the red part of the visible spectra

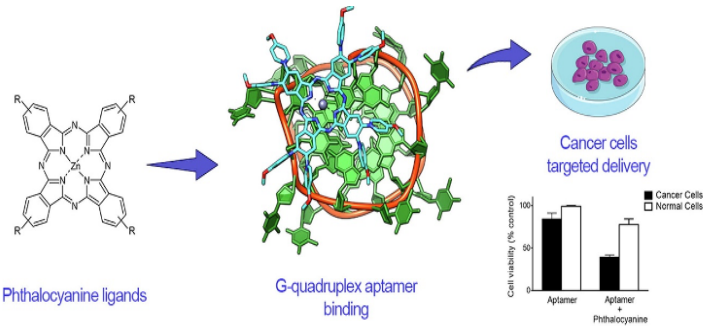


Novel hybrids based on graphene quantum dots covalently linked to glycol corroles for multiphoton bioimaging

Carbon 2020, 166, 164-174

HIGHLIGHTS

PHTHALOCYANINES FOR G-QUADRUPLEX APTAMERS BINDING



Tunable Color of Aggregation Induced Emission Enhancement in a Family of Hydrogen Bonded Azines and Schiff Bases.

Chemistry – A European Journal, 2018, 24, 17262-17267

The interactions of four Zn(II) phthalocyanines, previously reported as antibacterial photosensitizers and as binders of telomere GQ sequences, with the GQ AS1411 aptamer and its derivatives were studied by biophysical techniques, molecular docking and gel electrophoresis. Cell viability assay was also carried out to evaluate the antiproliferative effects of Zn(II) phthalocyanines.

The potential of the use of these aptamers as cancer-targeted drug delivery agents of the ZnPc ligands was evaluated. The study rationale is based on the ability of AS1411 to deliver a wide variety of cargoes to cancer cells, both by covalent and non-covalent conjugation strategies, without hampering its ability to target nucleolin at the surface of cancer cell.

This study demonstrates that the large π-planar structure of phthalocyanines derivatives (ZnPcs) is favorable for high-affinity binding to G-quadruplex (GQ) structures. Using a combined approach involving several biophysical techniques and in silico prediction analysis, their conformational properties were investigated towards GQ aptamers derivatives of AS1411.

The ZnPc functional substituents (methoxypyridinium or thiopyridinium units), the number of charges and their location affect the binding properties of these molecules. The octacationic ZnPc, with eight methoxypyridinium substituents, showed the highest affinity towards the studied GQ structures. Both CD profile and NMR results showed features that were attributed to the interaction of the ligands with the GQ structure, particularly in the case of the ZnPc with eight methoxypyridinium substituents.

The number and the location of charges in phthalocyanine core influenced the thermal stability of the GQ structure, ZnPc owning four and eight methoxypyridinium substituents showed to be the most stabilizing agents.

Molecular docking results provided further insights into the recognition between the ZnPc with methoxypyridinium substituents with four or eight positive charges and the AT11 GQ, highlighting π-π stacking and additional interactions of the positively charged side chains with the loops.

Results of cell viability assay also revealed a strong enhancement of cytotoxicity on HeLa cells upon complex formation of the tetracationic ZnPc (with four methoxypyridinium) with AT11 and AT11-L0 GQ and an attenuation of the cell toxicity in non-malignant cells

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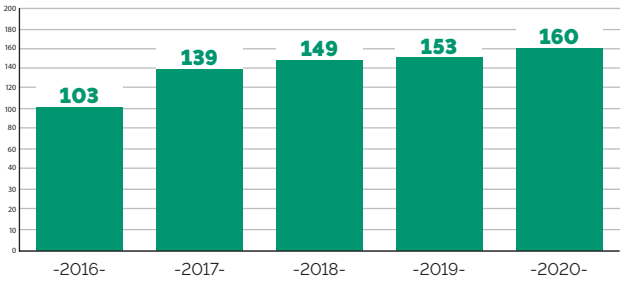
GROUP IN NUMBERS

SCIENTIFIC PRODUCTION

Articles published / Year



H-index: **89**

735 articles*
63515 citations

***2016-2020**
From WOS core collection

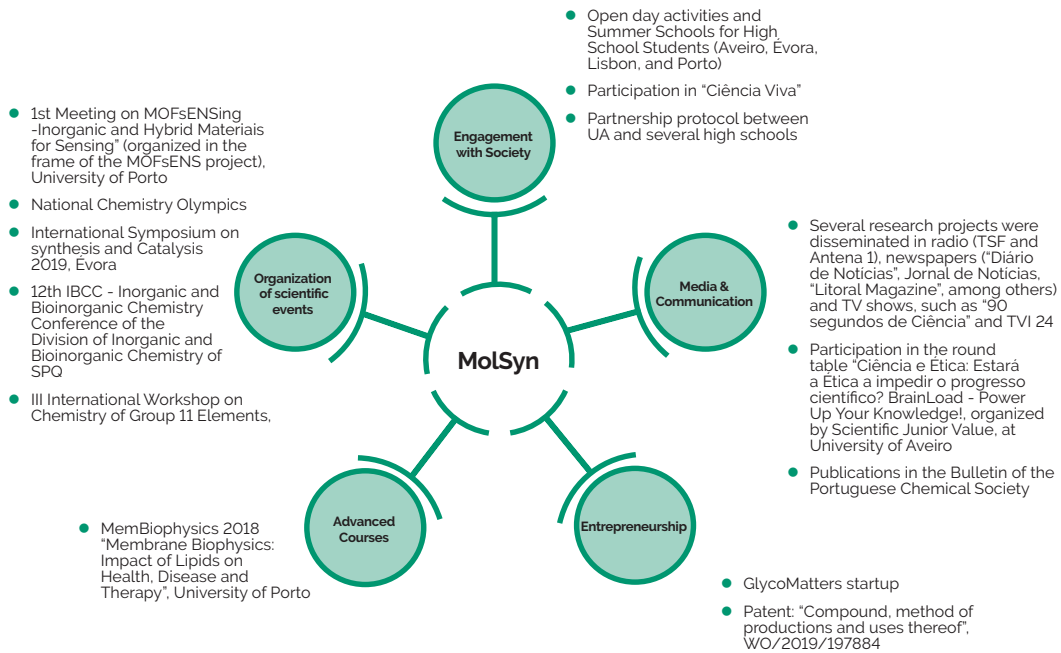
FUNDED PROJECTS *(Representative projects)*

- One-pot bimetallic catalyzed synthesis of challenging N-heterocycles.
  FCT, PTDC/QUI-QOR/0712/2020, Maria Manuel Marques (PI)
  Total Funding: € 247.034,00
- PAGE – Protein aggregation across the lifespan
  Centro-01-0145-FEDER-000003, Centro2020, Artur Silva (PI)
  Total Funding: € 1,598,206.47, Funding: € 569,787.00
- MOFsENS – Synthesis of metal-organic frameworks as optical gas sensors
  M-ERA.NET, Ana Margarida Silva (Local PI).
  Total funding: € 533,625.00, Funding: € 177,732.00
- ORGANIC REDOX MEDIATORS FOR ENERGY CONVERSIONs
  FCT, PTDC/QUI-QOR/7450/2020,Paula Branco (PI)
  Total Funding: € 248.344,28
- Supramolecular functionalization of carbon nanostructures with porphyrin and phthalocyanine derivatives for sustainable photoinduced energy and electronictransfer materials
  FCT, PTDC/QEQ-SUP/5355/2014, Leandro M. O. Lourenço (PI)
  Total Funding: € 171.408,00
- Novel C-glycosylated oxygen and nitrogen heterocyclic compounds as potential epigenetically active immune-stimulatory anticancer agents
  PTDC/QUI-QOR/29767/2017, Artur Silva (PI)
  Total Funding: € 239,581.00
- Organic-Inorganic Chemotypes as Anticancer and Anti-tumor Drugs
  Projects Portugal – Algeria, PT-DZ/0005/2015, Artur Silva (PI)
  Total Funding: € 99,840.00
- FERROCLOROSE – (Fe)rrying plants to prevent chlorosis
  FCT, PTDC/AGR-PRO/3515/2014, Maria Conceição Rangel (PI)
  Total Funding: € 199,721.00
- X-Sensors – Xanthene-based optical sensors
  FCT, POCI-01-0145-FEDER-29426, Ana Margarida Silva (PI)
  Total Funding: € 188,696.75
- FloWater – Fluorecent chelators for metal ion sensing in water
  FCT, POCI-01-0145-FEDER-28142, Andreia Leite (PI)
  Total Funding: € 239,178.47
- PepAlheira – Whey proteins and derived antimicrobial PEPtide-based active edible coatings for ALHEIRA industry
  FCT, POCI-01-0145-FEDER-31798, Cátia Teixeira (PI)
  Total Funding: € 234,885.90
- SilaSeco – Synthesis and Biological Evaluation of Sila-Secosteroids
  FCT, POCI-01-0145-FEDER-29059, José Enrique Borges (PI)
  Total Funding: € 233,261.97
- Two4Three - A small couple against the big three
  FCT, POCI-01-0145-FEDER-29786, Ricardo Ferraz (PI)
  Total Funding: € 230,771.39
- Amazing – AMAZonian snake toxins: creatING value from bioresources
  FCT, CIRCNA/BRB/0281/2019, Paula Gomes (PI),
  Total funding: € 298,857.55

INTERNATIONAL COOPERATION AND NETWORKING

- Algerian-Portuguese Bilateral Cooperation financed by FCT/ MESRS (PT-DZ/0005/2015), Centre de recherche scientifique et technique en analyses physico-chimiques (CRAPC) and University of Science and Technology Houari Boumediene, Argel
- Moroccan-Portuguese Bilateral Cooperation, Faculté des Sciences et Techniques de Béni Mellal, UNIVERSITÉ SULTAN MOULAY SLIMANE, Morocco
- 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.
- International Bilateral Portugal-Brazil Project: Programa CAPES
- COST ACTIONS 17104, 18132 and 18112
-

DISSEMINATION & OUTREACH



LABORATÓRIO ASSOCIADO
PARA A **QUÍMICA VERDE**

NATPRO

NATURAL PRODUCTS CHEMISTRY AND BIOACTIVITY

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

Group Coordinator:

Paula B. Andrade

The Natural Products – Chemistry and Bioactivity group conveys expertise in the discovery and elucidation of new chemical entities, either naturally-occurring or obtained by hemi-synthesis, as well as the evaluation of their biological activities. Among natural sources, we are particularly interested in plant and animal samples, both from terrestrial and marine origin.

Research activities are focused on drug discovery, namely for the treatment of cancer and diabetes, as well as inflammatory and neurodegenerative diseases. The group works to identify pharmacological modulators of human disease-related proteins, for which a targeted screening approach is employed that combines yeast, human cell lines, and animal models. We look for new targeted therapies with potential application in personalized therapy.

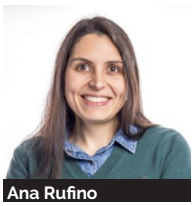
RESEARCH OBJECTIVES [2020-2023]

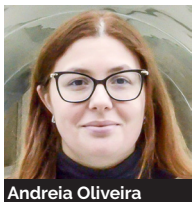
The major research objectives of the Natural Products – Chemistry and Bioactivity group are:

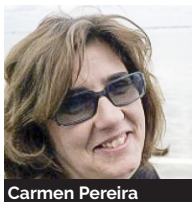
- development and application of chemical and instrumental methods for the study of natural matrices;
- development of green hemi-synthetic processes for obtaining novel bioactive molecules;
- chemical and pharmacological characterization of natural and hemi-synthetic bioactive compounds in a context of drug discovery, in the fields of cancer, diabetes, as well as inflammatory and neurodegenerative diseases;
- elucidation of the cellular mechanisms underlying inflammation, carcinogenesis, protein quality control disorders, mitochondrial dysfunctions, and their relationship with the pathophysiological events associated with the above-mentioned diseases;
- *in vitro* and *in vivo* assessment of the biological effects of the most commonly used nanoparticles in the food and health industries.
- study of the impact of emerging challenges in the biochemistry and metabolism of the cell, using multiple animal and plant models and tools.

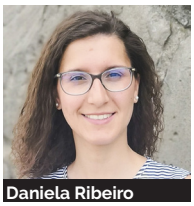
RESEARCH TEAM

SENIOR RESEARCHERS


Ana Rufino


Andreia Oliveira


Carmen Pereira


Daniela Ribeiro


David Pereira


Diana Pinto

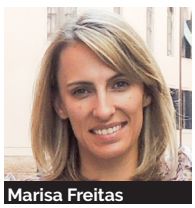

Eduarda Fernandes


Fátima Fernandes


Lucília Saraiva


Manuela Morato


Mariana Barbosa

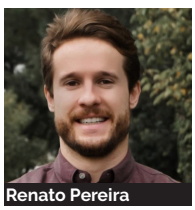

Marisa Freitas


Miguel Oliveira


Nelson Gomes


Patrícia Valentão


Paula B. Andrade


Renato Pereira


Romeu Videira


Susana Cardoso

RESEARCH TEAM

OTHER DOCTORATE RESEARCHERS
Áurea Carvalho
Ana Seca
Clementina Santo
Joana Terroso
Margarida Araújo
Mónica Válega
Patrícia Bacalhau

POST-DOCTORAL FELLOWS
Helena Ramos
Liliana Raimundo
Maria Dias

PhD STUDENTS
Adelaide Sousa
Adriana Januário
Adriana Silva
Ana C. Andrade
Ana R. Circuncisão
Ana Silva
Andrea Afonso
Andreia Silva
Ângela Oliveira
Carina Proença
Clarinda Costa
Daniela Mendes
Daniela Silva
Gonçalo Rosa
Joana Almeida
Joana Loureiro
João Bernardo
Juliana Calheiros
Karen João
Liliana Almeida
Márcia Araújo
Marcelo Catarino
Maria Rocha
Mariana Lucas
Pedro Gomes
Rafael Félix
Ricardo Ferreira
Rute Moreira
Sónia Rocha
Tânia Vicente
Tiago Macedo
Vera Ribeiro

MSc STUDENTS
Ana Campos
Ana Costa
Ana Monteiro
Beatriz Machado
Beatriz Silva
João Rebelo
Maria Faustino
Mariana Silva
Ricardo Santos
Rita Ribeiro
Valentina Pinheiro

RESEARCH GRANTEES
Carla Carvalho
Catarina Marçal
Nair Campos

OTHER RESEARCHERS
Rui Gonçalves

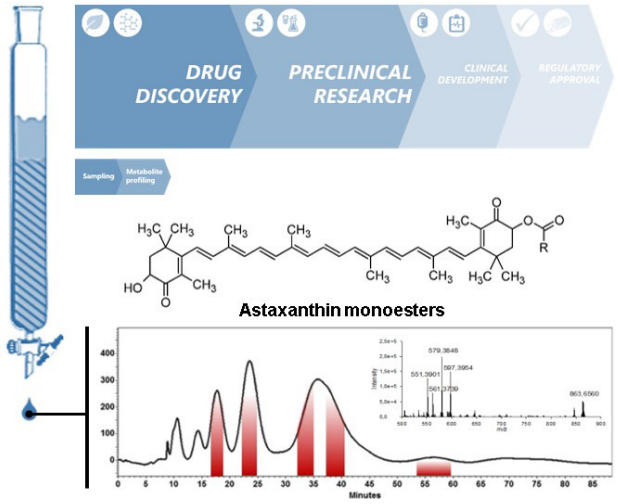
RESEARCH THEMES/
METABOLITE PROFILING AND ISOLATION OF BIOLOGICALLY ACTIVE NATURAL PRODUCTS

PROFILING AND ISOLATION

The screening of natural products for the identification of new lead structures to be used directly or as templates for the development of drugs has been one of the most successful strategies applied in drug discovery.

Metabolite profiling of natural-derived extracts assures the identity, authenticity, quality, and safety of natural matrices, particularly of those used in human nutrition and therapeutics. Furthermore, the chemical characterization of extracts and/or active fractions has been routinely applied, allowing the prioritization of new compounds considering unprecedented chemical scaffolds and/or potentially relevant biological properties.

To address the above, our group will continue to be actively engaged on the development, validation, and application of chromatographic-based techniques for the analysis of secondary metabolites in plants, marine organisms, and agro-industrial wastes. Ongoing research will cover also the isolation, structure elucidation, and pharmacological assessment of prioritized constituents, enabling to set of a platform for the development of new drug leads, functional foods, and cosmetics formulations. Chemical backbone of naturally-derived constituents displaying relevant biological properties in models of disease frequently serves as a template for the semisynthesis of derivatives, broadening the spectrum of potential drug candidates.



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14 S. J. Amarante, et al., Mar. Drugs, 2020, 18, 559. doi:10.3390/md18110559

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17 J. M. Pais, et al., Biomolecules, 2020, 10, 344. doi:10.3390/biom10020344

18 S. S. Ferreira, et al., Food Res. Int., 2020, 132, 109055. doi:10.1016/j.foodres.2020.109055

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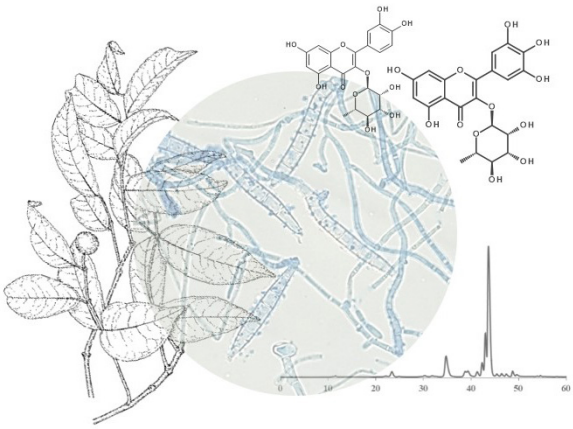
RESEARCH THEMES/ ETHNOPHARMACOLOGY

ETHNOPHARMACOLOGY IN DRUG DISCOVERY

Ethnomedicinal knowledge has been frequently driving research and drug discovery programs, remaining as one of the most fruitful strategies on the delivery of drug leads, as recalled by the 2015's Nobel Prize for Physiology or Medicine. Collaborations with research groups from Brazil, Guinea-Bissau, and Thailand put our group in a strategic position to ensure a privileged access to a large collection of plants used in folk medicine, in four continents.

Prioritization of plants based on their ethnomedicinal use has been frequently considered by the group, in order to tune the selection of biological and/or pharmacological properties to be investigated. We have already delivered experimental evidence on the relationship between the chemical constituents and the biological properties of several medicinal plants, contributing to the validation of their traditional use and providing insight into their efficacy and safety. Since data on the chemistry of many species are virtually absent, the group remains active on the elucidation of the structural complexity of their metabolites (e.g. alkaloids, sterols and phenolic constituents), and the related biological activities.

Such metabolites might have their medicinal chemistry developed into clinical candidates for the treatment of cancer, inflammation, diabetes, and neurodegenerative diseases.



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doi:10.1016/j.jep.2020.113177

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doi:10.3390/ijms21072421

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doi:10.1055/a-1023-8918

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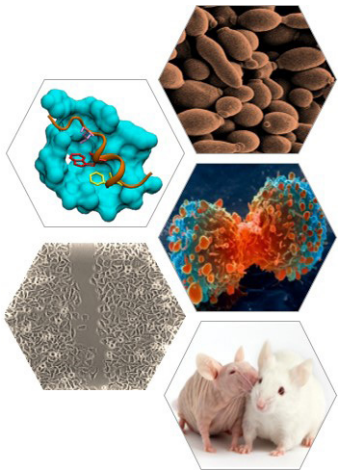
RESEARCH THEMES/ DRUG DISCOVERY

ANTICANCER DRUG DISCOVERY

As part of the ongoing program on drug discovery from natural sources and hemi-synthetic molecules, the group is interested in the evaluation and mechanism of action of molecules with potential use in cancer and inflammatory diseases.

Regarding cancer cells, the group focus its studies in the cell lines that are representative of the deadliest cancer types, including triple-negative breast cancers, hepatocarcinoma, and colorectal. The assessment of the anticancer effects of small molecules focuses on the impact upon mitochondrial function/status, p53 activity and expression, calcium dynamics, and chromatin status.

The high degree of conservation of cellular processes and molecular pathways between yeast and human cells has made *Saccharomyces cerevisiae* a powerful model system to study human proteins and molecular mechanisms underlying the pathobiology of several human diseases. If the gene encoding the protein of interest is conserved in yeast, its function can be directly studied in this organism. However, if the gene has no orthologues in yeast, its study is still possible by heterologous expression. This so-called humanized yeast model has been widely used by our group for biological and pharmacological studies of human proteins with a key role in cancer. Previous yeast models, as well as new yeast strains with humanized genes, will be constructed and used in association with yeast cell-based targeted screening approaches to the discovery of new therapeutic opportunities for cancer.



The group will continue to conduct anticancer research using a number of cancer models, including 2D/3D immortalized and patient-derived cancer cells and xenograft mice.

SELECTED PUBLICATIONS

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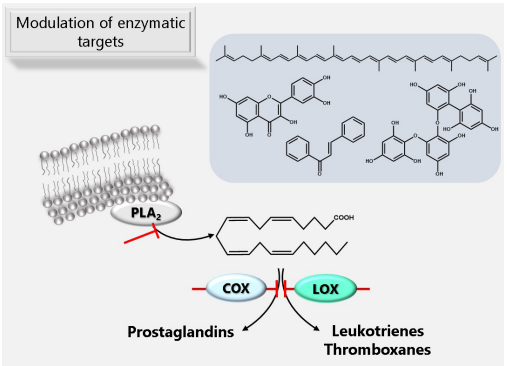
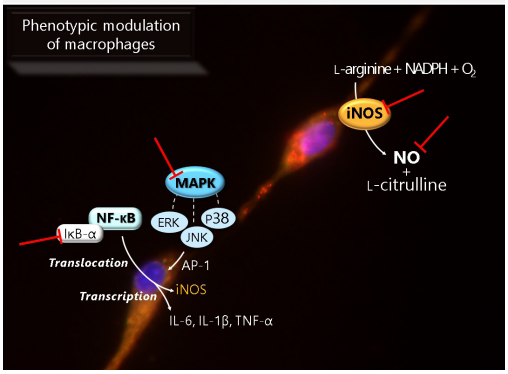
RESEARCH THEMES/ DRUG DISCOVERY

ANTI-INFLAMMATORY DRUG DISCOVERY

Normal inflammation is self-limiting, but anomalous resolution and prolonged inflammation are at the basis of a number of pathological processes in virtually any systemic or organ-specific diseases ranging from classical autoimmune diseases (e.g. rheumatic diseases, psoriasis) to cancer, passing through diabetes, inflammatory bowel disease, cardiovascular and neurodegenerative diseases. Additionally, the available drugs have significant side-effects and remain unable to counteract the increasing incidence and prevalence of chronic conditions with inflammatory status. Thus, the group have been actively enrolled in the search of candidates that may modulate the inflammatory response but also lead to fewer adverse effects.





Natural and synthetic molecules have been evaluated on their ability to modulate key targets in the inflammatory process, including enzymes (e.g. NADPH oxidase, phospholipase A2, cyclooxygenases, lipoxygenases, elastase, and hyaluronidase), 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-α and inducible nitric oxide synthase (iNOS). We will continue to investigate the impact of naturally-derived and synthetic compounds on the crosstalk between oxidative stress and inflammation, several cellular (human, murine) and non-cellular systems being used as research tools.

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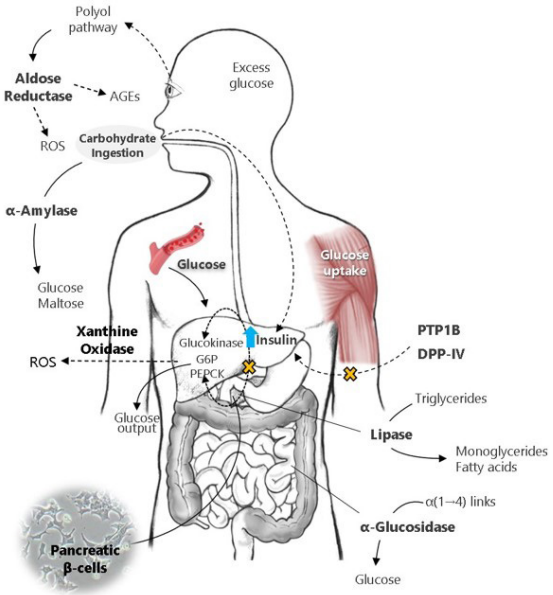
RESEARCH THEMES/ DRUG DISCOVERY

ANTIDIABETIC DRUG DISCOVERY

Diabetes mellitus is a metabolic disorder with multiple intertwined chronic complications that became one of the most serious and expensive epidemiological problems nowadays. Despite the therapeutics progress, the currently available antidiabetic drugs do not present the desired efficacy and are associated with serious adverse effects.

Multitarget activity of polyphenols has proved to act in several events associated with diabetes and related vascular complications. As this specific class of metabolites is abundantly found in natural sources, the group have been involved in the investigation of polyphenols obtained from plants and macroalgae. Their ability to improve insulin secretion, to overcome insulin resistance and/or to regulate blood glycaemic levels, has been assessed in enzymatic, cellular, and animal models.

As we seek to deliver new antidiabetic candidates with improved activity, preclinical research also deals with the synthesis of compounds bearing the polyphenolic backbone.



SELECTED PUBLICATIONS

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RESEARCH THEMES/ DRUG DISCOVERY

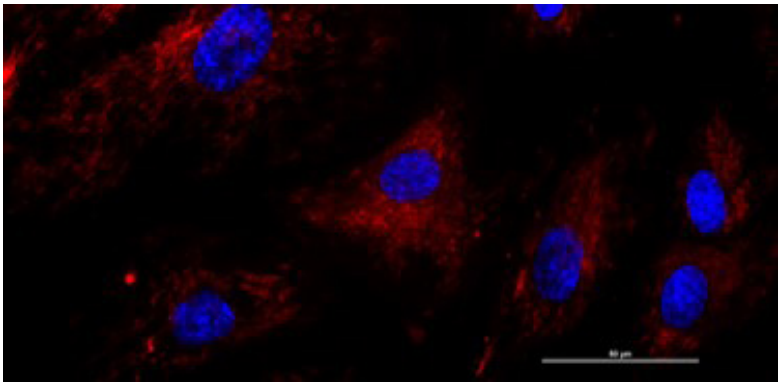
NEURODEGENERATIVE DISEASES AND DRUG DISCOVERY

The group is focused on the initial stages of brain degeneration associated with Huntington's, Parkinson's and Alzheimer's diseases (HD, PD, and AD), under the working hypothesis that mitochondrial dysfunction and proteome imbalance are transversal and key pathological features.

Cellular, zebrafish, and murine models of HD, PD, and AD have been used to investigate the molecular mechanisms underlying the homeostatic interconnectivity between the functional organization of the mitochondria and the cellular processes involved in the quality control of the proteome, aiming the identification of novel therapeutic targets.

The problem of age-related neurodegeneration has been addressed considering different therapeutic strategies to modulate mitochondrial function (e.g. energy, membrane lipids, homeostasis and signals) and/or to target endoplasmic reticulum and the unfolded protein response. In HD, mitochondrial damage emerges from the high generation of reactive oxygen species (ROS) triggered by unfolding huntingtin protein (mHtt) accumulation. Thus, we are investigating different redox-active compounds to select those that have ability to promote mHtt clearance and avoid the mitochondrial oxidative damage, whereby potential to support a disease-modifying HD therapy.

Regarding AD and PD, we will test therapeutic strategies based on cutting-edge nano-phytomedicinal tools, designed: i) to overcome the mitochondrial complex I deficiencies detected in AD and PD brains, ii) to tune the cell redox state, iii) to modulate the phospholipid composition of membranes, iv) to decrease the release of pro-inflammatory signs, and/or v) to modulate the activity of key enzymes of the catecholamine metabolism. The development of lipid-based nanocarriers for oral and nasal administration and delivery the phytochemicals for selected cellular targets are also under investigation.



SELECTED PUBLICATIONS

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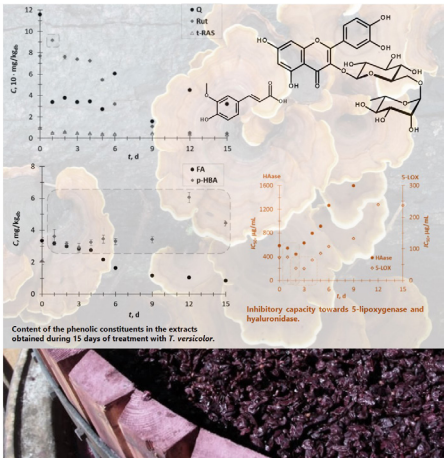
HIGHLIGHTS

VALORIZATION OF GRAPE POMACE UPON BIOTRANSFORMATION WITH TRAMETES VERSICOLOR

Within the circular economy context, grape pomace, the main winemaking by-product, was used as feedstock for *Trametes versicolor* fermentation under solid-state conditions, aiming the production of high-value bioproducts. Biotransformation with *T. versicolor* enabled to obtain extracts with an increased content of phenolic acids, flavan-3-ols and the flavonol rutin, particularly after 4-day fermentation. This approach allowed to improve the anti-inflammatory properties of a grape pomace extract, exhibiting significant inhibitory activity against 5-lipoxygenase and hyaluronidase. This simple and cost-effective biotechnological approach provides compounds with improved activity for pharmaceutical and nutraceutical industries.

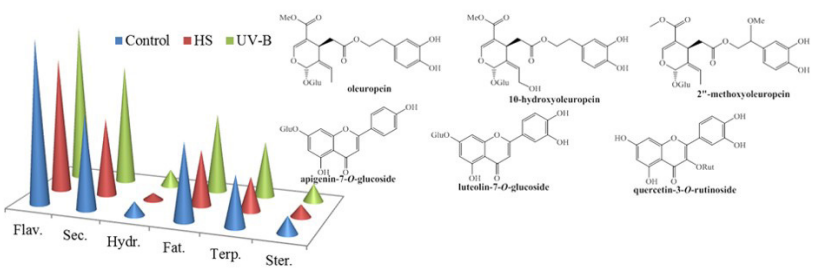


Enhancement of the anti-inflammatory properties of grape pomace treated by *Trametes versicolor*.

Food & Function, 2020, 11, 680-688

IMPACT OF CLIMATE-CHANGE-RELATED CONDITIONS ON OLEA EUROPAEA L. METABOLITE PROFILE

Olea europaea L. is a typical Mediterranean species with high economic value and important health benefits, but this region is particularly vulnerable to global climate change. Thus, special attention should be given to the impact that climate-change-related conditions can have on *O. europaea* metabolome. It was revealed that the profiles of flavonoids and secoiridoids is modulated by both UV-B radiation and heat shock exposure, as detected by increased levels of oleuropein, 10-hydroxyoleuropein, 2''-methoxyoleuropein, apigenin, luteolin, and quercetin derivatives. These bioactive compounds will enrich the plant and consequently improve its economic value and health-associated benefits.



The antioxidant system in *Olea europaea* to enhanced UV-B radiation also depends on flavonoids and secoiridoids.

Phytochemistry, 2020, 170, 112199

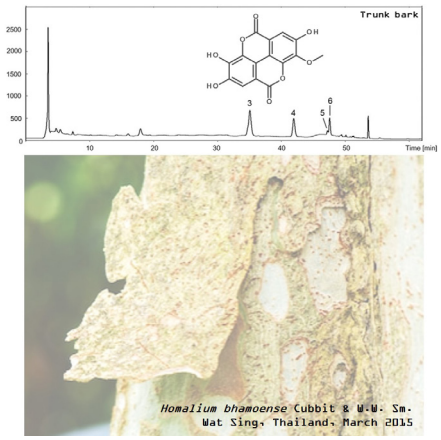
Physiological and metabolite reconfiguration of *Olea europaea* to cope and recover from a heat or high UV-B shock..

Journal of Agricultural and Food Chemistry, 2020, 68, 11339-11349

HIGHLIGHTS

ETHNOMEDICINAL USE OF PLANTS DRIVING THE DEVELOPMENT OF ANTI-INFLAMMATORY AGENTS

Medicinal plants still constitute the main therapeutic tool in several African and Asian countries, particularly by people inhabiting rural areas. Our ongoing research program on scarcely investigated species allowed identifying the leaves of *Xylopia aethiopica* and the trunk bark of *Homalium bhamoense* as sources of anti-inflammatory bioactives, the ethnomedicinal use of both species against conditions with an inflammatory background being reported. Extracts obtained from both plants were found to efficiently decrease the levels of the inflammatory cytokine IL-6 in macrophages, also eliciting significant inhibitory effects towards 5-lipoxygenase. Additionally, the chemical profile of both species has been characterized for the first time, allowing the identification of a series of structurally diverse phenolic constituents that appear to underlie the observed effects upon inflammatory events, and that might substantiate further research efforts as biological sources of new anti-inflammatory ingredients.

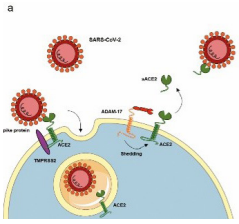


Inhibition of pro-inflammatory enzymes and attenuation of IL-6 in LPS-challenged RAW 264.7 macrophages substantiates the ethnomedicinal use of the herbal drug *Homalium bhamoense* Cubitt & W.W.Sm.

International Journal of Molecular Sciences, 2020, 21, 2421

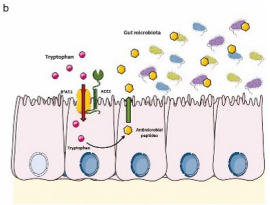
RENIN-ANGIOTENSIN SYSTEM (RAS) AS PHARMACOLOGICAL TARGETS IN INFLAMMATORY BOWEL DISEASE AND FETAL PROGRAMMING DISEASES

Fetal programming results from fetal stress that increases the susceptibility to cardiovascular diseases in adult age, including hypertension. Using an animal model, it was shown that the RAS, namely the AT1 receptor and ACE, have multifunctional activity associated with vascular hyper-sympathetic activation, involving a tonic facilitation of prejunctional AT1, which can justify, at least in part, the development of hypertension. Also, upregulation of ACE and ACE2 expression was found to enhance NADPH oxidase activity leading to pathological remodeling of arteries. Inflammatory bowel disease (IBD) is a chronic relapsing condition of the gastrointestinal tract that includes ulcerative colitis and Crohn's disease. ACE2 is a multifunctional protein with impact in IBD: (1) it balances the production of vasoconstrictor/vasodilator peptides; (2) controls the intestinal inflammation and nutritional status associated with neutral amino acids; (3) might modulate intestinal fibrosis and anti-integrin-mediated drug response; and (4) can influence the risk of infection by coronavirus such as the SARS-CoV-2, responsible for the present COVID-19 pandemic. Overall, these data identified RAS as key target, particularly ACE and ACE2, to reduce the FPH and IBD.



Unraveling the role of ACE2, the binding receptor for SARS-CoV-2, in inflammatory bowel disease.

Inflammatory bowel diseases, 2020, 26, 1787-1795



Insights into sympathetic nervous system and GPCR interplay in fetal programming of hypertension: a bridge for new pharmacological strategies.

Drug Discovery Today, 2020, 25, 739-747

HIGHLIGHTS

ADDING VALUE TO CHEMICAL DIVERSITY OF MARINE ORGANISMS

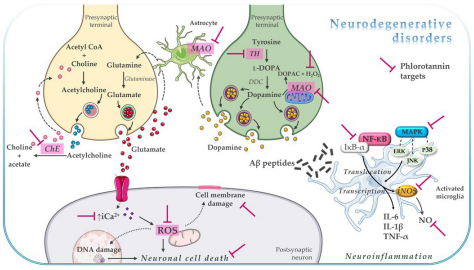
Phlorotannin-targeted extracts from Fucales (Ochrophyta, Phaeophyceae) open new windows for the management of human diseases with inflammatory background and unbalanced redox homeostasis, such as neurodegenerative disorders. Phlorotannin extracts exhibit multifunctional antioxidant properties, protect neuronal cells from glutamate-induced toxicity, decrease the cellular levels of the pro-inflammatory mediator nitric oxide and modulate the activity of enzymes that play a key role on cholinergic- and dopaminergic-dependent neuronal connectivity, including acetylcholinesterase, monoaminoxidase A, and tyrosine hydroxylase..

Polyphenols from brown seaweeds (Ochrophyta, Phaeophyceae): Phlorotannins in the pursuit of natural alternatives to tackle neurodegeneration.

Marine Drugs, 2020, 18, 654

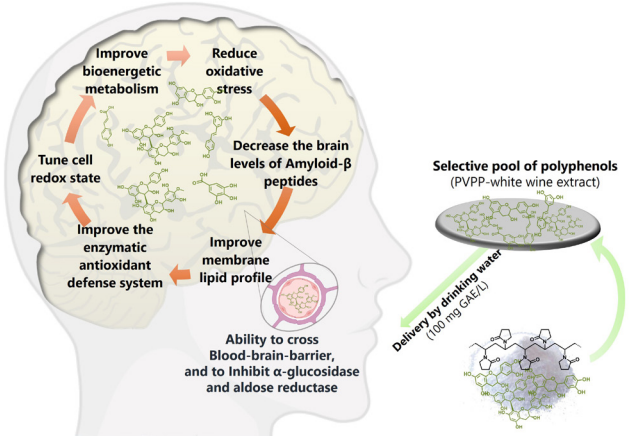
In vitro **multifunctionality of phlorotannin extracts from edible *Fucus* species on targets underpinning neurodegeneration**

Food Chemistry, 2020, 333, 127456



A MULTI-TARGET STRATEGY TO ADDRESS THE CHALLENGE OF ALZHEIMER'S DISEASE AND TYPE 2 DIABETES INTERLINK

A polyphenols-rich extract, obtained from polyvinylpolypyrrolidone (PVPP) winery residue, reveals neuroprotective effects and ability to modulate the kinetics of type 2 diabetes-relevant enzymes. These results expand the positive brain effects of PVPP-white wine extract previously revealed by us using an animal model for Alzheimer's disease. Thus, PVPP-white wine extract has potential to support the development of functional foods and/or nutraceuticals aiming neuroprotection and glucose homeostasis regulation, with high relevance in Alzheimer's disease and type 2 diabetes interlink.



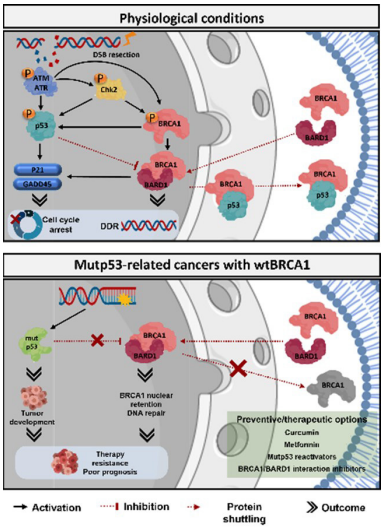
Adding value to polyvinylpolypyrrolidone winery residue: a resource of polyphenols with neuroprotective effects and ability to modulate type 2 diabetes-relevant enzymes

Food Chemistry, 2020, 329, 127168

HIGHLIGHTS

DISCOVERY OF NEW ANTICANCER DRUG CANDIDATES BY TARGETING TUMOR SUPRESSOR PROTEINS: FROM YEAST TO MICE MODELS

Innovative yeast targeted screening approaches were developed and used to identify new targeting agents of relevant tumor suppressor proteins, including 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 were validated. The identified compounds target major hallmarks of cancer through its antiproliferative, proapoptotic, antiangiogenic, anti-invasive and antimigratory properties. Additionally, they do not reveal toxic side effects in animal models. These preclinical results indicate that these compounds are promising drug candidates for anticancer therapy.

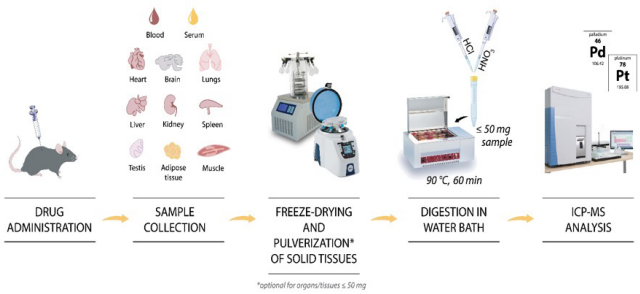


BRCA1/P53: Two strengths in cancer chemoprevention.

Biochimica et Biophysica Acta – Reviews on Cancer, 2020, 1873, 188339

ANTICANCER EFFICACY OF HOMO/HETEROMETALLIC COMPLEXES ASSOCIATED WITH BIOGENIC AMINES: TARGETS AND BIOACESSIBILITY *IN VITRO* AND *IN VIVO*

Palladium (Pd)-based complexes have significant similarities regarding structure and coordination chemistry with the platinum agents and have been studied regarding the treatment of triple negative breast carcinoma (TNBC), which has a particularly poor prognosis due to its high metastatic potential/aggressive biology. We developed a novel method to quantify by ICP-MS Pd and Pd-based drugs in animal pharmacokinetic/biodistribution studies. We described a favorable pharmacokinetics and biodistribution of Pd(II) complexed with spermidine (a biogenic amine), Pd2Spm, in vitro and in vivo. Also, metabolic changes induced by Pd2Spm in extracts of mice tissues are suggestive of potential lower negative effects of Pd2Spm administration. Overall, data indicates that Pd2Spm is a promising drug candidate with anticancer properties towards TNBC.



Fast and reliable ICP-MS quantification of palladium and platinum-based drugs in animal pharmacokinetic and biodistribution studies.

Analytical Methods, 2020, 12, 4806-4812.

HIGHLIGHTS

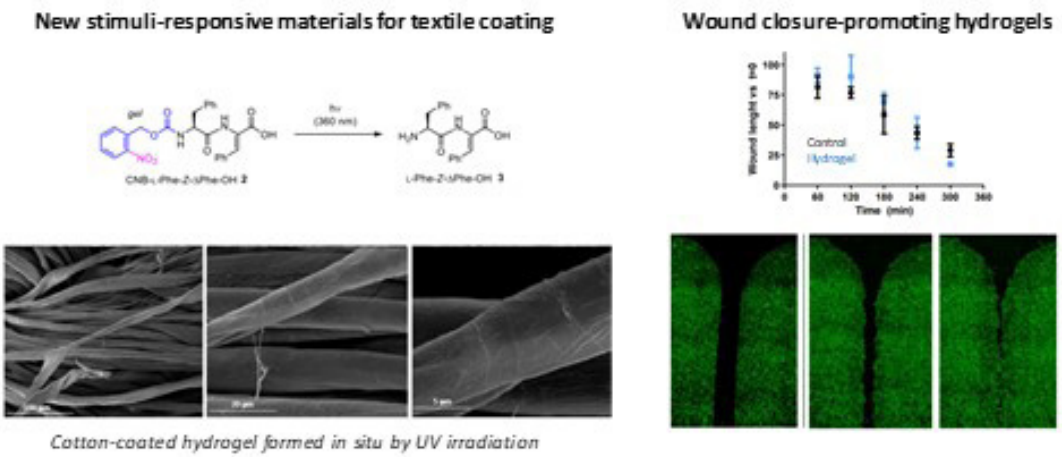
NATURE-INSPIRED AND STIMULI-RESPONSIVE NANOMATERIALS

Supramolecular hydrogels have attracted considerable attention due to their use as biomaterials for many biotechnological and biomedical applications, such as drug delivery, tissue engineering and theranostics. The building blocks of these materials can be diverse, however a subset of them can be obtained by mimicking natural-occurring dehydropeptides. The presence of a dehydroamino acid residue imparts increased proteolytic resistance into the hydrogels, thus contributing to their stability, further contributing to different physical properties that arise from decreased structural flexibility of the dehydropeptide chain. These materials have a diverse set of properties and can be applied in drug delivery, coating of textiles for enhanced biological properties, such as wound healing.

By incorporating magneto-responsive nanoparticles, we can add additional properties to the material, such as the capacity to be used in theranostics, temperature-controlled release of drugs by the action of an external magnetic field and also localized hyperthermia-based treatments

Dehydropeptide-based plasmonic magnetogels: a supramolecular composite nanosystem for multimodal cancer therapy.

Journal of Materials Chemistry B, 2020, 8, 45-64

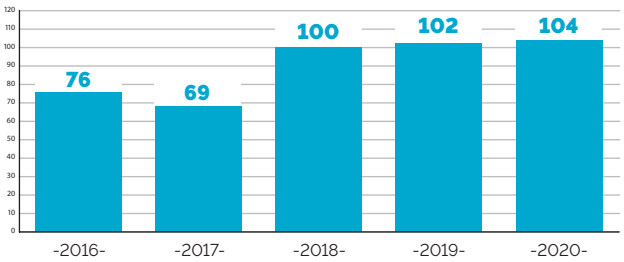


Cotton-coated hydrogel formed in situ by UV irradiation

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION

Articles published / Year



H-index: **98**

451 articles*
83053 citations

***2016-2020**
From WOS core collection

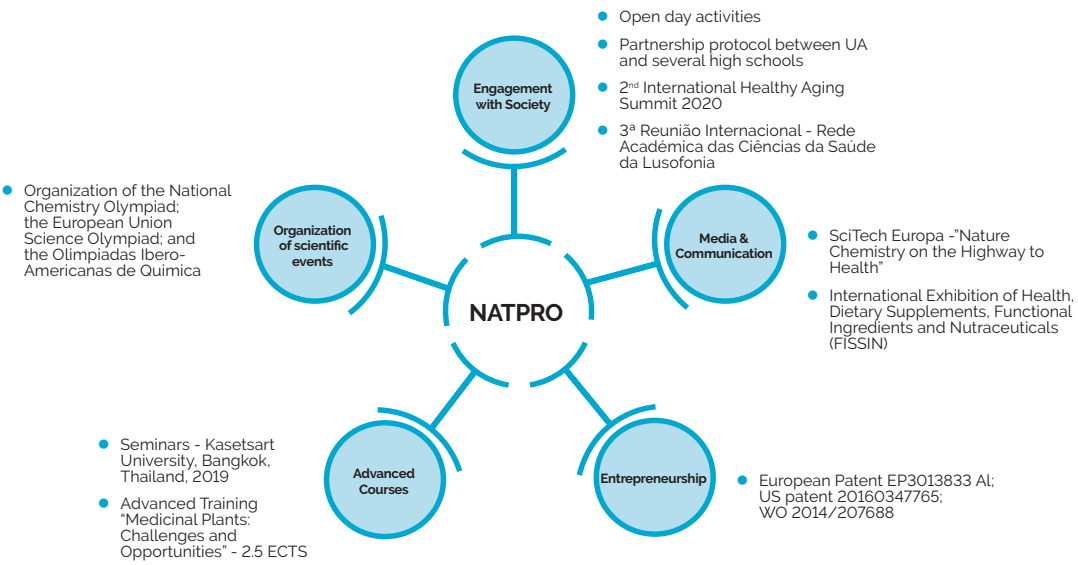
FUNDED PROJECTS *(Representative projects)*

- **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

INTERNATIONAL COOPERATION AND NETWORKING

- CYTED: CORNUCOPIA, Caracterización y evaluación funcional y de seguridad de compuestos bioactivos de frutas iberoamericanas como ingredientes alimentarios, Spain
- Consortium for Mitochondrial Research, University College London, UK
- MCR - Mitochondrial Biology Unit, University of Cambridge, UK
- CEBAS, Consejo Superior de Investigaciones Cientificas (CSIC), Murcia, Spain
- 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.

DISSEMINATION & OUTREACH




LABORATÓRIO ASSOCIADO
PARA A QUÍMICA VERDE

AnalytDev

ANALYTICAL DEVELOPMENT

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

Group Coordinator:

Marcela Segundo

The Analytical Development group is composed by researchers with established background in addressing real-life problems concerning quantification of small molecules in a plethora of matrixes. 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. To achieve these goals, research efforts will aim the miniaturization of devices and methods, the advanced data analysis through chemometrics, and the development of high-throughput methods mainly through intervention on sample preparation.

RESEARCH OBJECTIVES [2020-2023]

The research activity of the Analytical Development group will focus on the development of sustainable analytical solutions and comprehensive analysis. The main research objectives are the:

- 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

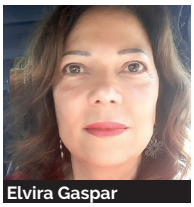
SENIOR RESEARCHERS


Agostinho Almeida


Alberto Araújo


Artur Figueirinha


Célia Amorim


Elvira Gaspar


Helena Soares


Inês Valente


João Paulo Noronha


João Prior


J. Rodrigo Santos


J. António Rodrigues

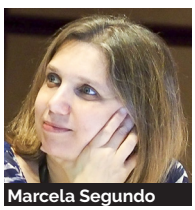

José L. Costa Lima


Júlia Magalhães


Liliana Martelo

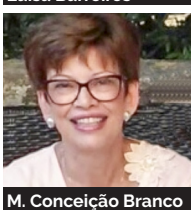

Luisa Barreiros


Mafalda Sarraguça


Marcela Segundo


Marco G. Silva


M. Beatriz Quinaz

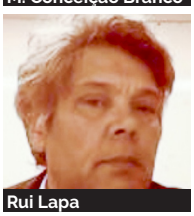

M. Conceição Branco


Nádia Silva

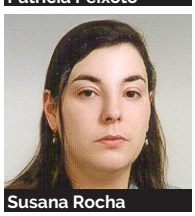

Patrícia Peixoto


Paulo Almeida


Ricardo Páscoa


Rui Lapa


Rui Ramos


Susana Rocha

RESEARCH TEAM

OTHER DOCTORATE RESEARCHERS

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Eduarda Silva
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Mary Duro
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M. José Pereira
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Sara Marques
Sónia Pedreiro

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Paula Melo
Pedro Costa

RESEARCH THEMES/
INNOVATIVE SAMPLE TREATMENT

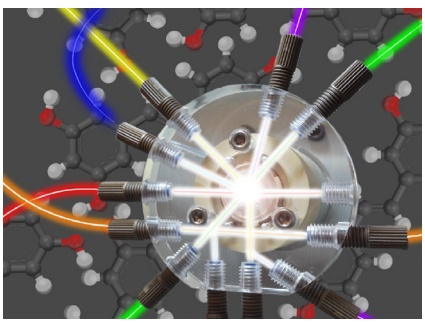
Sample treatment is the bottleneck of analytical procedures as it takes about 70% of total analysis time and is labor intensive. Almost all advanced instrumental methods of analysis require samples to be as much as possible free from interfering molecules, namely biomolecules and dissolved salts. Further, 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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1 J. A. Custodio-Mendoza, et al. J. Chromatogr. A. 2020, 1627. **doi:10.1016/j.chroma.2020.461397**

2 K. C. A. Francisco, et al. Int. J. Food Sci. Technol. 2020, 55, 248. **doi:10.1111/ijfs.14300**

3 C. A. L. Graca, et al. Water. 2020, 12. **doi:10.3390/w12123458**

4 B. J. R. Gregorio, et al. Molecules. 2020, 25. **doi:10.3390/molecules25061333**

5 M. Kohlova, et al. Macromol. Biosci. 2020, 20. **doi:10.1002/mabi.202000046**

6 D. Lograd, et al. Acta Medica Port. 2020, 33, 858. **doi:10.20344/amp.15216**

7 S. S. Marques, et al. Molecules. 2020, 25. **doi:10.3390/molecules25081879**

8 R. Mauricio, et al. Environ. Monit. Assess. 2020, 192. **doi:10.1007/s10661-020-8079-7**

9 R. Mauricio, et al. J. Environ. Sci. 2020, 89, 1. **doi:10.1016/j.jes.2019.09.019**

10 F. A. Miller, et al. Horticulturae. 2020, 6. **doi:10.3390/horticulturae6040060**

11 R. M. Ramos, et al. Food Anal. Meth. 2020, 13, 1088. **doi:10.1007/s12161-020-01730-6**

12 R. Salgado, et al. Environ. Technol. 2020, 41, 450. **doi:10.1080/09593330.2018.1502362**

13 N. Santarem, et al. Sci Rep. 2020, 10. **doi:10.1038/s41598-020-60067-6**

14 C. V. A. Santos, et al. LWT-Food Sci. Technol. 2020, 133. **doi:10.1016/j.lwt.2020.109893**

15 J. R. Santos, et al. Food Control. 2020, 108. **doi:10.1016/j.foodcont.2019.106879**

16 B. Sousa, et al. Environ. Pollut. 2020, 258. **doi:10.1016/j.envpol.2019.113762**

17 M. A. G. Valente, et al. J. Braz. Chem. Soc. 2020, 31, 2038. **doi:10.21577/0103-5053.20200104**

RESEARCH THEMES/
MULTIDIMENSIONAL METHODS FOR TOTAL ANALYSIS

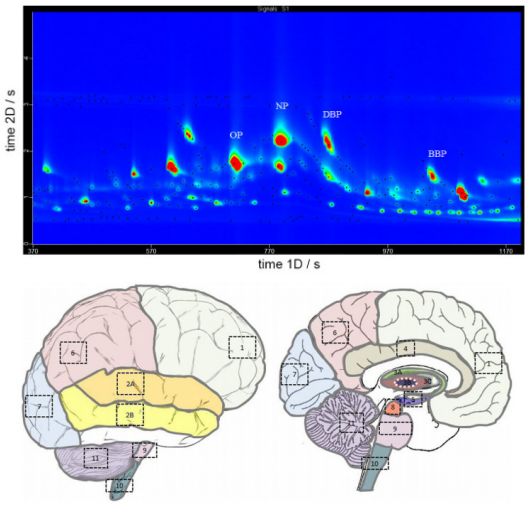
One of the trends in analytical sciences is the implementation of comprehensive methods, able to extract the maximum amount of information from a given sample within a single analytical run. This is possible using multidimensional setups, consisting of several detectors in series, orthogonal separative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



SELECTED PUBLICATIONS

18 A. Almeida, et al. J. Trace Elem. Med. Biol. 2020, 62. doi:10.1016/j.jtemb.2020.126580

19 F. Braham, et al. S. Afr. J. Bot. 2020, 129, 146. doi:10.1016/j.sajb.2019.04.001

20 S. Branco, et al. J. Appl. Entomol. 2020, 144, 41. doi:10.1111/jen.12701

21 M. M. S. Cabral-Pinto, et al. Expo. Health. 2020, 12, 629. doi:10.1007/s12403-019-00323-x

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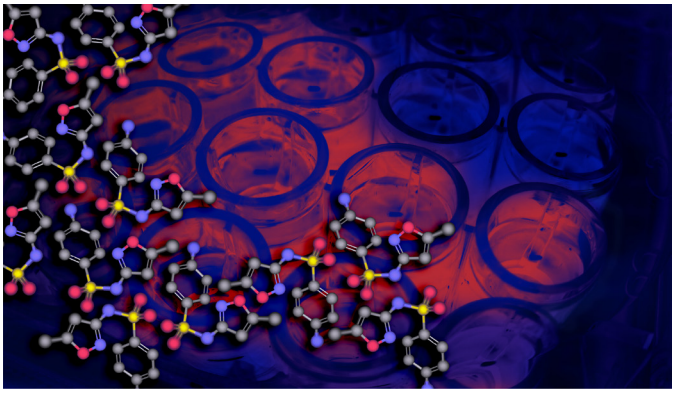
RESEARCH THEMES/
GREENER ANALYTICAL METHODS

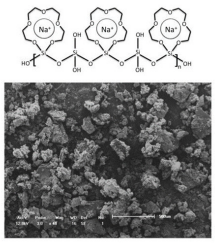
Sustainability is the key word in modern Chemistry. Analytical developments must embrace this paradigm and research within this topic will focus on providing analytical solutions with low environmental impact.

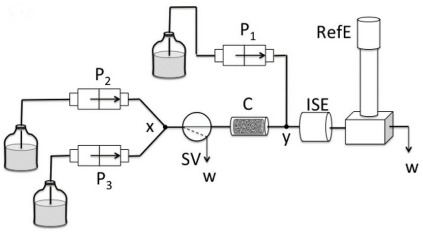
For this, methods based on the physical-chemical properties of target analytes will be sought, namely using electrochemical-based detectors and infrared/Raman spectroscopy associated to data fusion chemometrics.

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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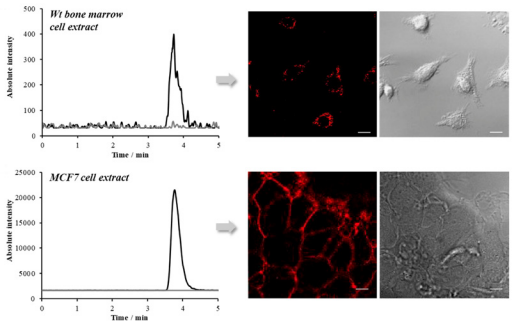
HIGHLIGHTS

DETERMINATION OF NEUROPEPTIDE Y Y1 RECEPTOR ANTAGONIST BIBP 3226 BY TARGETED ANALYSIS

Neuropeptide Y (NPY) is a peptide widely distributed throughout the body that is involved in various physiological processes, including the regulation of feeding behavior and energy homeostasis. BIBP 3226 is a selective NPY Y1 receptor antagonist with recognized application in bone regeneration studies, requiring quantification at picogram levels. A validated HPLC-MS/MS method has been developed with LOD and LOQ values as low as 0.1 and 0.3 pg in cell extracts and 16 and 48 pg in supernatant culture media, respectively. BIBP 3226 was successfully determined in cell extracts and supernatants obtained from internalization assays. Using similar exposure conditions, the amount of BIBP 3226 found in breast cancer cells (MCF7) was 72 to 657 times higher than that found in bone marrow cells (Wt C57BL/6 mice), providing an indirect indicator of NPY Y1 receptor expression.

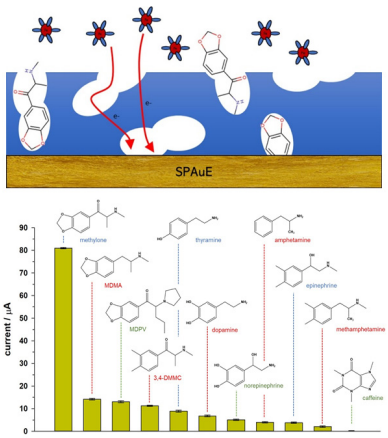


Determination of neuropeptide Y Y1 receptor antagonist BIBP 3226 and evaluation of receptor expression based on liquid chromatography coupled with tandem mass spectrometry.

Anal. Bioanal. Chem. 2020, 412, 6625-6632

ILLEGAL DRUG SCREENING BY MOLECULARLY IMPRINTING

Methylone, an illegal drug, is a synthetic cathinone which inhibits the uptake of amines at the central nervous system, similar to cocaine or amphetamines. An electroanalytical method for the selective quantification of methylone based on molecular recognition has been developed, targeting in-situ medical and forensic analysis. 2-Mercaptobenzimidazole (2-MBI) was chosen as monomer for electropolymerization, as it binds strongly with methylone (demonstrated by theoretical studies and molecular modelling) and the mercapto group provided good polymer-gold binding on gold electrodes. The molecularly imprinted polymer (MIP) was then electrosynthesized on the surface of a screen-printed gold electrode by polymerizing 2-MBI in the presence of methylone as template. This was subsequently extracted from the polymeric layer, resulting in a selective electrochemical sensor, which response was indirectly measured using ferricyanide/ferrocyanide pair as redox probe. The sensor displayed good sensitivity and selectivity in presence of chemically similar compounds. The analytical performance confirmed the sensor suitability for the facile electroanalytical quantification of methylone in human urine and blood.



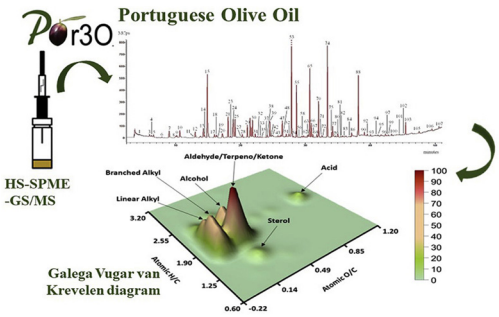
Methylone screening with electropolymerized molecularly imprinted polymer on screen-printed electrodes.

Sens. Actuator B-Chem. 2020, 316, 128133

HIGHLIGHTS

3D VAN KREVELEN DIAGRAMS FROM COMPREHENSIVE CHROMATOGRAPHY

A method based on head-space solid phase micro-extraction hyphenated to gas chromatography-mass spectrometry 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.

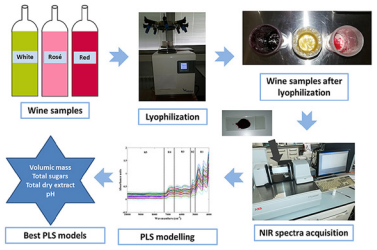


Revisiting 3D van Krevelen diagrams as a tool for the visualization of volatile profile of varietal olive oils from Alentejo region, Portugal

Talanta. 2020, 207, 120276

LYOPHILIZATION ENABLES FAST ANALYSIS OF WINES BY NEAR INFRARED SPECTROSCOPY

The implementation of near-infrared (NIR) spectroscopy for the quantification of major wine parameters is limited due to the aqueous nature of wines. Water molecules contribute to a poor signal-to-noise ratio and to suppress important groups' vibrations frequencies, hindering quantification. An alternative approach was proposed using lyophilized wine samples. A diversity of wine samples, including red, white and rosé, were lyophilized and analyzed by NIR spectroscopy (10,000 to 4000 cm−1). The partial least squares (PLS) regression models obtained were able to accurately quantify total sugars, pH, volumic mass and total dry extract with a range-error-ratio above 10. Nevertheless, alcoholic strength, total acidity, volatile acidity, free sulfur dioxide and total sulfur dioxide were not well predicted. The lyophilization process itself may change the concentration of volatile compounds and, therefore, different sample treatment conditions would be required.



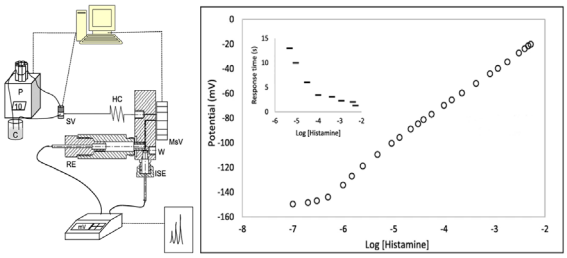
The application of near infrared spectroscopy to wine analysis: An innovative approach using lyophilization to remove water bands interference.

Talanta. 2020, 214, 120852

HIGHLIGHTS

POTENTIOMETRIC SENSOR FOR HISTAMINE DETERMINATION

Histamine (2-(4-imidazolyl)-ethylamine) is a biogenic amine with an important role in local immune and inflammation responses to pathogens and allergens, synthesized and released from several differentiated cells such as mast cells, basophils, platelets, and histaminergic neurons. Based on supramolecular organic frameworks, a histamine-selective electrode was proposed using cucurbit[6]uril (CB[6]) as ionophore, considering that the apparent stability constant of histamine-CB[6] (log) is 4.33. A polymeric membrane (PVC) was assembled, combining CB[6], 2-nitrophenyl octyl ether as solvent mediator, and potassium tetrakis(4-chlorophenyl)borate as anionic additive. Additionally, the enhancement of the detection limit was possible by the introduction of multi-walled carbon nanotubes in the membrane composition, providing a selective electrode with extended lifetime, fast response, and detection limit of 100 nM. The sensor was coupled to an automatic system, fostering the analysis of 30 samples per hour, requiring a sample volume < 200 µL. This strategy was successfully applied to quantification of histamine in biological samples after solid phase extraction.

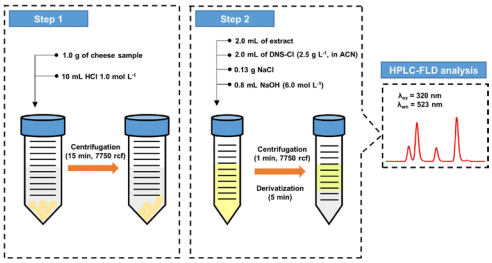


A simpler potentiometric method for histamine assessment in blood sera.

Anal. Bioanal. Chem. 2020, 412, 3629-3637

SALTING-OUT AS EFFECTIVE SAMPLE TREATMENT FOR BIOGENIC AMINES ANALYSIS

Neuropeptide Y (NPY) is a peptide widely distributed throughout the body that is involved in various physiological processes, including the regulation of feeding behavior and energy homeostasis. BIBP 3226 is a selective NPY Y1 receptor antagonist with recognized application in bone regeneration studies, requiring quantification at picogram levels. A validated HPLC-MS/MS method has been developed with LOD and LOQ values as low as 0.1 and 0.3 pg in cell extracts and 16 and 48 pg in supernatant culture media, respectively. BIBP 3226 was successfully determined in cell extracts and supernatants obtained from internalization assays. Using similar exposure conditions, the amount of BIBP 3226 found in breast cancer cells (MCF7) was 72 to 657 times higher than that found in bone marrow cells (Wt C57BL/6 mice), providing an indirect indicator of NPY Y1 receptor expression.



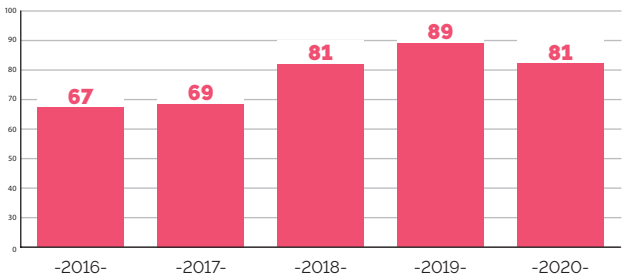
Development of a SALLE-HPLC-FLD analytical method for the simultaneous determination of ten biogenic amines in cheese.

Food Anal. Meth. 2020, 13, 1088-1098

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION

Articles published / Year



H-index: **70**

387 articles*
33250 citations

***2016-2020**
From WOS core collection

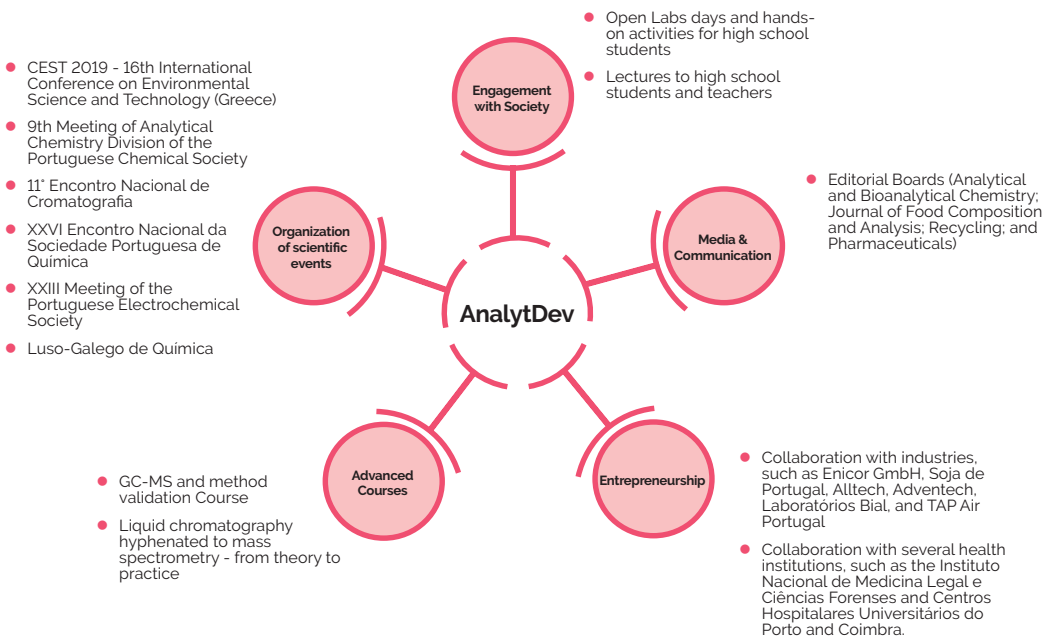
FUNDED PROJECTS *(Representative projects)*

- **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.
- **Screening of antibiotic contamination by mobile devices**
  FCT, PTDC/CTA-AMB/31756/2017, Marcela Segundo (PI).
  Total Funding: € 239,106.00.
- **Dialysis membranes by design: targeting neutrophil elastase to reduce inflammation/oxidative stress in end-stage renal disease**
  PTDC/MED-CAR/31322/2017, Conceição Branco (PI).
  otal Funding: € 232,938.00.
- **Sensitization of urologic tumors therapy driven by nanotechnology**
  FCT, PTDC/MED-QUI/29800/2017, João Prior (co-PI).
  Total Funding: € 239,938.00.
- **Rapid electrochemical detection of foodborne pathogens using bacteriophage nanoparticles**
  FCT, PTDC/NAN-MAT/31968/2017, Júlia Magalhães (PI).
  Total Funding: € 237,162.00.

INTERNATIONAL COOPERATION AND NETWORKING

- COST Action ES1407, "European network for innovative recovery strategies of rare earth and other critical metals from electric and electronic waste", from 2015-2019.
- COST Action CA16215, "PortASAP - European network for the promotion of portable, affordable and simple analytical platform", from 2018-2021.
- SENER- Ingeniería y Construcción, Barcelona, Spain
- Main strategic partner of STARSS - Specialized Team for Advanced Research on Separation Science (CZ.02.1.01/0.0/0.0/15_003/0000465) and of EFSA–CDN - Efficiency and safety improvement of current drugs and nutraceuticals: advanced methods – new challenge, Project CZ.02.1.01/0.0/0.0/16_019/0000841, Charles University, Czech Republic
- Team members of project CTM2017-84763-C3-2-R, Nestor Etxebarria (PI), University of Basque Country, Spain

DISSEMINATION & OUTREACH



LABORATÓRIO ASSOCIADO
PARA A **QUÍMICA VERDE**

BCO

(BIO)CHEMISTRY & OMICS

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

Group Coordinator:

Carlos Lodeiro

The (Bio)Chemistry & OMICS 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 and environmental problems using multidisciplinary approaches.

BCO comprises 25 senior researchers and 9 research labs in an integrative and cooperative approach, with a strong relationship with several International and National universities, hospitals, research centres, 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) Nanoproteomics | Proteomics and Oncoproteomics for the identification on tumor specific antigens; and vi) quantitative characterization post-translational modification in complex biological systems and in the analysis of bacteriology, mycology and viruses samples.

RESEARCH OBJECTIVES [2020-2023]

The (Bio)Chemistry & OMICS 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 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 (UNL).
- The identification and characterization of CO_2 reductases with biotechnological interest for the utilization of the abundant atmospheric CO_2 in the synthesis of added value compounds (UNL).

From 2018, the group has benefited from the incorporation of new members from the Universities of Aveiro and Porto. This circumstance potentiates the application of mass spectrometry in our research, both in terms of access to different equipment and of study other targeted analytes to an overall better comprehension of complexes and dynamic biological systems.

RESEARCH TEAM

SENIOR RESEARCHERS


Carla Miranda

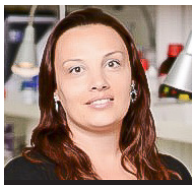

Carlos Lodeiro

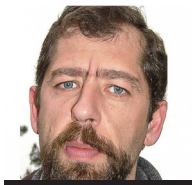

Conceição Santos


Cristina Cordas


Cristina Costa


Eliana Alves

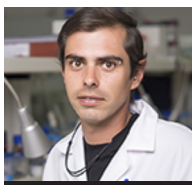

Elisabete Oliveira


Francisco Amado

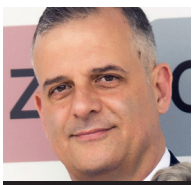

Gilberto Igrejas


Hugo Miguel Santos


Isabel Moura

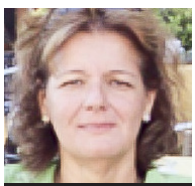

Javier Fdez -Lodeiro


Jorge Lampreia

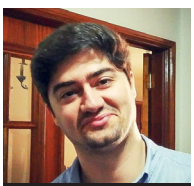

José Luís Capelo


José Moura


Luísa Maia


Maria João Nunes

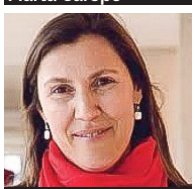

Marta Carepo


Miguel Ribeiro


Patrícia Poeta


Pedro Domingues


Pedro F. Oliveira


Rita Ferreira


Sílvia Coimbra


Sofia Guedes

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OTHER DOCTORATE RESEARCHERS
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Ana Pereira
Bruno Neves
Carla Carneiro
Luisa Helguero
Rui Vitorino
Stéphane Besson

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Ana Martins
Cíntia Carreira
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Fernando Ricardo
João Monteiro
Maria Maciel
Susana Aveiro
Susana Jorge

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Claudia Alfarela
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Frederico Duarte
Gabriel Valerio
Jessica Ribeiro
Joana Galhano
João Antunes
João Pinto
Liliana Denis
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Miguel Anjos
Paulo Pinto
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Tânia R. M. Ferreira
Tiago Costa

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Carolina Sabença
Pedro Bragança
Telma Sousa
Tiago Conde

OTHER RESEARCHERS
Cristian Cuerva
Cristina Barros

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

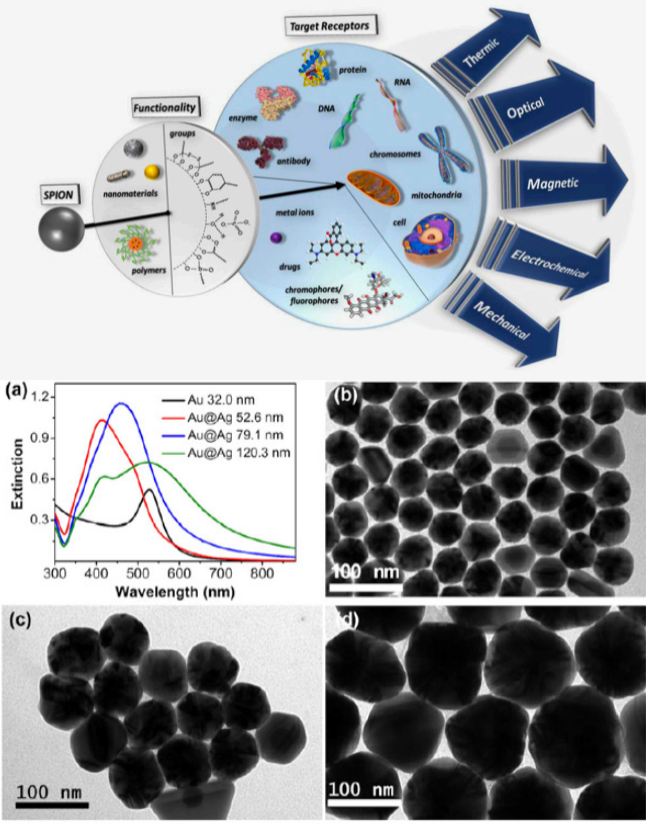
We have focused our work on the Synthesis of new Fluorescent and Colorimetric dyes, developing novel functionalized nanoparticles and composites (Au, Ag, Pt, Pd, SiO2, Fe2O3), doped polymers, mesoporous materials for drug cargo delivery, and nanoprobes for applications in environmental detection of Pollutants,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

NEW EMISSIVE LIQUID CRYSTALS AND SMART MATERIALS [1-2]

NANOMATERIALS FOR CATALYSIS AND OPTOELECTRONIC APPLICATIONS [3-4]

NANOMATERIALS AND DYES AS SCAVENGERS, DRUG DELIVERY AND IMAGING SYSTEMS [5-8]

BIOMEDICAL, TRANSLATIONAL, AND PROTEOMICS APPLICATIONS [8-10]



SELECTED PUBLICATIONS

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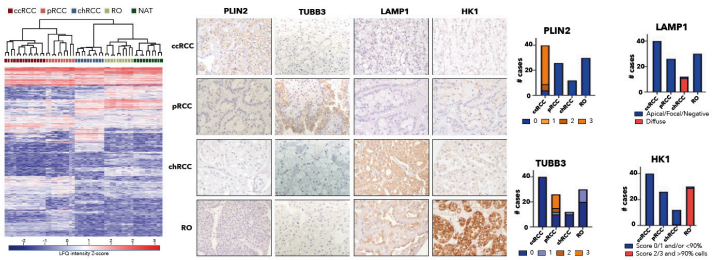
RESEARCH THEMES/
BIOANALYTICS & PERSONALIZED NANO@PROTEOMICS

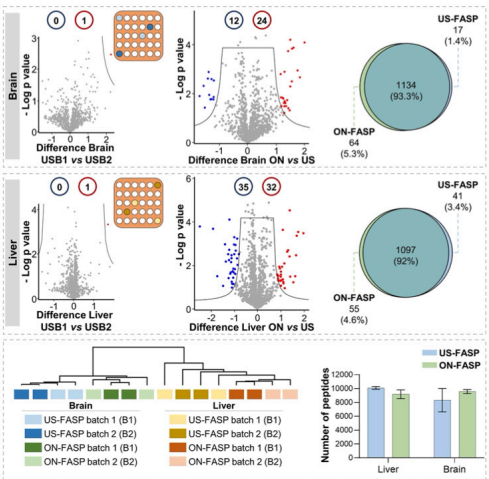
FUNCTIONAL ASSOCIATIONS OF POST-TRANSLATIONAL MODIFICATIONS & PRECISION HEALTH

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.[11-15]

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.[16-20]



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RESEARCH THEMES/ BIOLOGICAL CHEMISTRY AND DISEASE-RELATED MECHANISMS

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

NITROGEN BIOGEOCHEMICAL CYCLE – DENITRIFICATION

- mechanistic and structural characterization of all metalloenzymes involved in the denitrification pathway[21,22]
- biophysical and structural characterization of electron transfer complexes, and molecular recognition processes[21,22]
- development of effective disposable biosensors for nitrite, using nitrite reductases, and for nitric oxide, using nitric oxide reductase[23,24]

CARBON DIOXIDE REDUCTION[25-27]

- establishment of an innovative reaction mechanism for the formate dehydrogenase catalysis
- identification and characterization of a new and very efficient carbon dioxide reductase
- bioelectrochemical reduction of carbon dioxide

NOVEL HETEROMETALLIC CLUSTERS

- characterization of the novel and unique molybdenum/copper heterometallic cluster of the bacterial "Orange Protein"

HUMAN PATHWAYS FOR THE GENERATION OF NITRIC OXIDE

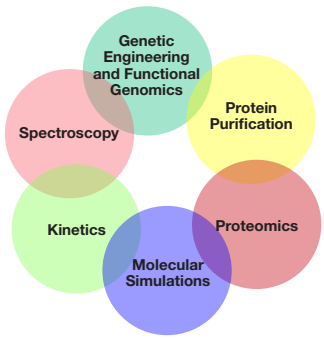
- characterization of new pathways for the generation of signaling nitric oxide in humans under hypoxic conditions, dependent on xanthine oxidoreductase and aldehyde oxidase[28]

BACTERIAL ROS METABOLISM AND DETOXIFICATION MECHANISMS[29-30]

- mechanistic characterization of hydrogen peroxide and superoxide detoxification in bacteria
- study of biological mechanisms of antityumoral ROS generating complexes by DNA cleavage assays and EPR
- study of new molecular systems involved in detoxification of metals, namely copper and molybdenum, and of arsenic-containing species

ARTIFICIAL PROTEINS

- development of spectroscopic probes, bioinorganic models of metalloenzymes and novel catalysts, using artificial metal-substituted proteins



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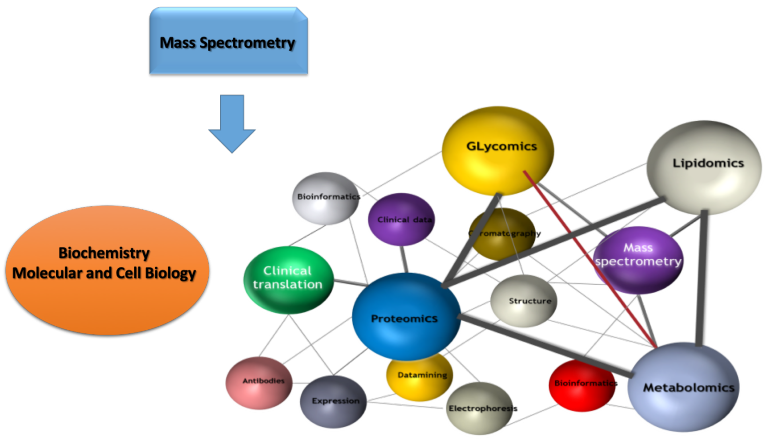
RESEARCH THEMES/ BIOLOGICAL CHEMISTRY AND DISEASE-RELATED MECHANISMS

METABOLOMICS, LIPIDOMICS, AND PROTEOMICS PROFILING OF METABOLIC SIGNATURES

This line of research focuses on the applications of mass spectrometry for the study of metabolism. We intend to elucidate the metabolic profile and the differential adaptation of the main metabolic pathways to different elicitors using an integrated metabolomic, lipidomic, proteomic, and phosphoproteomics approach. To date, the main work has been developed in the study of metabolic signatures as a means of identifying the mechanisms of adaptation of species to diseases and environmental agents.

THE MOLECULAR BASIS OF LIFESTYLE AND DISEASES

This line of research is concerned with the study of noncommunicable diseases using immunohistochemistry and proteomics as core methodologies and taking advantage of a diversity of experimental models (*in vitro, ex-vivo,* and *in vivo*) and human samples (body fluids and biopsies). Our research aims to study: i) cancer and cardiac cachexia; ii) disease biomarkers; iii) the impact of lifestyle on specific biochemical phenomena that influence human health (particularly muscle wasting conditions and male reproductive health); and iv) mitochondrial bioenergetics and plasticity in pathophysiological conditions.



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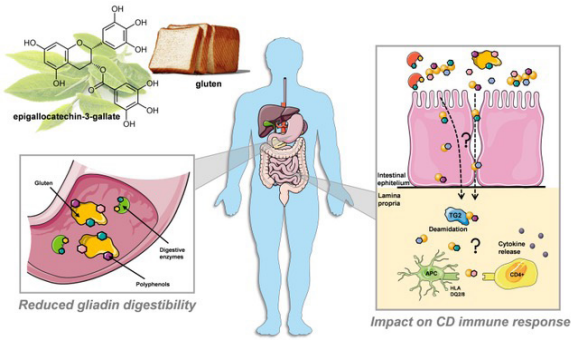
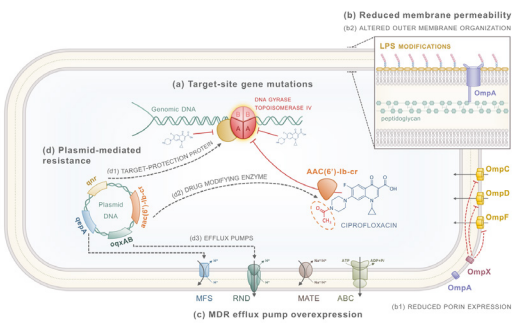
RESEARCH THEMES/
FUNCTIONAL GENOMICS AND PROTEOMICS

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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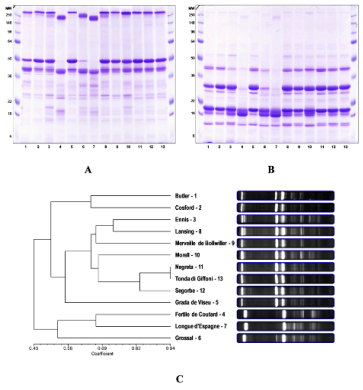
RESEARCH THEMES/
MicroART - MICROBIOLOGY AND ANTIBIOTIC RESISTANCE TEAM

The group aim to clarify mechanisms of multiresistant antibiotic resistance strains on an integrated and multidisciplinary scope by using genomics and proteomics; to characterize by biochemical and genetic methods the presumably news bacteriocins as bio-preservatives in the industry feed; to use Probiotics in biotechnology and health and to analyze the Bacterial Biofilm and its Role in the Pathogenesis of Disease

MECHANISMS OF MULTIDRUG RESISTANCE

The group drives part of its research activities on the detection of foodborne pathogens and specific spoilage organisms from food of animal origin along with different food production chains. Under these research subjects, important microbiological hazards (*Salmonella sp., E. coli*, MRSA) involved in foodborne outbreaks are analyzed. The group are also developing new approaches to analyze and interpret more complex and emerging microbial pathogen, using molecular, serotyping, and phylogenetic analysis. Furthermore, we are working to improve knowledge on prevalence and definition of contamination sources, risk to public health, and strategies to improve food safety and quality. The group analyze antibiotic resistance problem in a One Health concept.



BACTERIOCINS AS BIO-PRESERVATIVES IN THE FEED INDUSTRY

Phenotypic and genotypic profiles and proteomic patterns will be obtained to determine possible proteins involved in antibiotic resistance mechanisms, to evaluate the in vitro activities of new antibiotics against a serial of different strains already isolated and to study the application of bacteriocinogenic lactic bacteria as bio-preservatives in the feed industry. Our high quality research enables us to know which antimicrobial resistant bacteria variants are associated to each focus of infection, each animal species and in a particular each habitat, which is important to carry a greater control over the dissemination of zoonotic bacteria and better understand their transmissibility.

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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.

AGRIFOOD QUALITY AND SAFETY: FROM THE PLANT TO HUMAN CELLS[61-64]

We assess nanoparticles bioactivity/toxicity in different models (eg, plants, insects, human cells) and applications (eg, agrochemical delivery).
We unveil the dynamic relations and signaling between human pathogens (eg., Klebsiella spp.) and plant-hosts.

SIGNALING UNDER EXTREME EVENTS[65-67]

We disclose how extreme episodes associated to climate change shift plant´s signals, metabolism and physiology. We look for resistance genes/genotypes, for future exploitation on agrifood programs.

MOLECULAR PLAYERS INVOLVED IN SEED PRODUCTION[68]

We investigate 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[69]

Sugars are fundamental signaling molecules for many aspects of 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.

BIOTIC INTERACTIONS AND NEW BIOCONTROL STRATEGIES

We use (meta)genomics, transcriptomics, metabolomics and physiological tools to decipher pests' epidemiology, metabolic/functional shifts during biotic interactions, and pests response to new biocontrol solutions.

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HIGHLIGHTS

IRON(II) AS GREEN REDUCING AGENT FOR GOLD NANOPARTICLES SYNTHESIS

A highly versatile seed-mediated approach for the synthesis of citrate-stabilized gold, silver and palladium nanoparticles (NPs) with size control is reported. The use of iron(II) as a reducing agent enables the fabrication of monodisperse NPs in a wide range of sizes (from 15 nm to at least 120 nm (90 nm for Pd)) at room temperature. The citrate as capping ligand on the NPs surface facilitates its further surface modification with proteins and thiolated molecules.

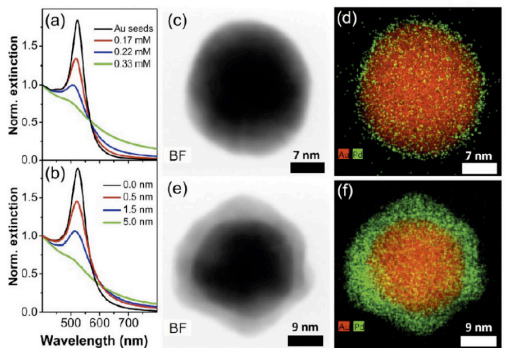


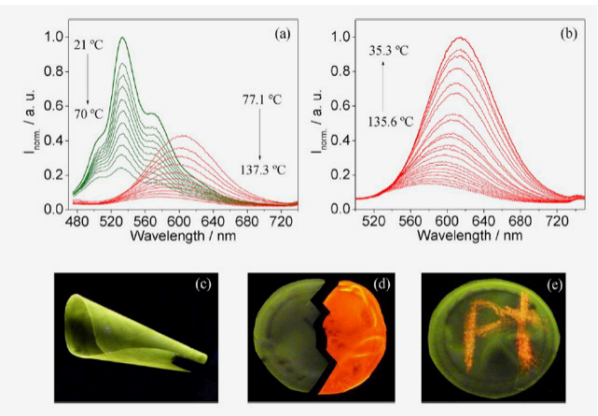
Fig. (a) Normalized extinction spectra of Au@Pd NPS upon reduction of different Pd salt amounts, as indicated. (b) Calculated extinction spectra of Au@Pd NPs with different Pd Thicknesses. (c-f) BF-STEM images and the corresponding EDX maps.

The versatility of Fe(II) in the synthesis of uniform citrate-stabilized plasmonic nanoparticles with tunable size at room temperature

Nano Research, 2020, 9, 2351-2355 (2020)

PLATINUM(II) METALLOMESOGENS AS DYES SENSITIVE FOR HG(II) AND STIMULI-RESPONSIVE LUMINESCENT POLYMER MATERIALS

The application of novel methodologies to the synthesis of nanomaterials is still a challenge in many different technological and scientific fields. New efficient and reproducible synthetic methodologies, that produce fewer residues and reduce the cost of raw materials, must be developed. We have explored the attractive possibility of applying the cheap iron (II) sulphate salt in the reduction process of the K_2PtCl_4 to produce colloids suspensions. The synthesis occurred in water and was assisted by sodium citrate (SC) using polyvinylpyrrolidone (PVP) as a surfactant. The adjustment of this novelty process allows to obtain well-dispersed and sub-20 nm dendrimer-type platinum nanoparticles (Pt D-NPs). Catalytic application of the Pt D-NPs has been explored in the reduction of p-nitrophenol (p-NP) to p-aminophenol (p-AP) in aqueous media at room temperature, obtaining a TOF value of 253 min^{-1}. Furthermore, it was also tested as artificial metalloenzyme showing catechol oxidase activity for oxidation of L-DOPA.



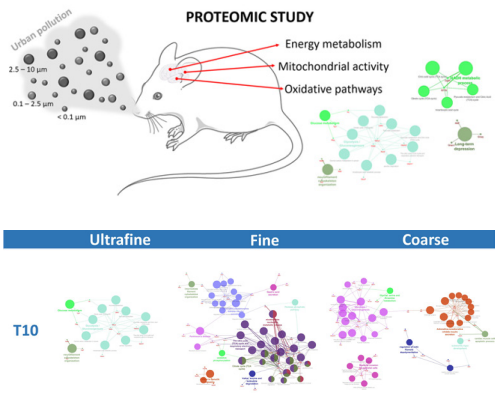
Aggregation-induced emission enhancement (AIEE)-active Pt(II) metallomesogens as dyes sensitive to Hg2þ _and dopant agents to develop stimuli-responsive luminescent polymer materials

Dyes & Pigments, 2020, 175, 108098.

HIGHLIGHTS

PROTEOMIC CHANGES DRIVEN BY URBAN POLLUTION SUGGEST PARTICULATE MATTER AS A DEREGULATOR OF ENERGY METABOLISM, MITOCHONDRIAL ACTIVITY, AND OXIDATIVE PATHWAYS IN THE RAT BRAIN

The adverse effects of air pollution have been long studied in the lung and respiratory systems, but the molecular changes that this causes at the central nervous system level have yet to be fully investigated and understood. To explore the evolution with time of protein expression levels in the brain of rats exposed to particulate matter of different sizes, we carried out two-dimensional gel electrophoresis followed by determination of dysregulated proteins through Coomassie blue staining-based densities (SameSpots software) and subsequent protein identification using MALDI-based mass spectrometry. Expression differences in dysregulated proteins were found to be statistically significant with p-value < 0.05. A systems biology-based approach was utilized to determine critical biochemical pathways involved in the rats' brain response.

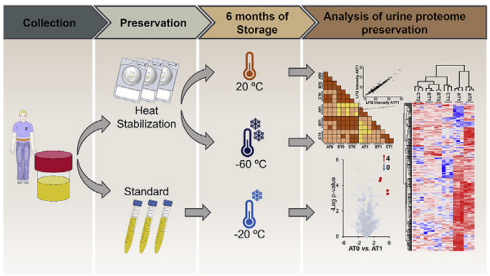


Proteomic changes driven by urban pollution suggest particulate matter as a deregulator of energy metabolism, mitochondrial activity, and oxidative pathways in the rat brain.

Science of the Total Environment, 2019, 687, 839-848.

SNAP-HEATED FREEZE-FREE PRESERVATION AND PROCESSING OF THE URINE PROTEOME USING THE COMBINATION OF STABILIZOR-BASED TECHNOLOGY AND FILTER AIDED SAMPLE PREPARATION

A new method to preserve and process urine proteins for proteomic analysis in a filter aided sample preparation (FASP) format was developed. The method combines the concentration of urine proteins in ultrafiltration devices, their thermal stabilization, allowing long term storage of the samples, and filter aided sample preparation. Proteomes of four different urines were preserved during 48h and 6 months using (i) the classic freeze preservation at 20˚C, (ii) snap-heated freeze-free preservation at laboratory temperature (20˚C), and (iii) snap-heated preservation at 60˚C. The three storage methods can effectively preserve the urine proteome for at least 6 months without significant alterations. Abundances of more than 500 proteins and specially 24 selected -cleared or -approved protein assayed in serum or plasma were found similar within the three preservation methods assessed.
The new method here proposed dramatically simplifies the conditions for preserving the urine proteome for biobanks in terms of space and storage, including lowering the risks of sample degradation caused by misfunction of the freezer. Furthermore, the shipping of large number of samples can be made without the need of freezing.



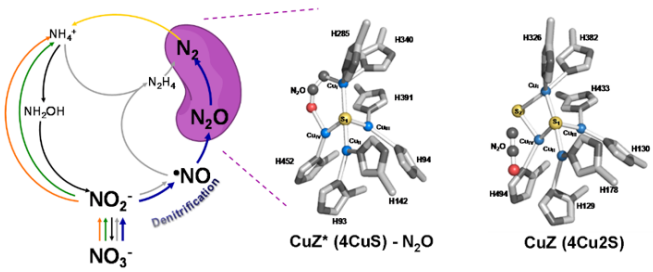
Snap-heated freeze-free preservation and processing of the urine proteome using the combination of stabilizor-based technology and filter aided sample preparation.

Analytica Chimica Acta, 2019, 1076, 82-90

HIGHLIGHTS

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.



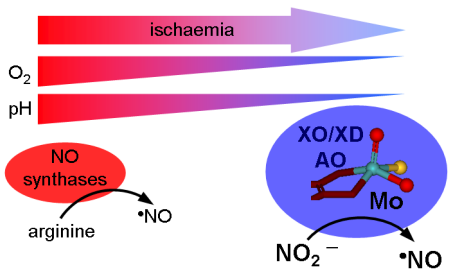
Spectroscopic definition of the CuZ* intermediate in turnover of nitrous oxide reductase and molecular insight into the catalytic mechanism.

Coordination Chemistry Reviews, 2019, 387, 436-449

NEW PATHWAYS TO GENERATE SIGNALING NO IN HUMANS UNDER HYPOXIC CONDITION

Nitric oxide radical (NO) is a signaling molecule involved in several physiological and pathological processes, and a new nitrate-nitrite-NO pathway has emerged as a physiological alternative to the classic pathway of arginine-dependent NO formation.

To contribute to elucidate the mechanisms behind the nitrite cytoprotective action observed under hypoxic conditions, we have been studying (characterizing kinetically and mechanistically) the ability of human xanthine dehydrogenase (XD), xanthine oxidase (XO) and aldehyde oxidase (AO) to reduce nitrate and nitrite to NO.



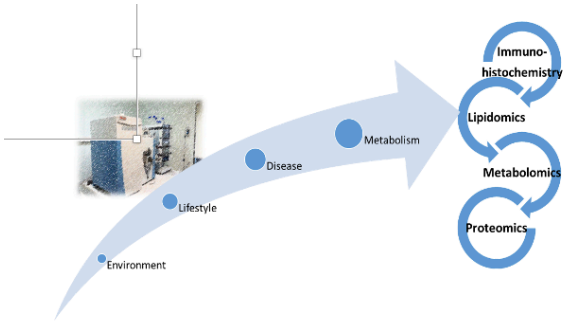
Human XD, XO, and AO catalyze the nitrite reduction to NO under hypoxic and acidic conditions, thus sustaining the •NO formation when the NO synthase activity is hampered.

Redox Biology, 2018, 19, 274-289

HIGHLIGHTS

TUMOUR RESECTION INDUCES ALTERATIONS ON SERUM PHOSPHOLIPIDOME OF LIVER CANCER PATIENTS

Hepatocellular carcinoma and cholangiocarcinoma are the most common primary malignant liver tumours. In a pilot study, we used a high-resolution HILIC-LC–MS lipidomic approach to study the serum phospholipidome profile of patients with liver cancer before and after tumour resection. We observed an upregulation of some phosphatidylcholine species, choline plasmalogens, and 1-O-alkyl-2-acyl-glycerophosphocholine in patients with liver cancer compared to the CT group, and a downregulation after tumour resection. These results show aberrant lipid metabolism in patients with liver cancer, which is altered by resection of the tumour, and that these changes can be detected by minimally invasive procedure through serum phospholipidome analysis.

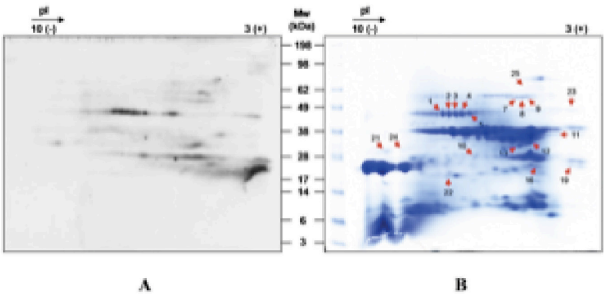


Tumor Resection Induces Alterations on Serum Phospholipidome of Liver Cancer Patients

Lipids. 2020 Mar;55(2):185-191.

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.



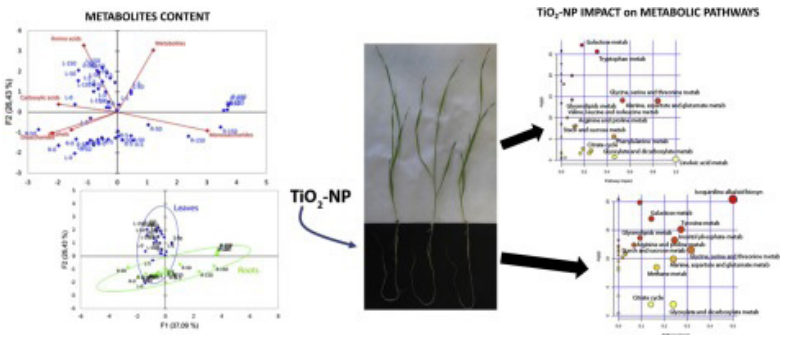
Multiomics Substrates of Resistance to Emerging Pathogens? Transcriptome and Proteome Profile of a Vancomycin-Resistant Enterococcus faecalis Clinical Strain.

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

HIGHLIGHTS

BIOACTIVITY OF ENGINEERED NANOPARTIVLES 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.



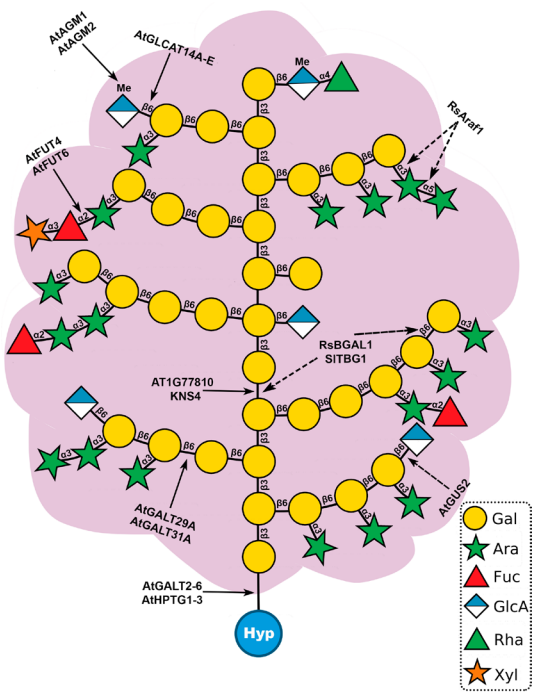
TiO2 nanoparticles induced sugar impairments and metabolic pathway shift towards amino acid metabolism in wheat.

J. of Hazardous Materials 2020, 399, 122982

HIGHLIGHTS

AGP BIOSYNTHESIS PATHWAY: THE SUGAR FACTORY

Arabinogalactan-proteins (AGPs) are a large and highly diverse class of heavily glycosylated cell wall proteins. The biosynthesis of AGPs comprises the addition and removal of amino acids, lipids, and carbohydrates. As some AGPs are composed of approximately 90% sugar, the AGP biosynthetic pathway resembles a candy factory occurring inside the cells. An N-terminal signal peptide directs AGPs toward the endoplasmic reticulum, where proline hydroxylation occurs and a GPI anchor may be added. AGPs are then transferred to the Golgi apparatus, where extensive glycosylation occurs by the action of a variety glycosyltransferase enzymes. Following glycosylation, AGPs are transported by secretory vesicles to the extracellular face of the plasma membrane. Here, we present an overview of the accumulated knowledge on AGP biosynthesis over the past three decades. The new challenge is to define how AGPs, after all the processes involved with their biosynthesis, act in the cells. Specifically, it will be important to elucidate the mechanism of action by which AGPs, and specifically their sugar epitopes, function. This will mean discovering the molecules, which interact with these sugar residues. These major challenges will be a stimulus for new future research developments on AGPs through the next 30 years.

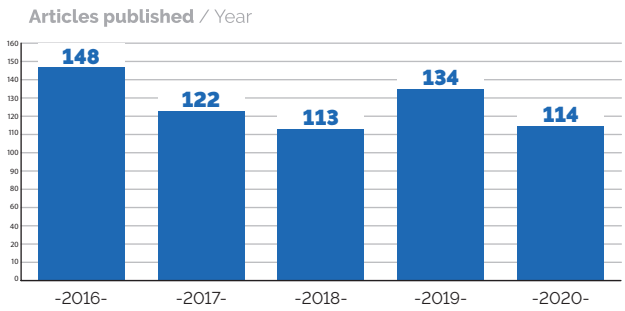


Three Decades of Advances in Arabinogalactan-Protein Biosynthesis.

Frontiers in Plant Science, 2020, 11, 610377.

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION



H-index: **88**

631 articles*
47873 citations

***2016-2020**
From WOS core collection

FUNDED PROJECTS

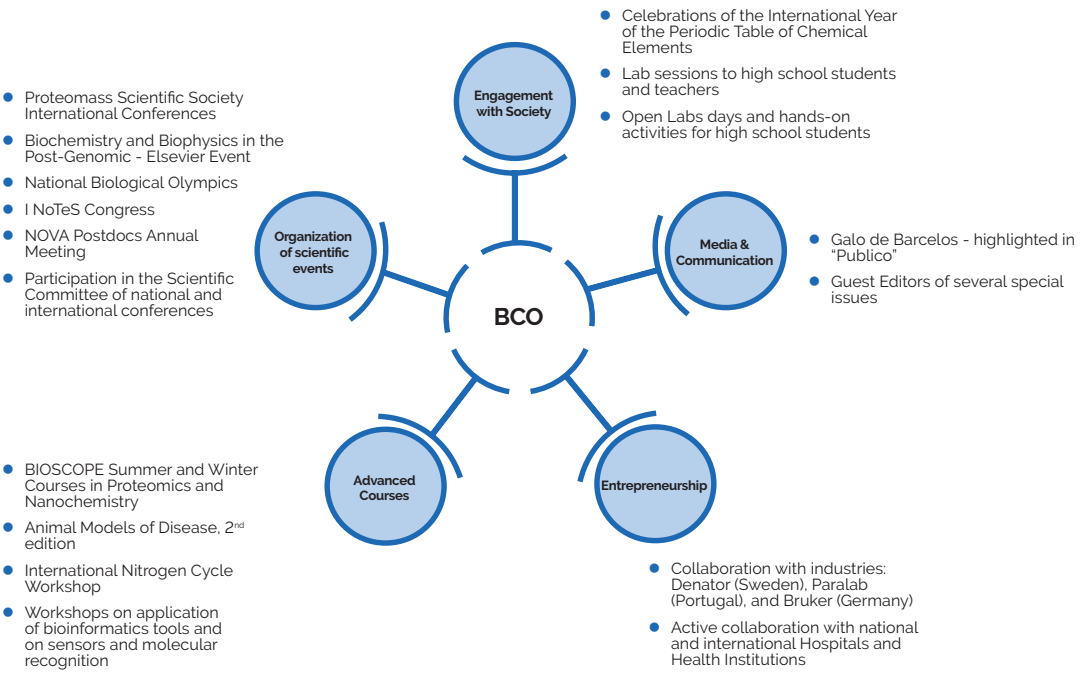
(Representative projects)

- MASS spectrometry Training in Protein Lipoxidation Analysis for Inflammation
  European Union, Innovative Training Networks, ITNH2020-MSCA-ITN-2015.
  Total funding: € 476,712.00
- Development of novel multifunctional nano-polyplexes as imaging and delivery vectors against triple negative breast cancer
  FCT, PTDC/QEQ-MED/2118/2014, Carlos Lodeiro (PI).
  Total funding: € 87,511.00
- Denitrification - How to deal with NO and N_2O
  FCT, PTDC/BBB-BQB/0129/2014, Isabel Moura (PI).
  Total funding: € 199,996.00
- OXYMOD - Optimized oxidative enzyme systems for efficient conversion of lignocellulose to valuable products
  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.
  Total funding: € 233,673.90
- Biomaterials for Regenerative Medicine Total
  CENTRO-07-ST24-FEDER-002030, Francisco Amado (PI).
  Total funding: €150.000,00
- SpermBoost – improving sperm preparation and cryopreservation for Assisted Reproductive Technologies
  By Merck®, 2019 – 2022, Pedro F. Oliveira (Co-PI).
  Total funding: € 300,000.00
- Physical and emotional stress biomarkers detection through non-invasive techniques
  FCT/MCTES, PTDC/SAU-SOC/28390/2017, Cristina Cordas (PI).
  Total funding: € 239,929.28
- Re-equipment "BIOSCOPE Laboratories – PROTEOMASS Scientific Society"
  Projects 2016-2019 Private Funding. (PI: C.Lodeiro, J.L Capelo, H. M. Santos, E. Oliveira, J. Fdez Lodeiro, and A. Fdez Lodeiro).
  Total funding: € 870,000.00
- Development of adjustable Silver@Silica nanocarriers and their stabilization in solid materials against drug resistant and non-resistant pathogenic bacteria. Towards advanced nano-antibiotics, wound dressing and anti-biofilm surfaces
  PTDC/QUI-COL/1517/2020. (PI: J. Fernández-Lodeiro, CoPI: C. Lodeiro).
  Total funding: € 233,038.50
- Comparative assessment of antimicrobial resistance in environmental biofilms through proteomics - towards innovative theranostic biomarkers — CAREBIO2", com referência n.º 030101, aviso 02/ SAICT/2017.
  Patrícia Poeta.
  Total funding: € 239.687,50
- 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

INTERNATIONAL COOPERATION AND NETWORKING

- COST Action FA1306, "The quest for tolerant varieties: phenotyping at plant and cellular level", 2014-2018.
- COST Action EuroMicropH 18113
- COST Action CAR182217. ENOVAT
- 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)
- Brazilian-Portuguese Bilateral Cooperation under a CNPq financed project (401797/2013-9), 2014-2018, Universidade de São Paulo, Brazil.
- Brazilian-Portuguese Bilateral Cooperation under a CAPES financed project (88881.062204/2014-01), 2014-2019, Universidade de Campinas, Brazil.
- 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.

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 predicaments.

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, control and remediation of soil; monitoring and treatment of water and wastewater, municipal and industrial solid wastes, as well as toxic and hazardous substances.

In addition, the field of Environmental Science relies heavily on analytical chemistry. Therefore, it also encompasses the development of screening methods and/or the improvement of the existing confirmatory methods for the analysis of the above-mentioned contaminants based on the principles of Green Chemistry, and environmental and economic sustainability. These methods have to meet current or proposed legislative requirements and are mainly based on chromatography, spectrophotometry, and biosensor tools.

RESEARCH OBJECTIVES [2020-2023]

The major research objectives of the Environmental Chemistry group are:

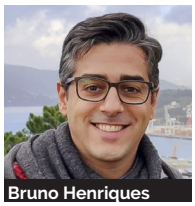
- to develop new analytical methods with higher performances, lower costs and environmental impacts for the quantification and monitoring of pollutants (pesticides, brominated flame retardants, pharmaceuticals, polycyclic aromatic hydrocarbons, metals,...) and contaminants in food (fresh and processed); 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 develop miniaturized and portable sensors (such as electrochemical and fluorescent) 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 and environmental 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.

RESEARCH TEAM

SENIOR RESEARCHERS


Álvaro Torrinha


Antonio Vega


Bruno Henriques


Clara Grosso


Cristina Delerue-Matos


Cristina Soares


Elena Surra


Elsa Vieira


Fátima Barroso


Francisca Rodrigues

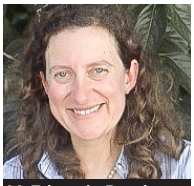

Hendrikus Nouws


Henrique Vicente

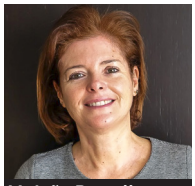

João Pacheco

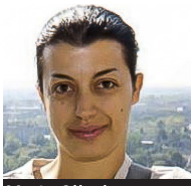

Manuela Correia


Manuela Moreira


M. Eduarda Pereira

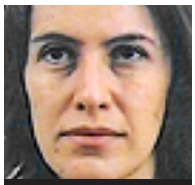

Maria Freitas

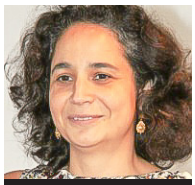

M. João Ramalhosa

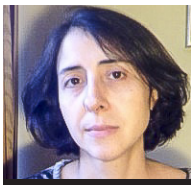

Marta Oliveira

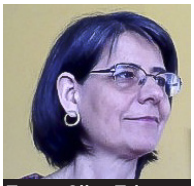

Nuno Lapa

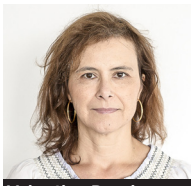

Olga Freitas


Salomé Teixeira


Simone Morais


Sónia Figueiredo


Teresa Oliva-Teles


Valentina Domingues


Vírginia Fernandes

 Group coordinator

RESEARCH TEAM

OTHER DOCTORATE RESEARCHERS

Carlos Vale
Claúdia Lopes
Estefanía Costa Rama
José Luis Vera
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Tomás Albergaria

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Diana Pinto
Diana Rede
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M. Aurora Silva
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Ana Almeida

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 distribution of micropollutants between water, soil, air, and biota is governed by their physicochemical properties, namely the fugacity, which may vary considerably, posing additional analytical challenges. 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 or subcritical fluid extraction, are privileged. The development of miniaturized and portable (bio)sensors for environmental control is another area of expertise.

Environmental monitoring allows to assess the degree of contamination and it is the basis for the development of treatment and remediation techniques. Monitoring data are to be gathered for the purpose of future policies and regulations.

SELECTED PUBLICATIONS

1 A. Maia, et al., Environ. Pollut. 2020, 259 113927. doi:10.1016/j.envpol.2020.113927

2 K. Slezakova, et al., Environ. Pollut. 2020, 258, 113648. doi.org/10.1016/j.envpol.2019.113648

3 M. Fernandes, et al., Chemosphere 2020, 239, 124729. doi:10.1016/j.chemosphere.2019.124729

4 J. Seco, et al., Environ. Pollut. 2020, 264, 114711. doi:10.1016/j.envpol.2020.114711

5 J. Seco, et al., Chemosphere 2020, 239, 124785. doi:10.1016/j.chemosphere.2019.124785

6 B. Jinadasa, et al., Food Addit. Contam. Part A-Chem. 2020, 37, 1004. doi:10.1080/19440049.2020.1733103

7 A. Maia, et al., Environ. Pollut. 2020, 259, 113927. doi:10.1016/j.envpol.2020.113927

8 L. Carvalho, et al., Water Air Soil Pollut. 2020, 231, 541. doi: 10.1007/s11270-020-04900-8

9 L. Barboza, et al., Sci. Total Environ. 2020, 717, 134625. doi: 10.1016/j.scitotenv.2019.134625

10 J. Queirós, et al., Environ. Res. 2020, 187, 109680. doi: 10.1016/j.envres.2020.109680

11 J. Queirós, et al., Mar. Environ. Res. 2020, 161, 105049. doi: 10.1016/j.marenvres.2020.105049

12 R. Matias, et al., Mar. Pollut. Bull. 2020, 158, 111447. doi: 10.1016/j.marpolbul.2020.111447

13 B. Barros, Environ. Int. 2021, 156, 106704. doi:10.1016/j.envint.2021.106704

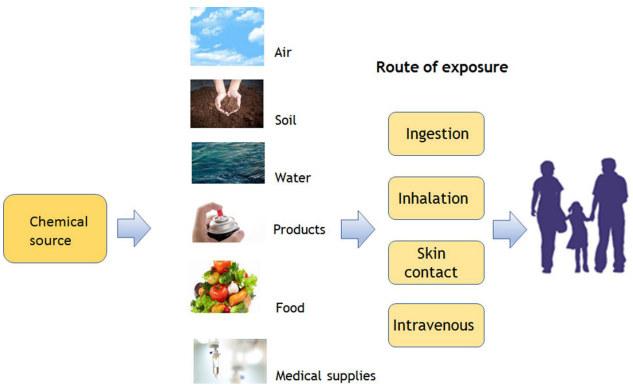
14 M. Oliveira, et al., Int. J. Environ. Res. Public Health 2021, 18, 230. doi:10.3390/ijerph18010230

RESEARCH THEMES/
MONITORING OF CONTAMINANTS AND TREATMENT

BIOMONITORING: SOURCES AND EXPOSURE ASSESSMENT

Exposure to environmental pollutants occurs through several routes, such as inhalation, ingestion, dermal absorption, and intravenous. Biomonitoring of exposure is a useful tool to assess environmental exposure. The body's burden of a specific pollutant is determined by several factors, such as the pollutant's concentration in a specific environmental medium, its physical and chemical properties, the timing of exposure, as well as individual factors, namely the uptake, metabolism, and excretion rates.

Biomonitoring provides the answer to the possible impact of chemicals on human health. By measuring these chemicals or metabolites in blood, urine, breast milk, adipose tissue, hair, or other clinical specimens, researchers can study the absorption extent of a chemical, and whether that chemical is being retained in the body. Biomonitoring can be used to determine people's exposure to a chemical following an incident, gather information on trends, whether a certain chemical is increasing or declining in a population or subgroup, and evaluate public health interventions to determine their success and prioritize environmental health resources.



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;
- establish reference values to determine whether a person or group has an unusually high exposure;
- assess the effectiveness of public health efforts to reduce exposure;
- determine whether exposure levels are higher among minorities, such as children and obese people;
- determine which chemicals get into the bodies of a population and at what concentrations.

SELECTED PUBLICATIONS

15 M. Oliveira, et al. Environ. Pollut. 2020, 266, 115243. doi:10.1016/j.envpol.2020.115243

16 T. Viana, et al., Environ. Pollut. 2020, 115458. doi:10.1016/j.envpol.2020.115458

17 S. Sousa, et al., J. Pharm. Biomed. Anal. 2020, 191, 113598. doi:10.1016/j.jpba.2020.113598

18 F. Coppola, et al., Water 2020, 12, 2148. doi:10.3390/w12082148

19 C. Leite, et al., Sci. Total Environ. 2020, 719, 134886. doi:10.1016/j.scitotenv.2019.134886

20 C. Leite, et al., Chemosphere 2020, 252, 126563. doi: 10.1016/j.chemosphere.2020.126563

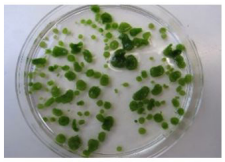
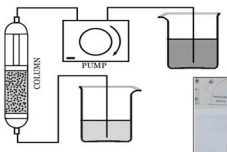
21 B. Barros, Environ. Int. 2021, 156, 106704. doi:10.1016/j.envint.2021.106704

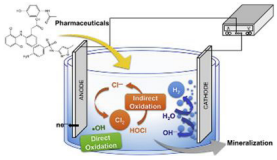
22 M. Oliveira, et al., Int. J. Environ. Res. Public Health 2021, 18, 230. doi:10.3390/ijerph18010230

RESEARCH THEMES/
MONITORING OF CONTAMINANTS AND TREATMENT

SUSTAINABLE AND SAFE WATER TREATMENTS

Water is one of the most precious resources for life on earth. The rapid growth of population and industrial processes are causing a huge impact on water quality. Both the lack of quality and water scarcity are issues of great concern. Ensuring its safety and availability to the population is one of the greatest present and future challenges.
Both domestic and industrial activities generate large amounts of wastewater that need to be efficiently treated. In developed countries, most wastewater treatment plants comprise secondary treatment; nevertheless, this treatment stage is not efficient in the removal of several micropollutants, such as pharmaceuticals and personal health care products in domestic wastewaters and metals and textile dyestuffs originated by industry. Moreover, agricultural activities, which uses large amounts of fertilizers and pesticides, contribute to the pollution of the aquatic environment.
To solve the water quality problem, the research group has been involved in the development of tertiary treatments using adsorption and advanced oxidation processes. The adsorption studies have been focused on the use of raw natural materials in their natural form (*e.g.* seaweeds, industrial and agriculture wastes, and clays) or after modification (physical, physico-chemical, and chemical) to produce environmental and economically sustainable materials with high performance in micropollutant removal. Approaches based on highly efficient nanomaterials have also been studied.




Due to water scarcity, water reuse is needed, increasing the demand for high quality treated water. This research group leads a JPI project (REWATER) aiming to develop and apply technologies, producing a final integrated solution for the reuse of treated wastewater for agricultural purposes. In another project, a 3D electrochemical process is developed for the removal of substances resistant to biological treatments. The economic and environmental evaluation, with SWOT and Life Cycle Assessment tools, of the proposed technologies are carried out. The systematic approaches in these projects will minimize potential negative impacts on the environment, decreasing the undesirable introduction of micropollutants and their spread within the food chain.

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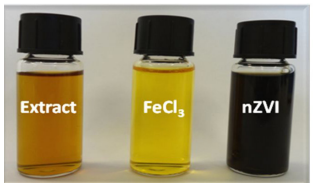
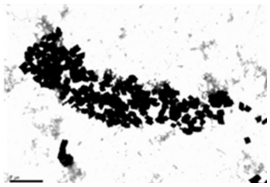
RESEARCH THEMES/
MONITORING OF CONTAMINANTS AND TREATMENT

GREEN TECHNOLOGIES FOR SOIL REMEDIATION

Soil contamination is a global environmental problem that still requires scientific innovative solutions, not only for the development of new, more efficient and cost-effective remediation technologies, but also for the monitoring of new and emergent contaminants.
The research group has always been on the frontline of these issues through the participation in European networks (such as Nicole - Network for Industrially Co-ordinated sustainable Land management in Europe) that allowed a close interaction with industry, consultants, legislators, and academic institutions; but also through funded European and national scientific projects that allowed the development of applied and innovative science. The development of the following new remediation technologies can be highlighted:

- Nanoremediation of soils is an efficient and recent technology that can be applied to a wide range of contaminants, from chlorinated organic compounds to heavy metals.
- Waste treatment methods and their value through biogeochemical processes may contribute to the protection of ecosystems. In these recovery processes, waste can be transformed into artificial soils (technosols) that are formulated and elaborated with specific properties. These technosols can be used in the recovery of contaminated and/or degraded urban and peri-urban environments.





The evaluation and comparison of the environmental and economic impacts of different remediation technologies through (i) ecotoxicity assays (toxicity for plants (phytotoxicity), bacteria, microalgae, crustaceans, and rotifers), (ii) Life Cycle Analysis and (iii) Life Cycle Cost Assessment methodologies contribute to a multivariate self-supported decision tool, which becomes more sustainable than the traditional decision only based in the decontamination efficiency.

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RESEARCH THEMES/ LIFE CYCLE THINKING

VALORIZATION OF AGRO-FOOD AND INDUSTRIAL WASTES

According to FAO, in Europe, around 90 million tons of food are annually wasted, and an additional 40% increase is expected until 2025. In addition, the intensification of the agricultural and food industrial sectors results in serious waste-related problems, which are subject of increasingly stringent regulations. In this sense, an integral analysis of the agricultural value chain is extremely urgent, including livestock and crop production, food processing, and retail sector, concerning economic and environmental sustainability standpoints. Our research group has been working on the valorisation of several residues from the agro-food industry (wine, chestnut, baby kiwi, spent grain, yeast, hop, beer, fish, dairy products, rice, and maize crop production), as well as marine (microalgae and seaweeds) and vegetable (chayote, apple, kiwano) residues and resources. These matrices are characterized by their high nutrient content, added-value compounds, or calorific value, making them excellent sources for valorisation into bioenergy, bioactive compounds, biomaterials, bio-fertilisers, animal feedstock, nutraceuticals, cosmetics, or even pharmaceuticals.

In this context, the main objective of the research group is to demonstrate and validate novel processes, practices and products for the sustainable use of agro-food and industrial by-products and wastes, contributing to the creation of sustainable value chains in the farming and processing sectors through the:

- development of "green" analytical methods (extraction and detection);
- characterization and validation of the biological activity of extracts by *in vitro* (and *in vivo*) assays;
- demonstration of technical feasibility of different valorisation technologies using laboratorial and pilot assays;
- deep and close collaboration with agriculture, food, cosmetic and pharmaceutical industries in order to promote a sustainable value-added chain and the development of new active ingredients.

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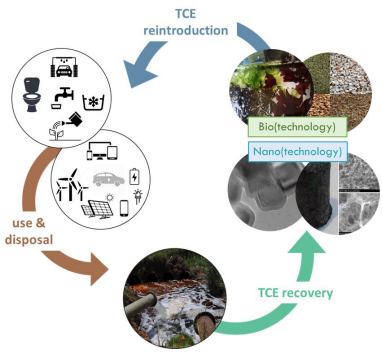
RESEARCH THEMES / LIFE CYCLE THINKING

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

Technology-Critical Elements (TCE) (*e.g.* rare earth elements) 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.

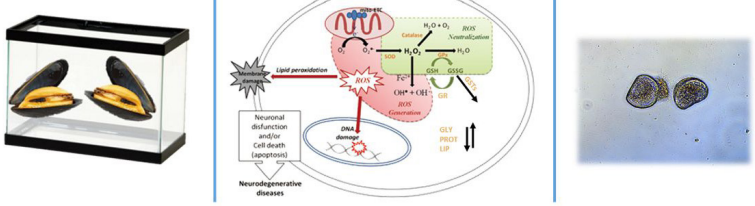
Due to technology proliferation, the rejection of TCE together with classical contaminants (*e.g.* Pb, Hg) through sewage is increasing but information on their occurrence and potential toxicity to aquatic organisms is very scarce. Also, waste electrical & electronic equipment (e-waste) is one of the fastest growing waste streams worldwide (3-5% year), representing a hazard if appropriate management strategies are not implemented.

This research group have been focusing on the development of environmentally sustainable and economically viable processes necessary for the TCE recovery from secondary sources (wastewaters and e-waste), with a view to its reintroduction into industrial processes.



The approaches followed focus on biotechnologies based on living seaweed and biosorbents (valorization of food/agro-industrial wastes), also including nanomaterials.

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 and bivalve's biochemical performance (biomarkers analysis).



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RESEARCH THEMES/ LIFE CYCLE THINKING

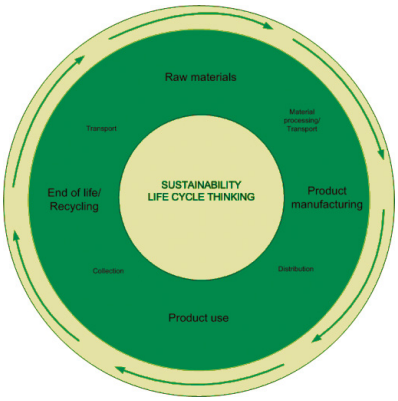
SUSTAINABILITY STUDIES AND LIFE CYCLE THINKING

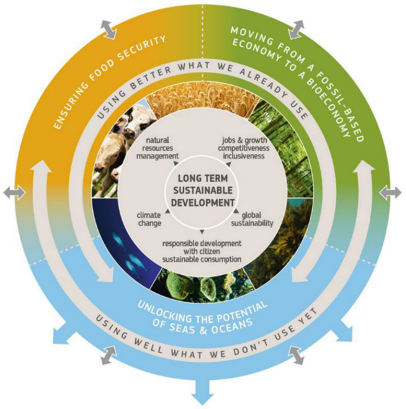
Nowadays there are several challenges that should be overcome, namely scarcity of raw materials, pollution, sustainable production and consumption, and issues concerning globalization and markets' stability. Sustainability studies considering the three pillars of sustainable development, especially with 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/ FOREST FIRES

IMPACT ON THE ENVIRONMENT AND POTENTIAL HEALTH RISKS FOR EXPOSED POPULATIONS

Forest fires frequency and severity have dramatically increased during the last years, principally in some high-risk countries, namely European Mediterranean countries (Portugal, Spain, Greece, and Italy), Australia, and in North America, thus causing significant ecological, economic, and social problems. Every year forest fires affect millions of people due to the released emissions. Therefore, it is becoming an important environmental, occupational, and public health issue. Forest fires release numerous hazardous pollutants to the environment, contaminating the air, soil, and water resources. Fire emissions may affect long-term health and quality of life of the general population, particularly of the most susceptible groups, and of occupationally exposed workers, the firefighting forces. Firefighters' occupational exposure is among the most hazardous occupations being classified as a possible carcinogen to humans. Fires emissions affect the quality of the air, soil, and water in the vicinity of burned areas, which raises additional scientific challenges. The impact of fire emissions on the health of exposed populations requires the development of additional analytical tools to evaluate the potential health risks, which will potentiate the establishment of prevention and mitigation strategies. Human biomonitoring represents a precious tool to complement information retrieved from environmental studies. Several methodologies based on the principles of green chemistry have been developed by this research group.

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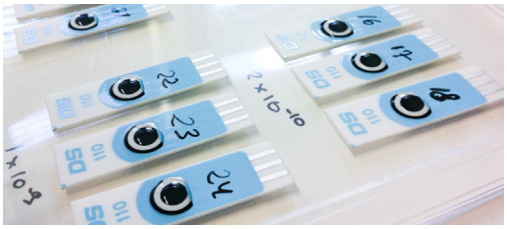
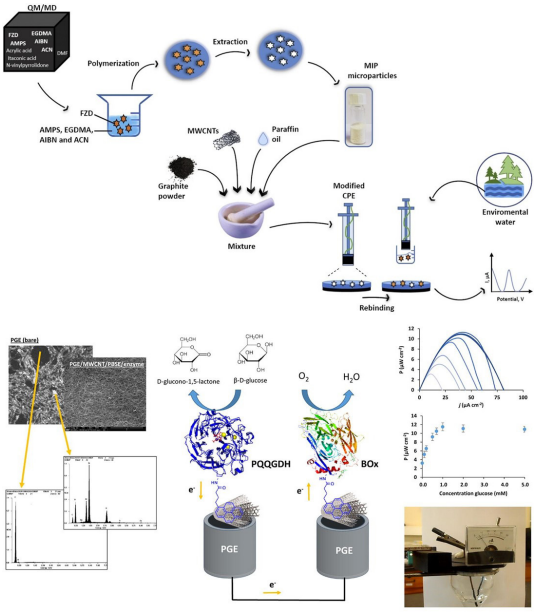
RESEARCH THEMES / ELECTROCHEMICAL (BIO)SENSING TOOLS

The advances in engineering and technologies have increased drastically in the last years, contributing decisively to the advancement of (bio)sensors as analytical tools. Electronic devices have become faster and smaller allowing their use as portable instruments to monitor concentrations in real-time and *in situ*. The accomplishments in nanotechnology assure that ultrahigh sensitivity, good selectivity, and low detection limit can be reached with (bio) sensors. Despite all the scientific advances, the development of (bio) sensors continues to be a challenge.



Despite the existing difficulties, research efforts are focused on various domains for which novel sensors, using chemical, biological, or bio-inspired molecular recognition elements, are developed: application 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, and pathogenic microorganisms), and disease diagnostics and follow-up (*e.g.* cancer, Alzheimer's and Parkinson's disease, and chronic kidney disease). Some of these challenges are the aim of several ongoing national and international projects.



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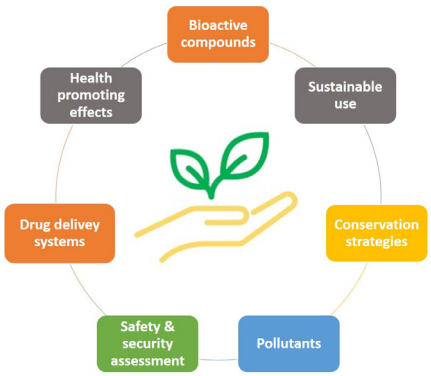
RESEARCH THEMES / PHARMACOLOGICAL ACTIVITY OF MEDICINAL PLANTS

According to the 2030 Agenda for sustainable development of the United Nations, one of the main goals to transform our world is to protect, restore, and promote the sustainable use of the ecosystems and prevent biodiversity loss. Biodiversity changes, as a result of anthropogenic activities and climate changes, affect ecosystem functioning with substantial consequences for plant and animal communities and for our societies. Almost 80% of the population from developing countries depend on traditional medicines as their primary health care system. Many of their treatments are based on medicinal plants, which most of them are collected from the wild. On the other hand, not only developing countries rely on medicinal plants but also pharmaceutical, cosmetic, and food industries take advantage of the vastness of bioactive compounds produced by these sources. Indeed, 60,000 species are estimated to be used for their medicinal and aromatic properties around the world, and every year more than 500,000 tons of material from such species are traded. This high demand for wild species associated with the unsustainable use of pesticides and other chemicals that present a severe negative impact on pollinators, and consequently, on plant reproduction, is responsible for plant populations declining, and one in five species is estimated to be threatened with extinction in the wild.



The research group has been actively engaged in the study of medicinal plants from different continents in order to contribute to raising awareness to all stakeholders responsible for the conservation of biodiversity programs. Our research focus on:

- quality control and authentication of plant species based on their chemical fingerprint;
- science- and evidence-based assessment of their health-promoting effects (by *in vitro* and *in vivo* assays);
- development of nanocarriers for natural products delivery;
- evaluation of the presence of different types of pollutants in plant matrixes and extracts, namely heavy metals, pesticides and other priority compounds.

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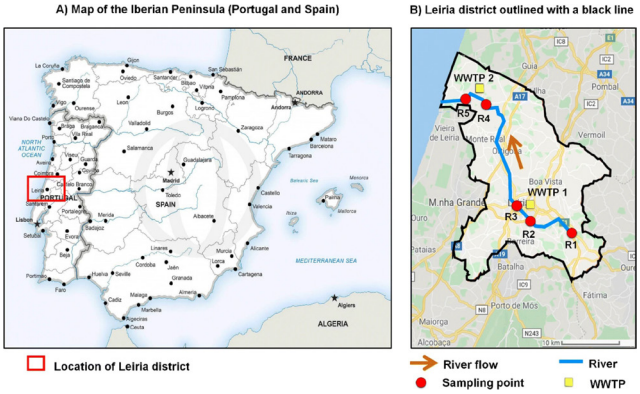
HIGHLIGHTS

ANALYSIS OF PESTICIDES IN RIVER- AND WASTEWATERS

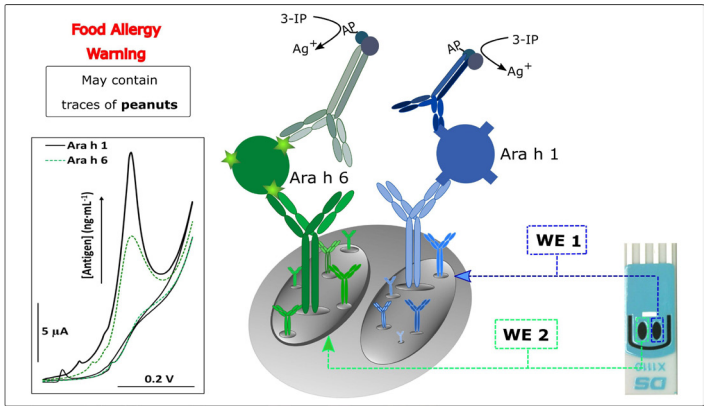
Three sampling campaigns were performed in the Lis River (Leiria, Portugal) in February of 2018, November of 2018, and May of 2019. River water and wastewater (influent and effluent) samples of two wastewater treatment plants were target of the study. A total of 25 samples were collected and 50 pesticides were monitored, including organochlorines, triazines, pyrethroids, and organophosphorus, among others. Most of the detected pesticides were insecticides and mainly organochlorines. Concentrations between 1.29 and 2134 ng/L were found. Aldrin, -HCH, and cypermethrin were detected in some samples in µg/L, being -HCH the pesticide most frequently detected with concentration in µg/L level. The pesticides with the highest detection frequency were (i) cypermethrin, HCB, methoxychlor, and -HCH in river waters; (ii) isoproturon, cypermethrin, methoxychlor, pyrimethanil, -HCH, dieldrin, diuron, -HCH, and -endosulfan in effluents; and (iii) diuron and isoproturon in influents. The detection of the organochlorides and their degradation products is a consequence of their persistence in the environment, as their usage has long been prohibited in the European Union. Pesticide toxicity index was determined in the samples collected in the river.



Multi-residue analysis of fifty pesticides in river waters and in wastewaters.

Environmental Science and Pollution Research, 2021

TRACKING PEANUT ALLERGENS IN FOODS



Electrochemical Immunosensor for the Simultaneous Determination of Two Main Peanut Allergenic Proteins (Ara h 1 and Ara h 6) in Food Matrices.

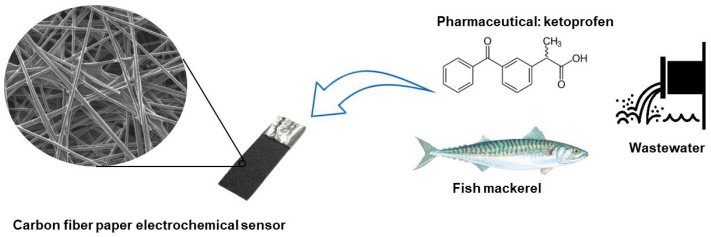
Foods 2021, 10, 1718

Efficiently detecting peanut traces in food products can prevent severe allergic reactions and serious health implications. This work presents the development of an electrochemical dual immunosensor for the simultaneous analysis of two major peanut allergens, Ara h 1 and Ara h 6, in food matrices. A sandwich immunoassay was performed on a dual working screen-printed carbon electrode using monoclonal antibodies. The antibody–antigen interaction was detected by linear sweep voltammetry through the oxidation of enzymatically deposited silver, which was formed by using detection antibodies labeled with alkaline phosphatase and a 3-indoxyl phosphate/silver nitrate mixture as the enzymatic substrate. The assay time was 2 h 20 min, with a hands-on time of 30 min, and precise results and low limits of detection were obtained (Ara h 1: 5.2 ng/mL; Ara h 6: 0.017 ng/mL). The selectivity of the method was confirmed through the analysis of other food allergens and ingredients (e.g., hazelnut, soybean and lupin). The dual sensor was successfully applied to the analysis of several food products and was able to quantify the presence of peanuts down to 0.05% (w/w). The accuracy of the results was confirmed through recovery studies and by comparison with an enzyme-linked immunosorbent assay. Tracking food allergens is of utmost importance and can be performed using the present biosensor in a suitable and practical way.

HIGHLIGHTS

CARBON PAPER-BASED ELECTROCHEMICAL SENSOR FOR PHARMACEUTICAL POLLUTANTS ANALYSIS

The exceptional electrochemical properties of an unmodified carbon paper were characterized and explored in the development of a sensor for the anti-inflammatory drug ketoprofen. The carbon paper sensor revealed excellent sensitivity for ketoprofen which resulted in a limit of detection at submicromolar level. This sensor also showed high selectivity in the presence of common interferents and other widely consumed anti-inflammatory drugs. When applied in real samples, a good accuracy was reached in wastewater and fish samples with acceptable recoveries. The particularities of the carbon paper sensor evidenced in this work can be important in the development of efficient and portable analytical systems for the environmental analysis of pharmaceuticals as well as other contaminants of emergent concern.

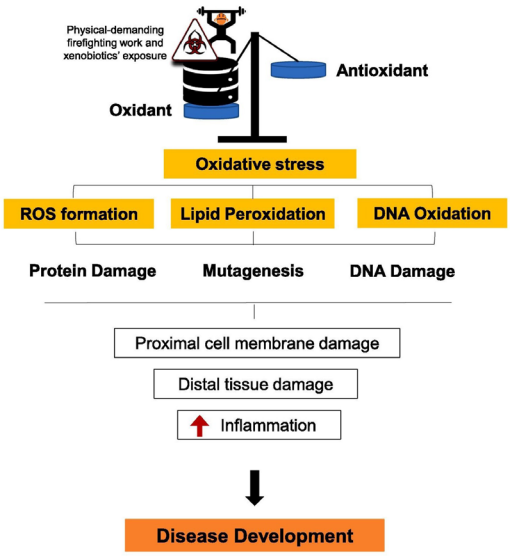


Carbon paper as a promising sensing material: characterization and electroanalysis of ketoprofen in wastewater and fish.

Talanta 2021, 226, 122111

FIREFIGHTERS' OCCUPATIONAL EXPOSURE

Firefighting is physically and physiologically exhausting besides encompassing exposure to toxic fire emissions. Studies have reported increased incidence of cardio-respiratory diseases and cancer in firefighters. Several recent studies proved an association between exposures to fire emissions and/or heat and significantly altered values of biomarkers of inflammation, vascular damage and tissue injury in firefighting forces. Moreover, preliminary data of DNA damage in blood, urinary mutagenicity and 8-isoprostaglandin in exhaled breath condensate suggest that these biomarkers of oxidative stress should be further explored. Since most of the reported studies are based on case/control or cross-sectional designs, broader studies based on longitudinal designs and strongly supported by the analysis of several types of biomarkers in different biological fluids are urgently required to gain deeper insights into the firefighters occupational related health hazards and contribute to implementation of new or improved surveillance programs.



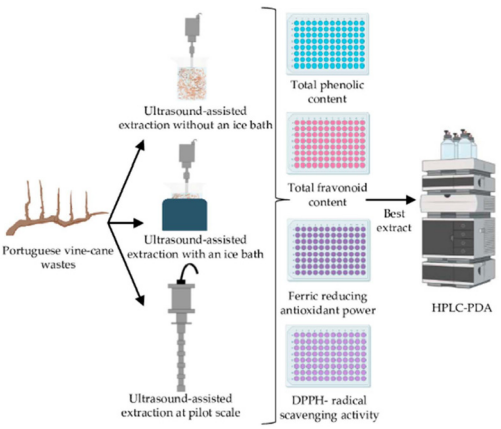
Firefighters' occupational exposure: contribution from biomarkers of effect to assess health risks

Environment International 2021, 156, 106704

HIGHLIGHTS

VINE-CANES VALORISATION

Wine production generates large amounts of vine-canes, a devalued by-product that could be used for the recovery of bioactive compounds. In this work, two vine-canes varieties, namely Touriga Nacional (TN) and Tinta Roriz (TR), were submitted to different ultrasound-assisted extraction (UAE) conditions. The highest phenolic and flavonoid content was observed for TR extract obtained at lab-scale without an ice bath and pilot-scale after 60 min of extraction (32.6 ± 2.1 and 26.0 ± 1.5 mg gallic acid equivalent/g dry weight (dw) and 9.5 ± 0.6 and 8.3 ± 0.8 mg epicatechin equivalents/g dw, respectively). Furthermore, all extracts demonstrated a high antioxidant activity to scavenge DPPH free radicals with the best value reached by TR at the lab-scale without an ice bath after 30 min and pilot-scale extraction after 60 min (34.2 ± 2.4 and 33.4 ± 2.1 mg trolox equivalents/g dw, respectively). The extracts' phenolic compositions were also evaluated by HPLC, demonstrating that resveratrol, myricetin, and catechin were the main compounds. This work represents an important step to the use of UAE as an industrial process to recover bioactive compounds.

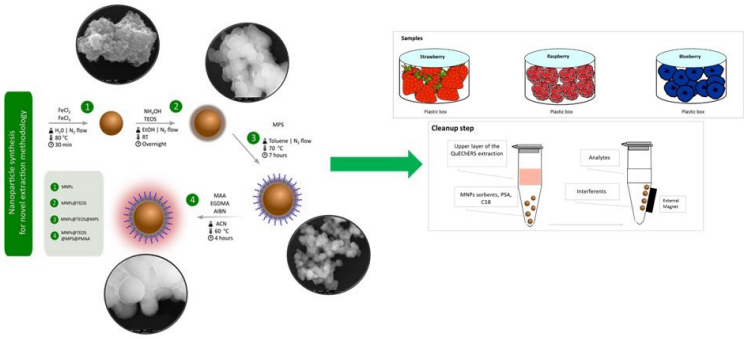


Vine-Canes Valorisation: Ultrasound-Assisted Extraction from Lab to Pilot Scale.

Molecules 2020, 25, 1739

APPLICATION OF MAGNETIC NANOMATERIALS IN SAMPLE PREPARATION

An innovative and efficient extraction method of food contaminants called magnetic micro dispersive solid-phase extraction (MµdSPE) was developed. Magnetic nanoparticles (MNPs) with different sizes and characteristics were synthesized to be used as QuEChERS sorbents for the determination 9 brominated flame retardants (BFRs) in red fruits (strawberries, blueberries, and raspberries). The MNPs sorbents as well as the lower amount used, proved to have an excellent adsorption ability for pigment matrix and other co-extracts. In comparison with the classic methods, the application of MµdSPE as a new cleanup showed excellent results. The method has been successfully applied to study BFRs in 12 red fruit samples from conventional and organic farming.



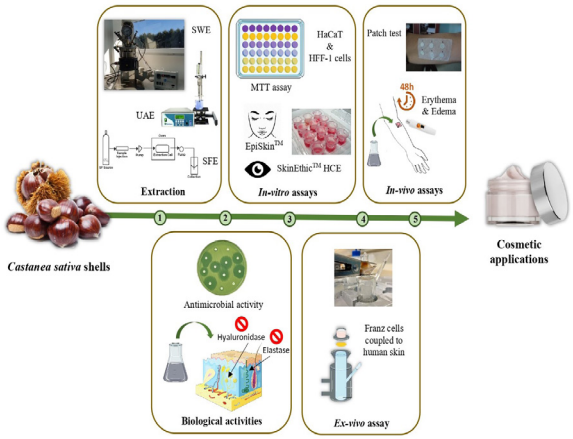
Evaluation of the QuEChERS and magnetic micro dispersive solid-phase extraction of brominated flame retardants in red fruits with determination by GC/MS.

Food Chemistry 2020, 309, 125572

HIGHLIGHTS

EXTRACTION OF A COSMETIC INGREDIENT FROM CHESTNUT SHELL USING ENVIRONMENTALLY FRIENDLY TECHNIQUES

Sustainability arises as a challenge in the last decades and the cosmetic field is not an exception. The search for new cosmetic active principles extracted from food byproducts through eco-innovative technologies has emerged as a novel concept. However, the European Regulation is very restrictive and different assays should be performed to guarantee the products' efficacy and safety. Considering a multidisciplinary approach, chestnut shell extracts prepared by three different green techniques – Subcritical Water Extraction (SWE), Ultrasound-Assisted Extraction (UAE) and Supercritical Fluids Extraction (SFE) – were compared regarding antimicrobial activity, hyaluronidase and elastase inhibitory activities, in-vitro cytotoxicity on dermal cells (HaCaT and HFF-1) and skin permeation (using Franz cells coupled to human skin). The best extract was tested on skin and ocular 3D models and through an in-vivo patch test to evaluate its irritancy and safety. The results demonstrated the antimicrobial properties of the extracts (particularly against Staphylococcus aureus) as well as the capacity to inhibit the hyaluronidase (IC50 = 0.76–54.36 mg/mL) and elastase (33.56-82.70% at 0.4 mg/mL) activities. Regarding in-vitro cell assays, UAE and SWE extracts revealed the best outcomes. Between 0.1 and 100 µg/mL, none of the extracts conducted to a decrease of cell viability in both cell lines (HaCaT and HFF-1). The ex-vivo assay proved that SWE extract led to a higher polyphenol's permeation (1061.6 µg/g dw), being selected for further assays. Ellagic acid was the major polyphenol that permeated the human skin (732.1–847.0 µg/g dw). The 3D skin and ocular models evidenced absence of irritation by SWE extract, without decreasing cell viability and releasing IL-1. Finally, an in-vivo patch test confirmed the absence of irritation in humans based on the acute irritation index of 0.50 achieved 24 h after the patch removal. This study validated a new cosmetic ingredient extracted from chestnut shells by in-vitro and in-vivo assays, in accordance with the European Regulation 1223/2009



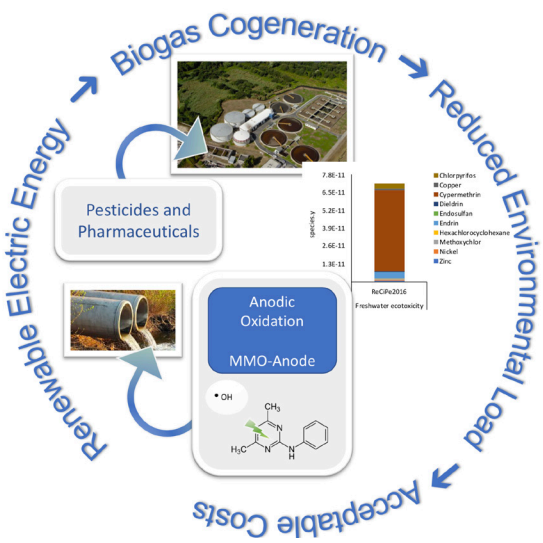
From soil to cosmetic industry: Validation of a new cosmetic ingredient extracted from chestnut shell through environmentally friendly techniques.

Sustainable Materials & Technologies 2021, 29, e00309

HIGHLIGHTS

LIFE CYCLE AND ECONOMIC ANALYSES OF WASTEWATER TREATMENT

Several pesticides and pharmaceuticals (PP) have been detected in the effluent of a full-scale Portuguese Wastewater Treatment Plant (WWTP). Their presence contributed to the environmental burdens associated with the existing treatment of the Municipal Wastewater (MWW) in the impact categories of Human Carcinogenicity, Non-Carcinogenicity, and Freshwater toxicities on average by 85%, 60%, and 90%, respectively (ReciPe2016 and USEtox methods). The environmental and economic assessment of the installation of an Anodic Oxidation (AO) unit for PPs' removal was performed through Life Cycle and Economic Analysis, considering two types of anodes: BoronDoped Diamond (BDD) and Mixed Metal Oxides (MMO). The operation of the AO unit increased the environmental burdens of the system by 95% on average (USEtox), but these impacts can be partially compensated by the avoided the production of non-renewable energy in the Portuguese electricity mix by biogas cogeneration at the WWTP. If the construction of the AO unit and the manufacturing of the electrodes are considered, the Human and Freshwater Toxicities are often higher than the environmental benefits derived from the PPs' removal. On the economic side, the MMO configuration is clearly more advantageous, whereas BDD is environmentally more favorable. The issue of the presence of PP in MWW effluents has to be addressed as an integrated solution both improving upstream PP's management and adopting PP's removal technologies strongly supported by renewable energies. Further insights are needed for the assessment of fate and of the environmental effects of PP in the sludge.



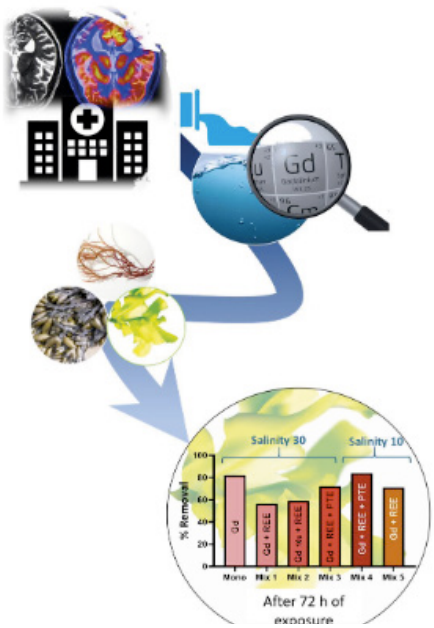
Life Cycle and Economic Analyses of the Removal of Pesticides and Pharmaceuticals from Municipal Wastewater by Anodic Oxidation.

Sustainability 2021, 13, 3669

HIGHLIGHTS

EVALUATION OF MARINE MACROALGAE POTENTIAL FOR GADOLINIUM REMOVAL AND RECOVERY FROM CONTAMINATED WATERS

The uptake of Gd (used in contrast agents for magnetic resonance imaging) by three living marine macroalgae *(Ulva lactuca, Fucus spiralis,* and *Gracilaria sp.)* from contaminated seawater was studied. Different Gd concentrations (10, 157, and 500 µg L^{-1}) were analysed along 72 h, comparing the capability of each macroalgae to remove and concentrate this rare earth element. Surface analysis (FTIR), water content, kinetic modelling, and Gd quantification in seawater and biomass were performed. All species were able to accumulate Gd, although green and red macroalgae showed better performance: green > red > brown. Removal efficiencies reached 85 %, corresponding to a bioconcentration factor of 1700. Findings show that macroalgae could be a countermeasure to the increasing anthropogenic enrichment of Gd in the aquatic environment. The ecological technology macroalgae-based kept its efficient even in more complex solutions that intended to mimic real contaminated environments, namely mixtures with other rare earth elements (Y, La, Ce, Pr, Nd, Eu, Tb, Dy), and with potentially toxic elements commonly found in wastewaters (Cr, Ni, Cu, Cd, Hg, Pb), at two salinities (10 and 30). Removal efficiencies were 84 and 88 % for green and red macroalgae, respectively.

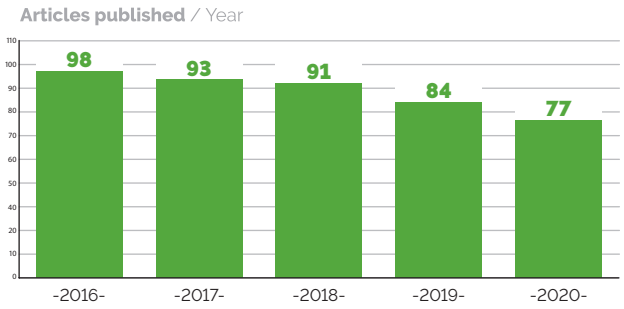


Gadolinium removal by living marine macroalgae *(Ulva lactuca, Gracilaria sp.*, and *Fucus spiralis)* under different relevant contamination scenarios

Science of Total Environment, 2020, 749, 141488

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION



H-index: **67**

434 articles*
24977 citations

*2016-2020
From WOS core collection

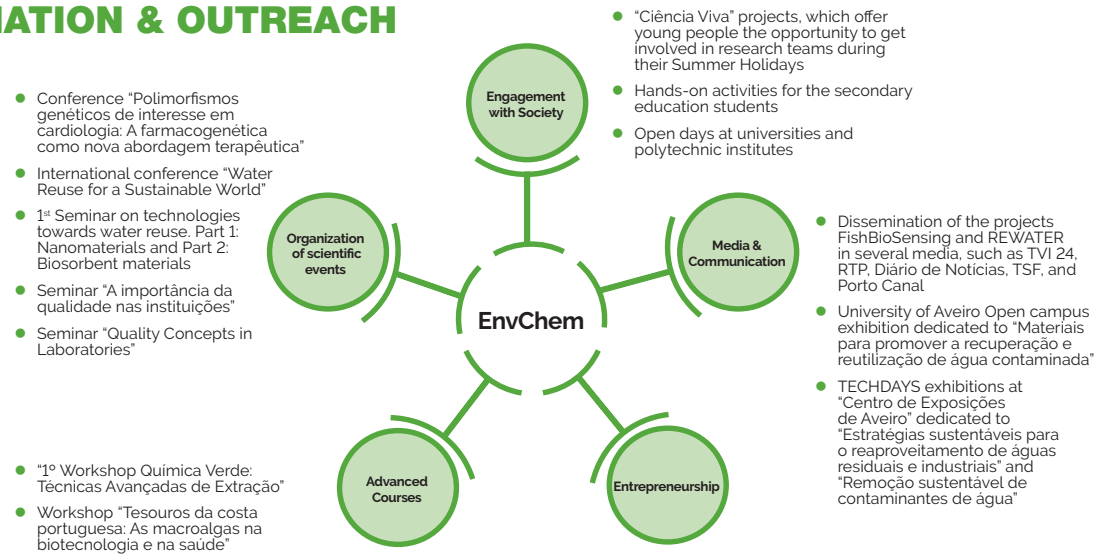
FUNDED PROJECTS *(Representative projects)*

- **Biorefinery for the Production of Low- and High-Grade Activated Carbon from forestry wastes, maize residues and biogas digestate - Bio-FESS**
  ERA NET LAC 2014, Isabel Esteves (PI), Nuno Lapa (Local PI)
  Total Funding: € 536,227. National funding: € 99,548
- **REWATER – Sustainable and safe water management in agriculture: Increasing the efficiency of water reuse for crop growth while protecting ecosystems, services and citizens' welfar**
  WaterJPI/0007/2016, Cristina Delerue-Matos (PI)
  Total Funding: € 555,960
- **TERRAMATER – Medidas innovadoras de recuperación preventiva en áreas quemadas**
  INTERREG-POCTEP 0701_TERRAMATER_1_E,
  Cristina Delerue-Matos (Local PI)
  Total Funding € 1,107,000
- **FFCastanea – Castanea sativa shells as a new source of active ingredients for Functional Food and Cosmetic applications: a sustainable approach**
  Funded by the Portuguese Foundation for Science and Technology - FCT (PTDC/ASP-AGR/29277/2017), Francisca Rodrigues (PI)
  Total Funding: € 231,622
- **CECs(Bio)Sensing – (Bio)sensors for assessment of contaminants of emerging concern in fishery commodities**
  Funded by the Portuguese Foundation for Science and Technology - FCT (PTDC/ASP-PES/29547/2017), Simone Morais (PI)
  Total Funding: € 234,245
- **Silver Brain – From sea to brain: Green neuroprotective extracts for nanoencapsulation and functional food production**
  Funded by the Portuguese Foundation for Science and Technology - FCT (PTDC/OCE-ETA/30240/2017), Clara Grosso (PI)
  Total Funding: € 239,966
- **TracAllerSens – Electrochemical sensors for the detection and quantification of trace amounts of allergens in food products"**
  Funded by the Portuguese Foundation for Science and Technology - FCT (PTDC/QUI-QAN/30735/2017), Hendrikus Nouws (PI)
  Total Funding: € 239,245
- **BioFirEx – Um painel de (bio)marcadores para a vigilância da saúde e da segurança do bombeiro**
  Funded by the Portuguese Foundation for Science and Technology - FCT (PCIF/SSO/0017/2018), Simone Morais (PI)
  Total Funding: € 299,625

INTERNATIONAL COOPERATION AND NETWORKING

- Coordination of the Portuguese-Serbia Bilateral Cooperation project (Development of functional foods incorporating a chestnut shells extract obtained by subcritical water - 5537 DRI, Sérvia 2020/21)
- Coordination of the FCT-CAPES project "MultiSNPsensor aplicado à farmacogenética cardiovascular" (88881.156344/2017-01)
- 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, United States of America
- Supervision of PhD students in cotutelle (Italy and Spain)
- 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 international projects: SeaFoodTomorrow (H2020); COCKLES (INTERREG ATLANTIC), and ASARISAFE (FCT/NSFG China)

DISSEMINATION & OUTREACH



- "Ciência Viva" projects, which offer young people the opportunity to get involved in research teams during their Summer Holidays
- Hands-on activities for the secondary education students
- Open days at universities and polytechnic institutes

- Conference "Polimorfismos genéticos de interesse em cardiologia: A farmacogenética como nova abordagem terapêutica"
- International conference "Water Reuse for a Sustainable World"
- 1st Seminar on technologies towards water reuse. Part 1: Nanomaterials and Part 2: Biosorbent materials
- Seminar "A importância da qualidade nas instituições"
- Seminar "Quality Concepts in Laboratories"

- Dissemination of the projects FishBioSensing and REWATER 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"

- "1º Workshop Química Verde: Técnicas Avançadas de Extração"
- Workshop "Tesouros da costa portuguesa: As macroalgas na biotecnologia e na saúde"
- Workshop "Macroalgas da costa portuguesa: uma abordagem económica e nutricional"
- Workshop "Análise Sensorial: Princípios e Aplicações no Desenvolvimento de Novos Produtos"
- Introductory course on scientific research

- Portugal 2020 - Co-Development TR&D projects (OXI-e3D; FarmaSense; and iCanSea)
- Active collaborations with several industries, namely Venti1AQUA S.A.; Castelbel S.A.; WedoTech -Companhia de Ideias e Tecnologias, Lda; Sogrape Vinhos S.A.; Fábrica de Conservas La Gôndola S.A.


LABORATÓRIO ASSOCIADO
PARA A QUÍMICA VERDE

BCPE

(BIO)CHEMICAL PROCESS ENGINEERING

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

Group Coordinator:

Rui Oliveira

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
- Water treatment/valorisation/reuse and pollution control
- Sustainable energy
- Digitalization

RESEARCH OBJECTIVES [2020-2023]

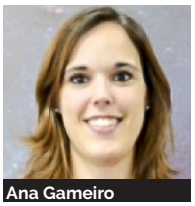
- Functionalized ionic liquids and eutectic solvents for delivery of biomolecules, protein crystallization, microfluidics, electrochemical devices, and gas separation;
- Extraction and fractionation of high added-value compounds present in by-product streams, using ionic liquids, eutectic solvents, enzymatic 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 new functional materials, such as membranes and adsorbents, with the ability to establish specific molecular interactions with target solutes and/or regulate their selective transport;
- Development of integrated processes for water/wastewater treatment, valorisation and reuse;
- Development of new approaches for process monitoring – at molecular/nanoscale, online, real-time, 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.

RESEARCH TEAM

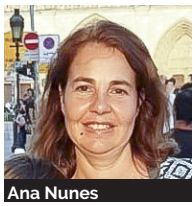
SENIOR RESEARCHERS


Alexandre Paiva


Alfredo Carvalho


Ana Gameiro


Ana Machado

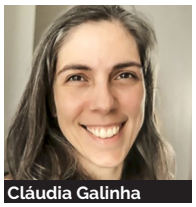

Ana Nunes


Ana B. Pereiro


António Canto


Carla Brazinha


Carla Portugal


Cláudia Galinha

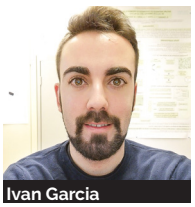

Fernando Cruz


Filipa Pires


Gonçalo Carrera


Isabel Coelhoso


Isabel Esteves


Ivan Garcia


João Araújo

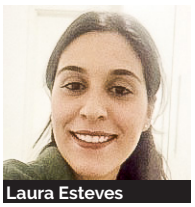

João G. Crespo


João Ramalho


José Esperança


José Lopes

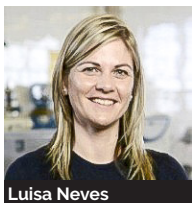

José P. Mota


Laura Esteves


Liliana Tomé


Luis Martins


Luís P. Rebelo

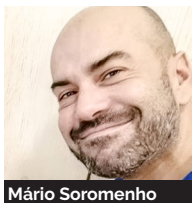

Luisa Neves


Madalena Dionísio


Manuel da Ponte

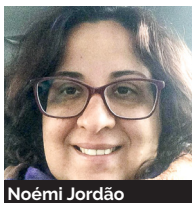

M. Margarida Cardoso


Mário Eusébio


Mário Soromenho


Mohammad Tariq


Nicole Vieira


Noémi Jordão

RESEARCH TEAM


Patricia Reis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Rui Oliveira


Rui Ribeiro


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Sylwin Pawlowski

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Liane de Meneses
Luís G. Barreira
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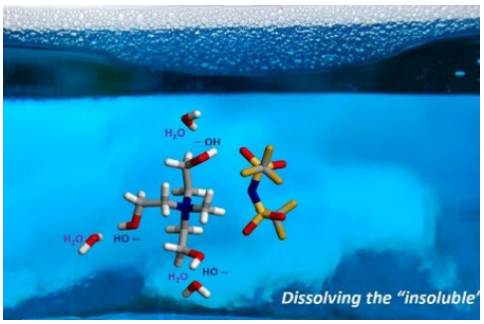
Tamara P. Leite
Tânia M. Neto
Elsa C. Mestre

RESEARCH THEMES/
ALTERNATIVE GREENER SOLVENT

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.

- Fluorinated Ionic Liquids(IL): Influence of nanosegregation on the behaviour of IL. Usage as drug delivery systems. Enhanced tunability afforded by aqueous biphasic systems and ILs. Increase of the surfactant behaviour and solubilization capacity of ionic liquids
- Functionalized ILs: Protonic ammonium nitrate ILs. Charge-inverted IL pairs. ILs for the crystallization of proteins. Magnetic ILs and their applications on the development of high performance materials. Playing with ionic liquids structure to discover unusual properties and applications.
- Nature inspired ILs: Carboxilate-based ILs to enhance the dissolution, properties and applications of nucleic acid bases. 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.
- Deep eutectic solvents (DES) have been used to decrease cellulose crystallinity; also DES have been used on the production of stable nanoemulsions using novel membrane emulsification approaches;
- Development of environmentally friendly ionic liquid (IL) – gas hydrate (GH) based biocompatible systems to address some of the societal challenges, namely clean energy (transportation/storage) and climate change (CO2 capture). Ionic liquids are used as GHs inhibitors (GHIs) to mitigate the flow assurance issues in the oil/gas industry. Design of ionic liquids that can be used as GHPs promoters to enhance the formation rate of hydrates for rapid energy storage and CO2 capture aiming to convert natural gas into solid pellets so that it can be transported easily across the borders in a compact form.



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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 and preparation of 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. The formulation and fabrication of structured materials, especially in monolithic form, with tailored structural, chemical and mechanical properties, are under intensive research using extruder/3D Printing techniques.
- Novel materials based on agarose and ionic liquids to separate cytostatic from the urine of cancer patients avoiding cytostatic release into the environment (Collaborative project with CICECO).
- Agarose-based materials as affinity (or most probably multimodal) chromatographic supports in the development novel purification schemes for pDNA which enables to obtain it with a purity that meets pharmaceutical specifications, at a competitive cost and with a much smaller environmental footprint (Collaborative project with CICECO and CICS)
- 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 (80 K) without vibration or mobile components, using an innovative technology based on adsorption organo-metallic pumps.
- Development of heterogeneous catalysts consisting on homogenous complexes anchored on carbon supports and metal nanoparticles deposited on oxide supports for reactions of industrial importance, such as oxidation of alcohols and hydrocarbons.

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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. Another problem is the proper digestate handling from biogas plants. A biorefinery is proposed in BioFESS ERA-NET project that take advantage of these low-cost materials to produce high-quality activated carbon (AC) from biomass residues in a self-sustainable biorefinery. AC is used as adsorbent of impurities in liquid/gaseous media and to recover CH4 from biogas.
- The extraction and fractionation of added-value compounds using supercritical technology: there has been a strong interest from industry which has already translated into 2 projects with DELTA Cafés for the valorisation of spent coffee grounds and for the decaffeination of coffee beans. Also, there has been industry-financed projects with AMORIM for the extraction of TCA from cork using this technology. There is an open collaboration contract with the company EXMCeuticals Portugal for the use of this technology for the extraction of cannabinoids and cannabis oil from cannabis. This is a mature technology with already industrial application and viability.
- Subcritical water has also been studied for the valorisation of agro-industrial by-products and wastes. Subcritical water is a green technology (using water without any additive) with a low energetic load (up to 80% of the energy used can be recovered). BCPE has developed antioxidant-rich extracts for the cosmetic industry, the use of oligomer-rich extracts in polymers, food packaging, nutraceutical, civil and biotech industries. The interest of a Portuguese wine company in this technology for the valorisation of their wastes led to the creation of a start-up by LAQV members.
- The “Susfishwaste” project, which aims to develop a sustainable strategy for the valorisation of fish waste into high added value products, contributing to one of Portugal’s priority challenges in the coming years: a more efficient, safer and sustainable use of our marine resources, in particular the by-products and residues of associated industries, through their valorisation in the development of new products and processes in key areas such as biomedicine, pharmaceuticals, cosmetics and food.
- The “3SLYCO” project, which aims to valorise the presence of carotenoids such as lycopene in the residues of the tomato industry by creating new topical formulations for the treatment of inflammatory skin disorders, such as atopic dermatitis, urticaria and psoriasis.

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

- The "Silverbrain" project, aims at the extraction of bioactive compounds from macroalgae from integrated multitrophic aquaculture harvested on the Portuguese coast. This project has a strong framework in the priority domain Saúde (Health) as well as in the priority domain Economia do Mar (Sea Economy) of the National Intelligent Specialization Strategy (ENEI).
- Several national and European projects were focused on the use of membrane processing for the recovery, transformation and fractionation of target added-value compounds from complex agro-industrial subproduct streams. These projects comprised the harvesting of microalgae (EC projects D-Factory and SaltGae) and their biorefining (EC projects D-Factory and Multi-Str3am), the valorization of corn wastes for the production of bio-vanillin (funded by COPAM) and the recovery of bioactive compounds from Cynara cardunculus for biomedical use.
- Mixed microbial cultures are sued in several projects for the treatment and valorisation of by-products and waste streams from different types agro-forest, domestic and other industries
- .

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RESEARCH THEMES/
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:

- Production of cleaner fuels by the reduction of sulphur and nitrogen in collaboration with GALP refinery, to process diesel and jet fuel in order to reduce the presence of these elements.
- To create a sustainable and cost-effective solution to produce low-sulfur marine fuels (Heavy Fuel Oil) to accomplish the actual legislation, contributing to the international economy of maritime and to the development of clean marine fuels, which is crucial to mitigate the global sea pollution, particularly in the "Portuguese international waters".
- 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. This involves not only the development of membranes with the ability to selectively transport lithium against these two other metals, but also the development of a new concept, a Lithium Membrane Flow Capacitive Delonization prototype, using flow electrodes.
- Active participation on the Collaborative Laboratory CoLAB NET4CO2, together with Galp Energia, S.A., Universidade do Porto, Universidade de Lisboa, Laboratório Ibérico Internacional de Nanotecnologia and Change Partners, SCR, SA. LAQV contributes to the development of new products and processes for a circular economy of sustainable CO2. LAQV is particularly involved in projects for mitigation of CO2, development of biofuels and renewable sources of energy, and devices for energy conversion.
- In the SunStorage project, technologies are developed for converting 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.
- In the CO2usE project, the reaction between CO2 and biomass derived diols was explored for the production of renewable organic carbonates. This reaction produces high quantities of water, which constitutes a severe technical limitation. Promising results were obtained using hydrophobic ionic liquids (with high CO2 up-take) as solvents for metal-based catalysts, in order to increase CO2 concentration in the liquid phase and to simultaneously remove in-situ the water from the reaction mixture.

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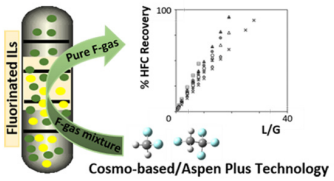
RESEARCH THEMES/
CLIMATE CHANGE MITIGATION AND POLLUTION CONTROL

WATER TREATMENT/VALORIZATION/REUSE

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

- BCPE has been involved in several industrial projects with EPAL, Águas de Portugal and GALP, targeting the 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.
- Additionally, BCPE developed in collaboration with Águas do Tejo Atlântico - Grupo Águas de Portugal a new process for wastewater treatment combining membrane filtration (ultrafiltration and/or nanofiltration) with photocatalytic degradation of rejected pollutants. Also in collaboration with this company, a new project is focused on membrane wastewater treatment aiming its reuse for irrigation in the production of fruits.
- BCPE developed the concept of ion-exchange membrane reactor for the removal and recovery of arsenic from drinking water supplies. A new project is starting in collaboration with an Indian partner in order to establish a pilot plant for extended tests and validation in the field (in India).
- BCPE is involved in the development of real-time, online techniques that allow for process monitoring, namely using techniques such as two-dimensional fluorescence, use of molecular probes and online mass spectrometry.
- The design and optimization of systems for the separation of azeotropic mixtures of refrigerant F-gases (fluorinated greenhouse gases) into their individual components, in a pilot scale, using the best multi-Key Enabling Technologies (multi-KET).
- Development of composite carbon or metal oxide based materials for water purification (from dyes, metals and drugs by adsorption or photocatalysis) and air cleaning (from nitrogen oxides, carbon dioxide, volatile organic compounds, etc).



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RESEARCH THEMES/ DIGITALIZATION

BCPE is committed to the development and application of data science and systems analysis for process engineering, covering the emerging fields of Artificial Intelligence and Machine Learning, but also the traditional First Principles/mechanistic/phenomenological modelling approaches :

- Computational Fluid Dynamics (CFD) to model flow patterns in highly porous monolithic columns with a wide variety of applications, including chromatography, due to increased surface area and good accessibility to the ligands and reduced diffusional hindrances.
- HYBMOD: HYBMOD is a long-term project, running over several funding cycles, aiming at the development of hybrid systems theory for the integration of Artificial Intelligence/Machine learning with traditional first Principles/mechanistic engineering models. It follows the principle of *Augmented Engineering.* Novel semi-symbolic formalisms are being exploited to decrease computation power and to increase scalability. This project has originated two startups, 5 PhDs, and more than 40 papers. This project is evolving towards an open-source software, SBML compatible and web-accessible to the scientific community.
- Hybrid AI/genome-scale modelling. This project seeks for 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: Novel systems approaches for fast (bio)process development resorting to M3C (Measurement, Modelling, Monitoring and Control). 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. The SILICOMEDIA project is currently funded by GlaxoSmithKline, Brussels, Belgium.
- Digital solutions for industrial biotechnology and better health: Development and application of new systems engineering techniques (ML algorithms, data analytics and computational modelling) for (bio-)clinical data analysis and decision-making.
- Use of Artificial Intelligence(AI) approaches for phase equilibrium prediction and comprehension. AI modelling of physico-chemical properties of ionic liquids and organic molecules. Development of novel machine-learning methodologies in order to improve predictive capacity. Novel codification strategies to unveil the mechanisms behind a certain chemical system's behaviour.

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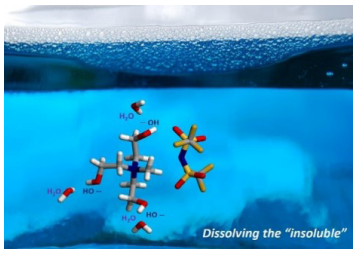
HIGHLIGHTS

ALTERNATIVE GREENER SOLVENTS: ILS HIGHLIGHT



By chemical manipulation of the quaternary ammonium cation with hydroxyethyl moieties we were able to obtain bistriflimide-based ionic liquids completely miscible with water, even below room temperature. The underlying reason is the full integration of the OH groups of the cation in the continuous H-bonded network of water. There is a strong evidence that the replacement of a methyl group by a hydroxymethyl group in the cation has an almost-null contribution to the overall molar volume of the ionic liquid. Molecular dynamics simulations have been performed to explain from a structural perspective the obtained results. Hydrogen bonding between hydroxyl groups or between them and the charged moieties of the ionic liquid can lead to further contractions of the free volume that annuls the intrinsic volume contribution of the OH group. These ILs showed a significantly lower cytotoxicity than other well-known and commonly used fluorinated ILs. The capability of these ILs to form ABS with a series of carbohydrates, allowed us to design a process to separate carbohydrates and antioxidants from real food waste samples.

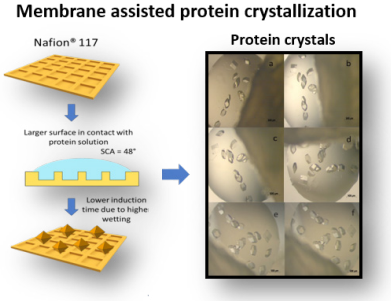
Evidences for a Null Molar Volume Contribution by Hydroxyl Groups in Ammonium Bistriflimide-Based Ionic Liquids.

Journal of Chemical Engineering, 2019, 11, 4932

Simultaneous Separation of Antioxidants and Carbohydrates From Food Wastes Using Aqueous Biphasic Systems Formed by Cholinium-Derived Ionic Liquids.

Frontiers in Chemistry, 2019, 7, 459

FUNCTIONAL MATERIALS FOR PROCESS INTENSIFICATION



Ion-exchange membrane processes were used for consecutive protein crystallization and crystal derivatization, leading to protein crystals with good structural stability and high x-ray diffraction quality, as required for protein structural resolution – protein crystallography. Magnetic-responsive membranes were designed and have shown to allow for a non-invasive magnetic modulation of protein adsorption and transmembrane transport, thus offering the possibility of fouling and mass transport control. Magnetic-responsive membranes were used as tissue scaffolds allowing for the magnetic regulation of angiogenesis processes, with a promising application on the development of novel therapies for vascular diseases and cancer.

Enhanced Protein Crystallization on Nafion Membranes Modified by Low-Cost Surface Patterning Techniques.

Crystal Growth & Design, 2020, 20, 2174–2186

Functional alumina monoliths with hierarchical porous structures were prepared using a single-stage sol-gel emulsification methods and functionalized with a simple and expedite technique for effective purification of immunoglobulins.

Photocatalytic membranes with highly retentive properties have been prepared with TiO_2 and TiO_2 doped materials using magnetron sputtering and sol-gel techniques. The membranes developed have been tested in a novel membrane photocatalytic reactor for the treatment of various effluents, namely from olive oil production.

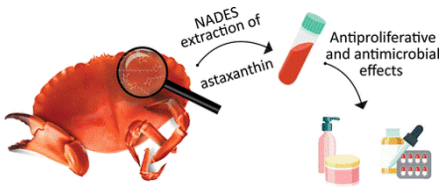
HIGHLIGHTS

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.

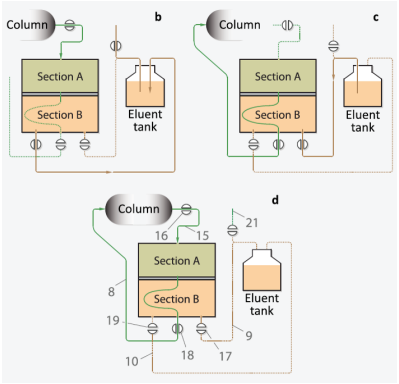
Terpene-Based Natural Deep Eutectic Systems as Efficient Solvents To Recover Astaxanthin from Brown Crab Shell Residues.

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



PROCESS INTENSIFICATION IN DOWNSTREAM BIOPROCESSING

We have explored the concept of batch chromatography with recycle lag, concluding with the design, construction, and experimental validation of a prototype that embodies the physical realization of this new concept. Moreover, the apparatus is simple to set up in particular in view of large-scale applications. By resorting to selected examples, namely GE Healthcare Bio-science's three-column periodic countercurrent chromatography, Novasep's sequential multicolumn chromatography, and a few hypothetical multi-column processes, we showed how the theory can be operationalized. Finally, we have designed a device or apparatus—an eluate recycling device (ERD)—to physically realize the proposed concept. The ERD implements an approximate "first in, first out" method for organizing and manipulating the to-be-recycled fractions of eluate collected from the chromatography column, where the oldest (first) amount fluid, or 'head' of the fraction, is the first to exit and be recycled to the column. The setup was validated experimentally with success using the separation of a nucleoside mixture by reversed phase chromatography as a model problem. It was also shown that by redesigning the fluid distributor using 3D printing technology the ERD performance can be improved.



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

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

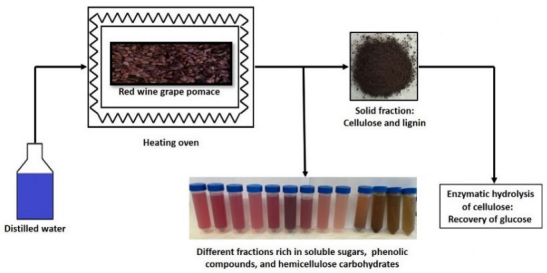
HIGHLIGHTS

(BIO)CATALYSIS & BIOREFINERY: FRACTIONATION OF RED WINE GRAPE POMACE BY SUBCRITICAL WATER

Grape pomace, the byproduct that is generated in the wine making process, is a valuable source of cellulose, hemicellulose, and lignin, as well as of proteins, lipids, and phenolic compounds with antioxidant capacity.

The use of subcritical water extraction/hydrolysis to fractionate red wine grape pomace (RWGP) into different useful fractions, following the biorefinery concept towards the full utilization of the carbon content of biomass, was studied in a semi-continuous reactor.

A temperature profile at 100 bar featuring plateaus at 50, 100 and 190 °C allowed the recovery of virtually all hemicellulose, leaving in the residue essentially all the lignin and cellulose. The latter was readily enzymatically hydrolyzed to glucose. RWGP extracts were rich in phenolics as well as in hemicellulose-derived carbohydrates, mostly in the form of oligomers, with favorable antioxidant capacity.

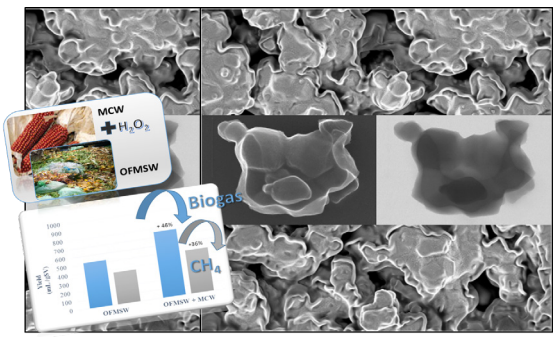


Fractionation of red wine grape pomace by subcritical water extraction/hydrolysis.

The Journal of Supercritical Fluids, 2020, 160, 104793

(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)

Ionic Liquid-Impregnated Metal–Organic Frameworks for CO2/CH4 Separation.

ACS Applied Nano Materials, 2019, 2, 12, 7933

Porous carbons derived from hydrothermally treated biogas digestate.

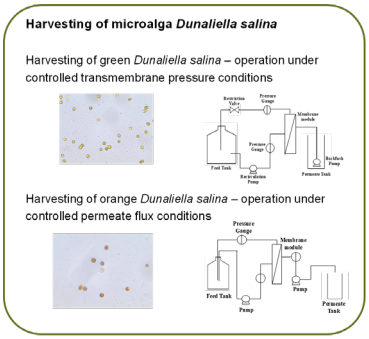
Waste Management, 2020, 105, 170

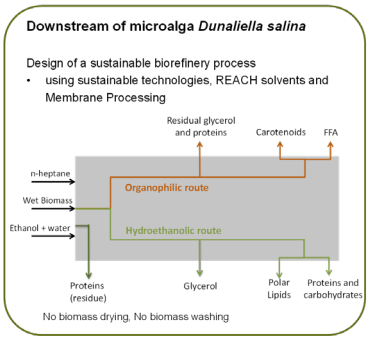
HIGHLIGHTS

(BIO)CATALYSIS & BIOREFINERY: MICROALGAE

The development of harvesting and design of sustainable downstream processes were achieved for microalga *Dunaliella salina* (known for the production of carotenoids) under the European project D-Factory. Harvesting of other microalgae species was also studied under the European project H2020 SaltGae. Monitoring using 2D Fluorescence spectroscopy was successfully achieved for the production of *Dunaliella salina* and *Nannochloropsis oceanica*.

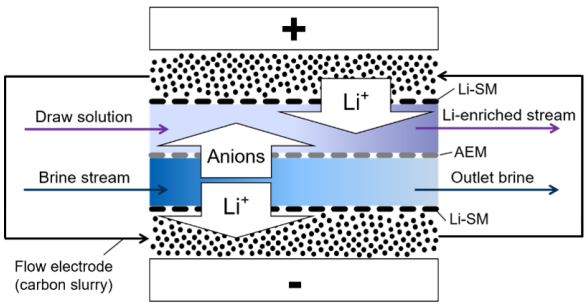
FP7 PROJECT D-FACTORY
FP7-KBBE- 613870





SUSTAINABLE RECOVERY OF LITHIUM FROM SALINE STREAMS BY FLOW CAPACITIVE DEIONIZATION (FCDI)

Lithium is becoming an essential metal in the global energy economy due to its applications in electric car batteries; however, its recovery from land resources is geographically limited and not environmentally friendly. Although lithium can be extracted from seawater, the so far proposed processes have limited efficiency. They require cyclic charging and discharging of the electrodes (capacitive deionisation - CDI) or are based on frequent regeneration of adsorbent material (adsorption processes). In order to increase the degree of lithium recovery from seawater (or any other saline streams such as for example saltworks' bittern) and to make the process continuous and selective, the static electrodes in CDI devices will be replaced by novel flow-electrodes (recirculated in a loop arrangement between cathode and anode) and lithium-selective membranes (Li-SMs) will be developed by electrospinning. The geometry of such flow-electrode capacitive deionisation (FCDI) device with integrated Li-SMs will be optimised by computational fluid dynamics (CFD) studies and the first-ever prototype will be constructed using 3D printing.

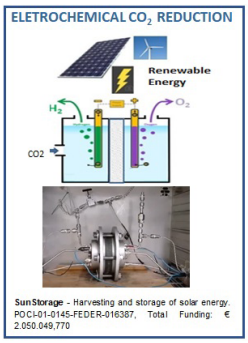


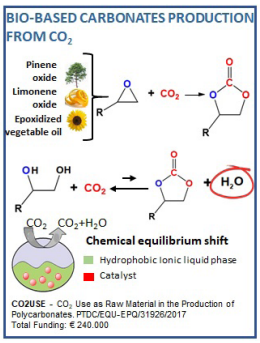
This project has received funding from the European Union's Horizon 2020 research and innovation programme under Grant Agreement No. 869467 (SEArcularMINE -Circular Processing of Seawater Brines from Saltworks for Recovery of Valuable Raw Materials) and FCT-MCTES IC&DT project PTDC/EQU-EQU/6193/2020 (Se(L)ect(i)vity - Design of tailored composite membranes for lithium recovery from brines and seawater).

HIGHLIGHTS

SUSTAINABLE ENERGY: CO_2 CAPTURE AND PROCESSING

CO2 capture and utilization will be a key pillar in the new paradigm energy system. The group is involved in the reductive CO2 conversion into energy vectors and non-reductive conversion of CO2 into chemicals and materials. Research has been focused in the following areas (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 (vi) the production of fully renewable organic carbonates from CO2 and bio-based substrates.; (vii) the integration of reaction and product separation step; and (viii) chemical equilibrium shift through ionic liquid/high-pressure CO2 biphasic reaction systems.





CO2 + ionic liquid biphasic system for reaction/product separation in the synthesis of cyclic carbonates.

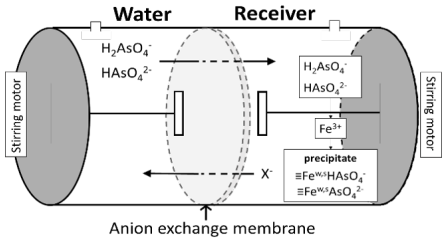
The Journal of Supercritical Fluids, 2018, 132, 71-75.

Electrochemical production of syngas from CO2 at pressures up to 30 bar in electrolytes containing ionic liquid.

Reaction Chemistry & Engineering, 2019, 4, 1982-1990

WATER TREATMENT AND POLLUTION CONTROL

A new type of clean integrated process referred to as "ion exchange membrane reactor" (IEMR), especially suitable for detoxification of drinking water sources, containing toxic ions has been developed and validated for a number of important applications in drinking water treatment, such as removal of arsenic from contaminated groundwater (in 2021, pilot-scale on-site validation will be performed for arsenic removal from groundwater in India); removal of heavy metals (*e.g.*, ionic mercury); removal of disinfection by-products; nitrate removal in closed marine systems (validated with water from the Oceanarium of Lisbon); and perchlorate removal from groundwater successfully validated with collaboration with the Ben Gurion University at the Negev, Israel. The quality of the liquid wastewater effluents of the GALP refinery in Sines has been optimized. Novel treatment methods for recovery of phosphorus and chromium from industrial effluents with collaboration with an Algerian university and purification of mine drainage and electroplating industry acidic effluents have been developed in collaboration with the company LanXESS, Germany. Valorisation of wastewater streams (*e.g.*, olive wastewaters) has been also investigated with the collaboration of Portuguese olive producing factories.



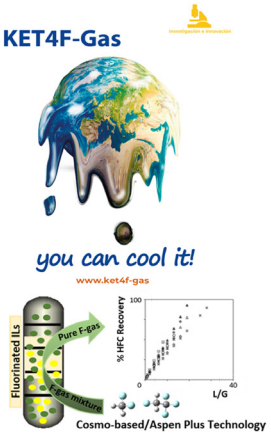
Optimisation of arsenate removal from water by an integrated ion-exchange membrane process coupled with Fe co-precipitation.

Separation & Purification Technology, 2020, 246, 116894

HIGHLIGHTS

MITIGATION OF THE ENVIRONMENTAL IMPACT OF FLUORINATED GASES

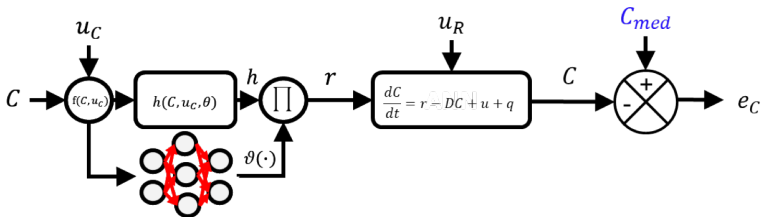
The European project KET4F-Gas aims the design and optimization of systems for the separation of azeotropic mixtures of refrigerant F-gases (fluorinated greenhouse gases) into their individual components, in a pilot scale, using the best multi-Key Enabling Technologies (multi-KET). Moreover, the construction, validation, and optimization of the multi-KET pilot system in an industrial partner (No Waste, Lda) are being carried out, with the registration of 2 patents for reducing emissions of fluorinated compounds. Two prototypes have been constructed for the efficient recovery of value-added compounds from high global warming potential (GWP) refrigerant blends in the end-of-life, for reutilization purposes in novel environmentally-friendly refrigerant mixtures with low-GWP, applying circular economy. These two prototypes are based on two different advanced separation processes that provide high yields and have low energy requirements. The consortium of KET4F-Gas project is composed of 19 partners: 6 industrial partners, 6 academic institutions, 1 public administration, 1 European platform, 1 Environmental Federation, 1 NGO, 1 Innovation Cluster and 2 public foundations.



Fluorinated Ionic Liquids as F-Gas Absorbents.
Environmental Science & Technology, 2020, 54, 12784−12794

HYBRID AI/ENGINEERING SYSTEMS FOR PROCESS DIGITALIZATION

HYBMOD is a long term project at BCPE for the development and dissemination of Augmented Engineering methodologies through digital hybrid systems. The vision is that emerging AI tools should not "replace" the vast wealth of human engineering knowledge. Emerging AI tools should rather complement human engineering knowledge and human decision making. BCPE maintains a software package on the emerging digitalization topic of hybrid AI/mechanistic systems to make AI compatible with human knowledge abstraction. BCPE is recognized as a significant scientific contributor to this particular scientific topic by the international community. A biennial hybrid modelling summer school is organised. Supported by the research developed, several startups operating in the systems biotechnology arena were launched: Mediaomics SA, NOVASIGN SA, and GycoMatters Lda.

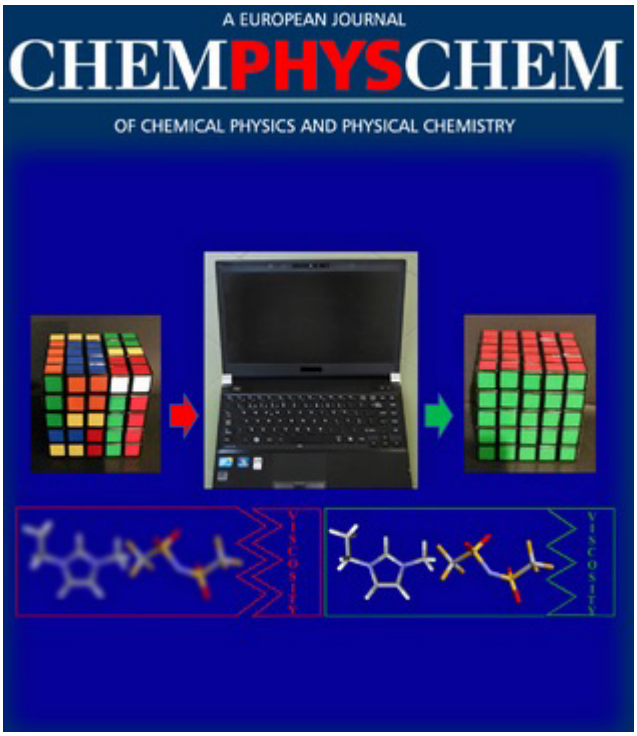


Hybrid modelling as a QbD/PAT tool in process development: an industrial *E. coli* case study.
Bioprocess and Biosystems Engineering, 2016, 39, 773–784

HIGHLIGHTS

DIGITALIZATION OF CHEMICAL SYSTEMS BY CHEMOINFORMATICS AND ARTIFICAL INTELLIGENCE

A Chemoinformatic approach based on Artificial Intelligence were applied to predict viscosity and to generate mechanistic hypothesis underlying the observed behaviour. The chemical systems under study were Ionic Liquids (ILs) and its combinations with other ILs or organic molecules. A straightforward encoding framework permits to compare systems of different nature, with varying number of components and proportions. The Molecular Maps of Atom-level Properties (MOLMAPs) are applied for encoding. It consisted on a pattern of activation, of the atoms of a chemical system, in a fixed length matrix (Kohonen neural network). The position of each atom depends on its atomic properties profile. The combination between this encoding approach and the Random Forest (RF) algorithm enabled to obtain a generical chemical system's class prediction and to unveil the structural features underlying the system behaviour.



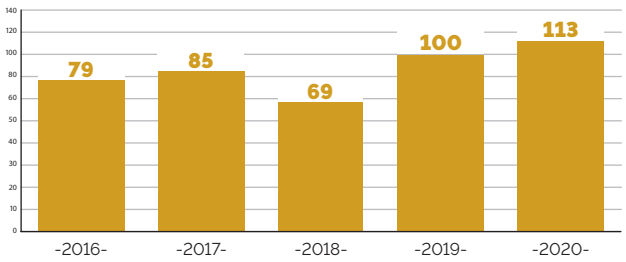
Chemoinformatic Approaches to Predict the Viscosities of Ionic Liquids and Ionic Liquid Containing Systems.

ChemPhysChem, 2019, 20 (21), 2720-2720

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION

Articles published / Year



H-index: **96**

446 articles*
46659 citations

***2016-2020**
From WOS core collection

FUNDED PROJECTS

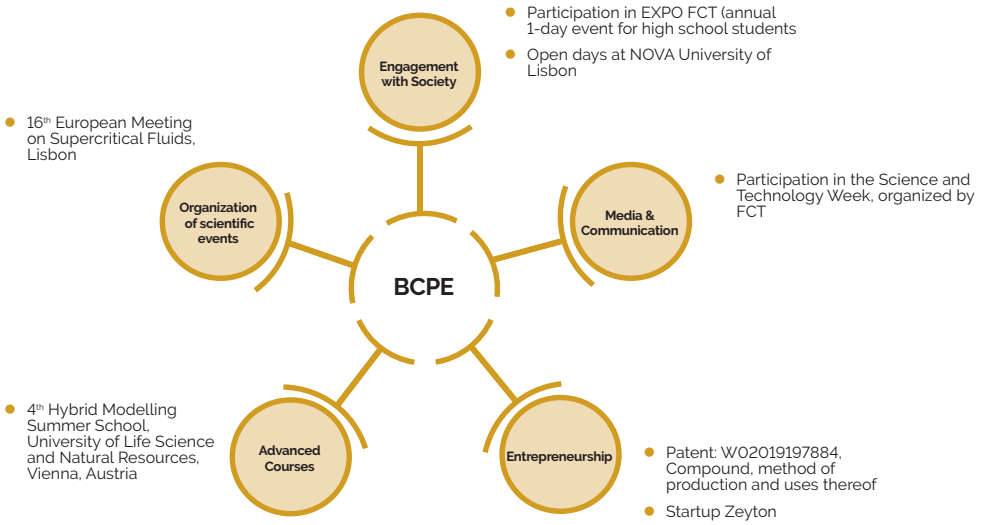
(Representative projects)

- AQUAMONITRIX - Enhanced Portable Sensor for Water Quality Monitoring, moving to genuinely integrated Water Resource Management.
  LIFE17 ENV/IE/000237, João G. Crespo (Local PI).
  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 2017, Ana Estévez and L. P. Rebelo (PI).
  Total Funding: € 1,742,800.00
- CryoDES - Development of Nature-inspired Criopreservation Systems using Natural Deep Eutectic Solvents.
  FCT, PTDC/EQU-EQU/29851/2017, Alexandre Paiva (PI).
  Total Funding: € 236,736.00
- Fluorinated Ionic Liquids: New Engineering Solvents for Separation Processes.
  FCT, PTDC/EQU-EQU/29737/2017, Ana Pereiro (PI).
  Total Funding: € 238,984.62
- ARTINTELPHASEQ - Inteligência Artificial Aplicada à Previsão de Equilíbrio de Fases.
  FCT, PTDC/EQU-QUE/30060/2017, Gonçalo Carrera (PI).
  Total Funding: € 228,641.57
- CMILE - Estruturas nanoporosas compósitas à base de carbono derivadas de redes orgânometálicas (MOFs)- Um novo meio adsorvente aperfeiçoado sob medida e com potencial promissor para aplicações de adsorção e separação de gases.
  FCT, PTDC/CTM-CTM/30326/2017, Isabel Esteves (PI).
  Total Funding: € 239,984.13
- InnovIL4SkinDrug - Desenvolvimento de biomateriais usando líquidos iónicos para libertação de fármacos através da pele.
  FCT, PTDC/CTM-CTM/29869/2017, Luisa Neves (PI).
  Total Funding: € 238,857.73
- SusfishWaste - Desenvolvimento de um processo de biorefinaria sustentável para a valorização de resíduos de processamento de peixe.
  FCT, PTDC/ASP-PES/28399/2017, Pedro Simões (PI).
  Total Funding: € 221,288.42
- CleanMemBrains - Sustainable power generation by reverse electrodialysis with novel monovalent ion perm-selective membranes with antifouling properties.
  FCT, PTDC/EQU-EPQ/29579/2017, Svetlozar Velizarov (PI).
  Total Funding: € 217,230.08
- HILT - The multiple faces of ionic liquids for natural gas hydrates: Inhibitors, promoters, anti-agglomerates and synergists.
  FCT, PTDC/EQU-EQU/32050/2017, Mohammad Tariq (PI.
  Total Funding: € 239,992,85

INTERNATIONAL COOPERATION AND NETWORKING

- EUDIME: Erasmus Mundus Doctorate in Membrane
- CATSUS - Catalysis and Sustainability Ph.D. program
- EM3E-4SW: Erasmus Mundus Master in Membrane a Sustainable World;
- Student exchange at Master's level with the University (Brazil) and University of Pamplona (Colombia);
- Participation in EIT RawMaterials activities (as members of Co-location Centre CLC West);
- Founding member of the CO2 Value Europe Association.
- Member of the COST Action: Greenering
- Participation in the INTERREG Project(EMPORIA 4KT) in the teaching courses of Systems Thinking,Technology Transfer in Pratice and Reverse Engineering/Technology Development
- Cooperation with IFREMER- Centre Bretagne, Brest, France in a PhD program
- Member of the Modeling, Monitoring, Measurement and Control (M3C) section of the European Society of Biochemical Engineering Sciences

DISSEMINATION & OUTREACH




LABORATÓRIO ASSOCIADO
PARA A QUÍMICA VERDE

Charm

CULTURAL HERITAGE AND RESPONSIVE MATERIALS

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

Group Coordinator:

J. C. Lima

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.

RESEARCH OBJECTIVES [2020-2023]

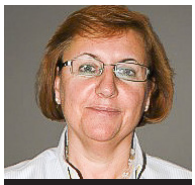
The CHARM group is strongly committed in the next years to find sustainable solutions in the field of energy conversion and storage: improvement of natural dyes performance in DSSCs, tailored ionic liquids for redox flow batteries and CO_2 to fuel conversion and up and down conversion emitting glasses to increase energy efficiency. The electrochromic display technology developed in the group in the last years has achieved a mature state, and dissemination and translation of the technology into applications with societal impact is another key objective for the next years.

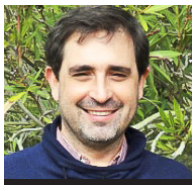
We aim at consolidating our position as members of LAQV@REQUIMTE, bridging Chemistry and Art. As such, we will keep a strong focus on the development of Interdisciplinary Approaches, in particular to Medieval Iberian Heritage and to the conservation of 19th century and contemporary heritage. The latter includes contributions for a history of plastics in Portugal, preserving historic photographic collections in the framework of the European project NEMOSINE, and enabling the online access to the Winsor & Newton artist materials supplier database. We have a long-term involvement with the W&N 19th century archive, creating a page-image database of over 17,000 records covering recipes for pigments, binders, and varnishes which are being researched by DCR Masters & CORES Ph.D. students.

RESEARCH TEAM

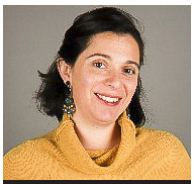
SENIOR RESEARCHERS


A. Jorge Parola

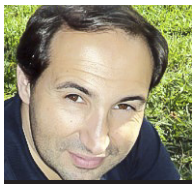

Ana M. Ramos


César Laia

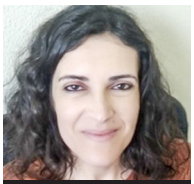

Fernando Pina

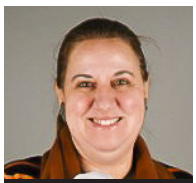

Joana L. Ferreira


J. C. Lima


Luís C. Branco


M. João Melo


Sandra Gago


M. C. Casanova


Leslie Carlyle

RESEARCH TEAM

OTHER DOCTORATE RESEARCHERS
Angelica Bartoletti
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Claúdia Pereira
Élia Roldão
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Isabel P. Cardoso
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Miguel Santos
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Paula Nabais
Patrícia Máximo
Pedro Mateus
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Zeljko Petrovski
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Elin Howard
Eva M. Angelin
Filipa Santos
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Hermine Grigoryan
Inês Martins
Joana M. Devesa
João Sarrato
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Juliana B. Oliveira
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Rafael J. Hidalgo
Rafael Mamede

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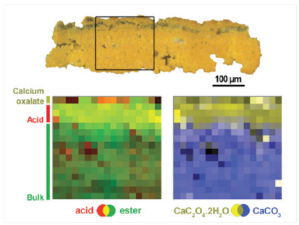
Dong-Min Lee
Massimo Tosolini
Sílvia Sequeira
Verónica Diniz

RESEARCH THEMES/ CULTURAL HERITAGE

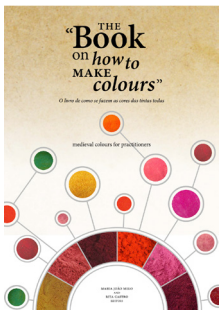
CAUSES AND MECHANISMS OF ALTERATION

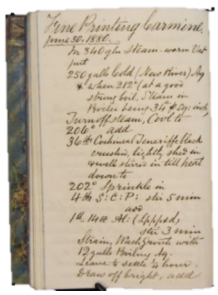
- Medieval illuminated manuscripts.[1, 2]
- Material culture studies in polychrome sculpture and the codex.[3,4]
- Amadeo de Souza-Cardoso and 19th century artists' paints.[5]
- 19th century, Modern & Contemporary Cultural Heritage.[6-13]
- Cinematographic and photography films.[14, 15]

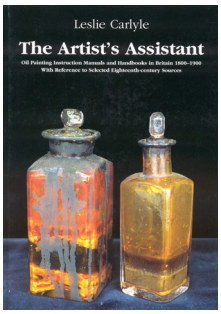


HISTORICAL RECONSTRUCTIONS DATABASE

- The book on how to make colours.[16]
- The Winsor & Newton artist materials supplier, 19th century archive.

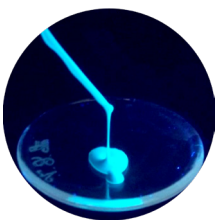


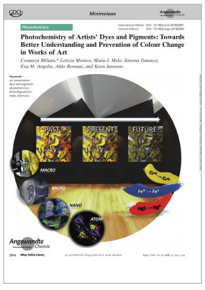


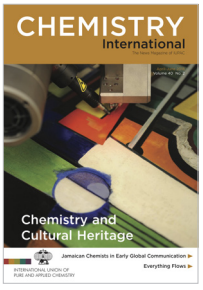


SUSTAINABLE INNOVATIVE METHODS

- Applications of super critical and liquid CO2.
- Applications of ionic liquids and nanomaterials in conservation.
- Responsive materials for cultural heritage.[17]
- Historical dyes: applications & advanced methods of analysis.[2, 18-20]







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18 S. Sharif et al. Molecules. 2020, 25, 908. **doi:10.3390/molecules25040908**

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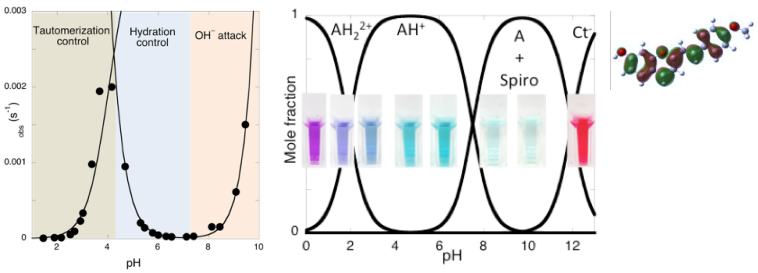
RESEARCH THEMES/ RESPONSIVE MATERIALS

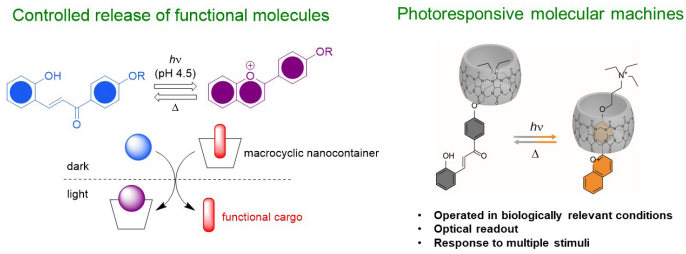
ANTHOCYANINS AND FLAVYLIUM SALTS

- Uncovering color mechanisms in anthocyanins.[21-23]
- New dyes for DSSCs.[24-26]
- Isomeric styrylflavylium systems.[27]



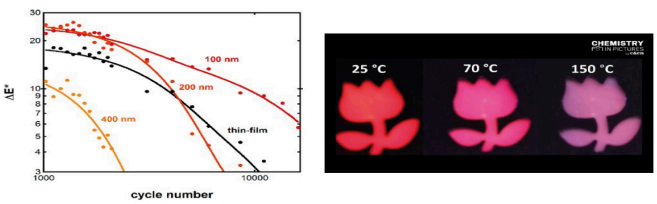
PHOTOCHROMIC AND PHOTOSWITCHING SYSTEMS

- Photochromic systems in micelles.[28]
- Molecular machines based on flavylium photoswitches.[29]
- Host-guest functional systems.[30-32]



ELECTROCHROMIC AND THERMOCHROMIC SYSTEMS

- Development of electrochromic polymer nanoparticles.[33]
- Luminescent thermochromic systems.[34-36]



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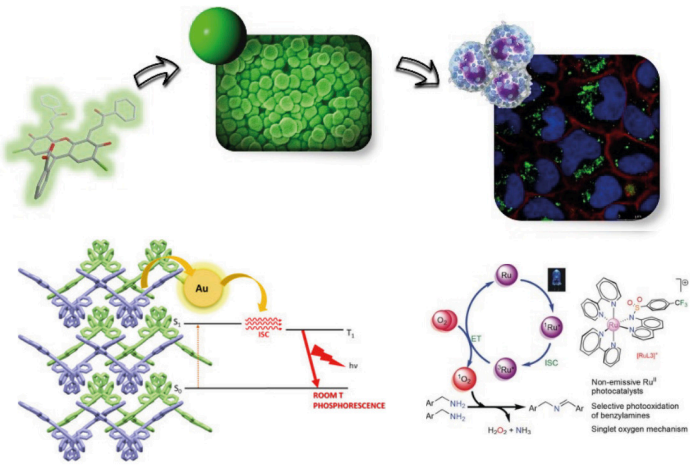
RESEARCH THEMES/ RESPONSIVE MATERIALS

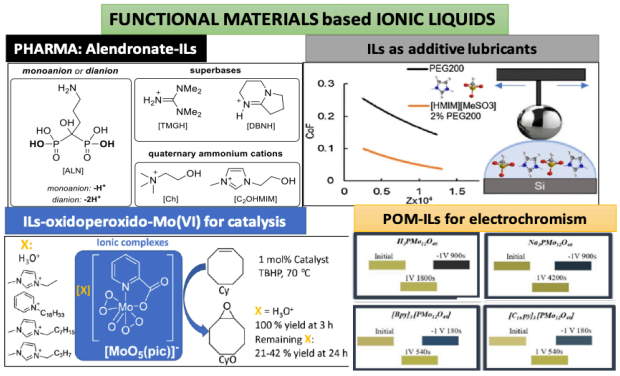
LUMINESCENT MATERIALS AND SENSORS

- Zeolite photoluminescence for LEDs and light management applications.[37]
- Copper-, Silver- and Gold-based materials.[38-45]
- Fluorescence sensors for biological[46-49] and catalytic[50] applications.



FUNCTIONAL MATERIALS BASED ON IONIC LIQUIDS

- Innovative active pharmaceutical drugs based ionic liquids.[51-54]
- Functional Materials for energy[55] and ionic liquids based polyoxometalates for electrochromism and solar cells.[56, 57]
- Alternative lubricants based on ionic liquids for silicon surfaces.[58, 59]
- Task-specific Ionic liquids for sustainable synthesis[60] & catalysis.[61,62]



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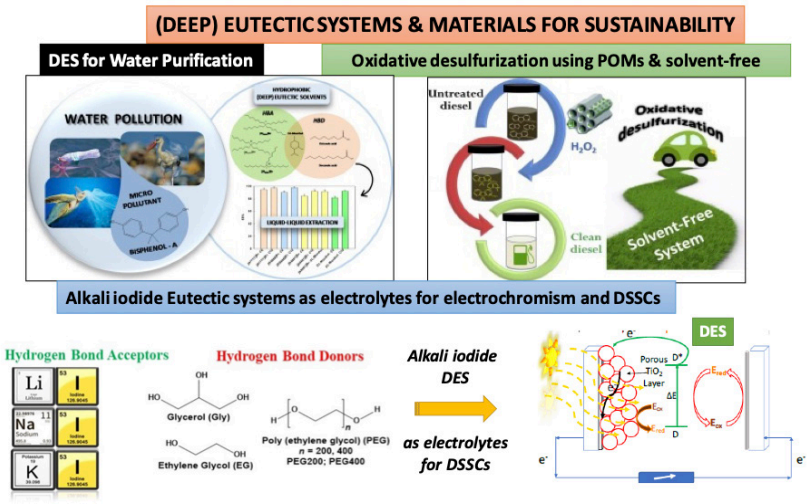
RESEARCH THEMES/ RESPONSIVE MATERIALS

DEEP EUTECTIC SOLVENTS AS GREEN SOLVENTS

- Water purification using hydrophobic DES.[63]
- Eutectic Systems based on alkali metals as green electrolytes for electrochromism and solar cells.[64]
- Extractive desulfurization of fuels using eutectic systems[65] and solvent-free processes.[66]



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HIGHLIGHTS

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

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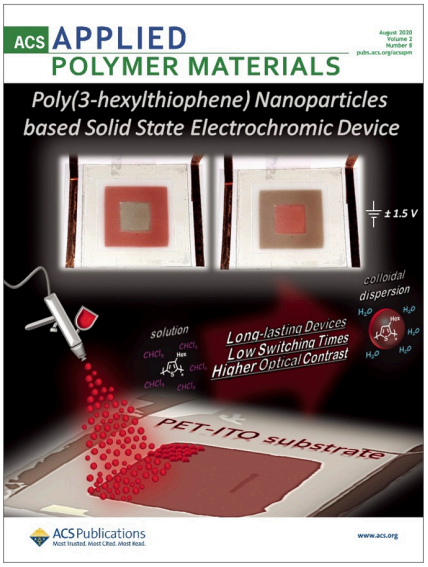
A 1000-year-old mystery solved: Unlocking the molecular structure for the medieval blue from *Chrozophora tinctoria*, also known as *folium*

Science Advances, 2020, 6, eaaz7772

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.

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.



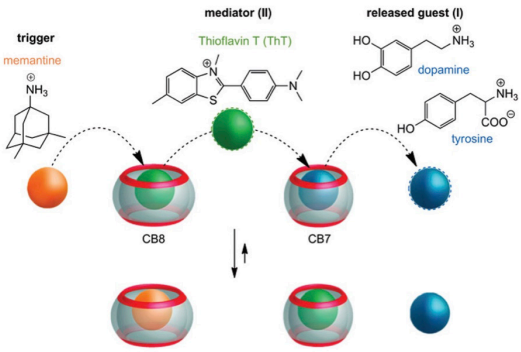
Semicrystalline polythiophene-based nanoparticles deposited from water on flexible PET/ITO substrates as a sustainable approach towards long-lasting solid- state electrochromic devices

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

HIGHLIGHTS

FUNCTIONAL SUPRAMOLECULAR HOST-GUEST SYSTEMS IN WATER

Signal transduction is the process by which chemical information is communicated along a pathway in a cell. Mimicking such archetypal processes with stimuli-responsive chemical structures is an important goal in supramolecular and systems chemistry, where regulatory functions and chemical communication are key features.
In collaboration with researchers from the University of Huelva, we pursue the use of a four-component system, consisting of two guests (I and II) and two cucurbituril macrocyclic receptors (i.e. CB7 and CB8), to demonstrate externally triggered chemical communication that yields the stimuli responsive release of bio-relevant cargo I (i.e. the neurotransmitter dopamine or the essential amino acid tyrosine), reminiscent of a cascade reaction.

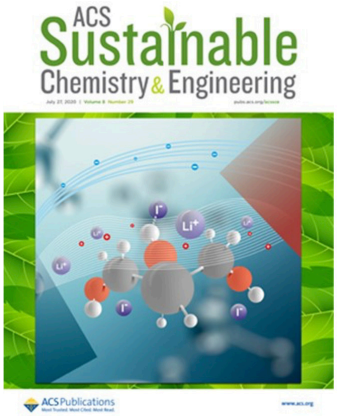


Chemical Signal Cascading in a Supramolecular Network

Chem. Commun., 2020, 56, 3737-3740

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.



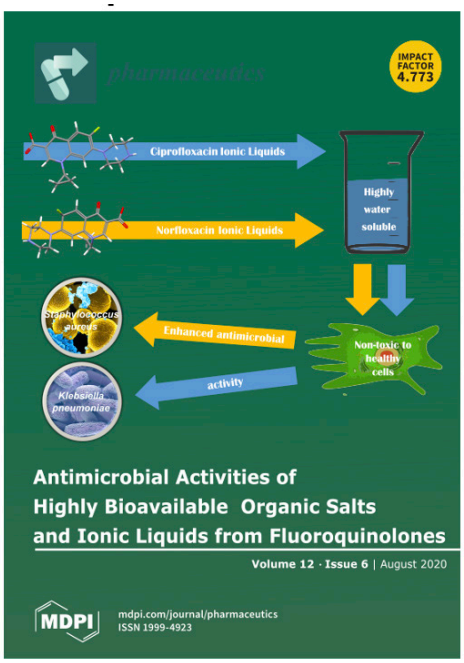
Alkaline Iodide-Based Deep Eutectic Solvents for Electrochemical Applications

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

HIGHLIGHTS

ORGANIC SALTS AND IONIC LIQUIDS BASED FLUOROQUINOLONES

As the development of novel antibiotics has been at a halt for several decades, chemically enhancing existing drugs is a very promising approach to drug development. Herein, we report the preparation of twelve organic salts and ionic liquids (OSILs) from ciprofloxacin and norfloxacin as anions with enhanced antimicrobial activity. Each one of the fluoroquinolones (FQs) was combined with six different organic hydroxide cations in 93–100% yield through a buffer-assisted neutralization methodology. The prepared compounds were not toxic to healthy cell lines and displayed between 47- and 1416-fold more solubility in water at 25 and 37 °C than the original drugs, with the exception of the ones containing the cetylpyridinium cation. In general, the antimicrobial activity against Klebsiella pneumoniae was particularly enhanced for the ciprofloxacin-based OSILs, with up to ca. 20-fold decreases of the inhibitory concentrations in relation to the parent drug, while activity against Staphylococcus aureus and the commensal Bacillus subtilis strain was often reduced. Depending on the cation–drug combination, broad-spectrum or strain-specific antibiotic salts were achieved, potentially leading to the future development of highly bioavailable and safe antimicrobial ionic formulations.



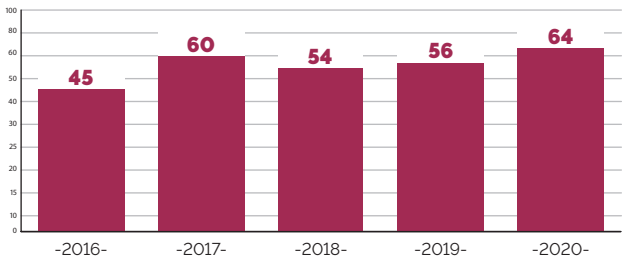
Antimicrobial Activities of Highly Bioavailable Organic Salts and Ionic Liquids from Fluoroquinolones

Pharmaceutics 2020, 12(8), 694.

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION

Articles published / Year



H-index: **72**

279 articles*
25344 citations

***2016-2020**
From WOS core collection

FUNDED PROJECTS

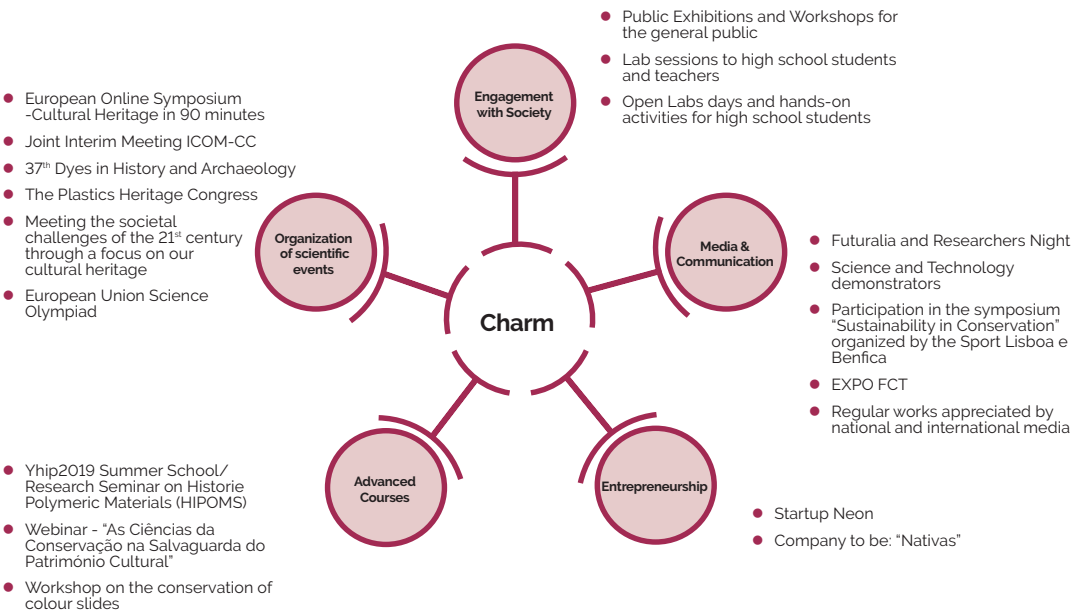
(Representative projects)

- **NEMOSINE - Innovative packaging solutions for storage and conservation of 20th century cultural heritage of artefacts based on cellulose derivatives**
  H2020-NMBP-2017-two-stage - grant 760973-2, Ana Ramos (Portuguese coordinator)
  Total funding: € 7,293,911.20
- **CHARISMA - Entrepreneuring Chemical Irreversibility to Prototype Responsive Smart Labels**
  H2020-MSCAITN-2018 grant N. 814292, A. Jorge Parola (Portuguese coordinator)
  Total funding: € 2,422,010.16
- **INFUSION - Engineering optoelectronic INterfaces: a global action intersecting FUndamental conceptS and technology implementatION of self-organized organic materials**
  H2020-MSCA-RISE-2014 - grant 734834, A. Jorge Parola (Portuguese coordinator)
  Total funding: € 1.237.500.00
- **DecoChrom - Decorative Applications for Self-Organized Molecular Electrochromic Systems**
  H2020-NMBP-2017-two-stage - grant 760973-2, César A. T. Laia (Portuguese coordinator)
  Total funding: € 6,688,150.88
- **Active Pharmaceutical Ionic Liquids as new platform for Effective Treatment of Tuberculosis (TB-ILs)**
  PTDC/QUI-QOR/32406/2017, Luís Branco (PI)
  Total funding: € 237.425,18
- **Photoresponsive Self-Assembled Nanomaterials for Drug and Gene Delivery**
  PTDC/QEQ-QFI/1971/2014, Nuno Basílio (PI)
  Total funding: € 238 923.58
- **Polyphenols in Art - Chemistry and biology hand in hand with conservation of cultural heritage**
  PTDC/QUI-OUT/29925/2017, Maria João Melo (PI)
  Total funding: € 239.062,08
- **SupraPhoR - Supramolecular Photochemical Control of Fluid Rheology**
  PTDC/QUI-QFI/30951/2017, A. Jorge Parola (PI)
  Total funding: € 231 426.21
- **Dye Sensitized Solar Cells based on ionic liquids and synthetic flavylium compounds**
  PTDC/QEQ-QFI/1971/2014, Fernando Pina (PI),
  Total funding: € 156,768.00
- **SunStorage - Harvesting and Storage of Solar Energy**
  POCI-01-0145-FEDER-016387, Adélio Mendes (PI, FCUP)
  Total funding: € 2,050,049.77
- **Repurposed antimalarial and anti-Ebola drugs as Organic Salts and Ionic Liquids to prevent and fight COVID-19**
  Miguel Santos (PI)
  Total funding: € 40,000.00

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)

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) Catalysis for a Sustainable Environment; ii) Renewable Energy and Climate Change Mitigation; iii) Environmental Protection and Remediation; iv) Drug Delivery and Tissue Regeneration; and v) 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 or through the creation of University spin-offs, with the goal of contributing to innovative products/technologies for society.

RESEARCH OBJECTIVES [2020-2023]

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.
- 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.

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

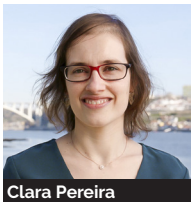

Ana Aguiar-Ricardo


Ana Rita Duarte


Andreia Peixoto


Bruno Jarrais


Carlos Granadeiro


Clara Pereira


Cristina Freire


Diana Fernandes


Diana Julião


Fátima Mirante


Inês Matos

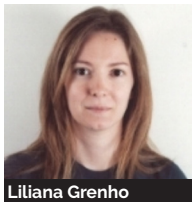

Isabel Cansado

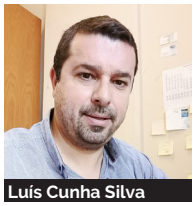

Isabel Fonseca


Iwona Kuzniarska-Biernacka


Joaquim Vital

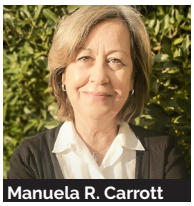

José Domingos Santos

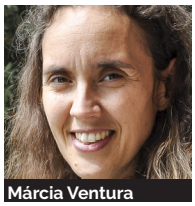

Liliana Grenho

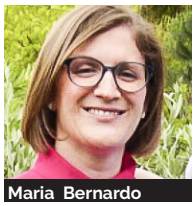

Luís Cunha Silva


M. Ascensão Lopes


M. Helena Fernandes


Manuela R. Carrott


Márcia Ventura

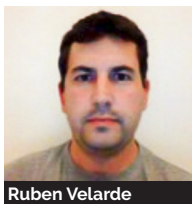

Maria Bernardo


Marta Susete Nunes


Paulo Mourão


Pedro Sousa Gomes

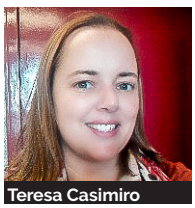

Raquel Viveiros

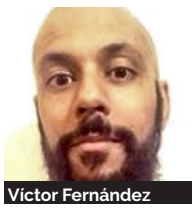

Ruben Velarde


Salete S. Balula


Susana L. H. Rebelo


Svitlana Lyubchyk


Teresa Casimiro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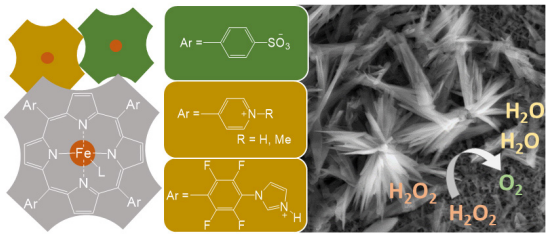
RESEARCH THEMES/
(BIO)MATERIALS ENGINEERING AND PRODUCTION

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) with reduced particle size and enhanced magnetic properties prepared by coprecipitation in aqueous media using organic alkaline agents, hydrothermal process and thermal decomposition.
- **Core-shell gold-coated magnetic nanoparticles** for sensing applications.
- **Light-responsive hybrid silica nanoparticles** with tailored photochromic response and wider color palette based on silylated naphthopyran dyes (microwave-assisted synthesis) or polyoxometalates.
- **Light-responsive hybrid tungsten oxide nanoparticles** with tailored morphology, particle size, and photoswitchable properties through hydrothermal and solvothermal processes.
- **Multifunctional hybrid carbon/metal oxide nanomaterials** with fine-tuned morphological, chemical (redox), electrical, and/or magnetic properties through coprecipitation, hydrothermal and ball milling processes.[1]
- **Biochar-based materials** to prepare carbon-based catalysts by heteroatom doping and metal/sulfonic acid funcionalization.
- **Doped bismuth-based dieletric ceramic materials** produced by mixed oxide method and sintering by pressureless sintering method.[2,3]
- **Optical sensors based on lanthanide-containing MOFs** for the detection of heavy metal ions in water.
- **Magnetic porous, nanoporous and nanostructured adsorbents,** for the removal of organic contaminants and/or recovery of metals and rare-earth elements.[4-7]
- **Metalloporphyrin based (nano) materials** as new enzyme models for catalytic antioxidants.[8]



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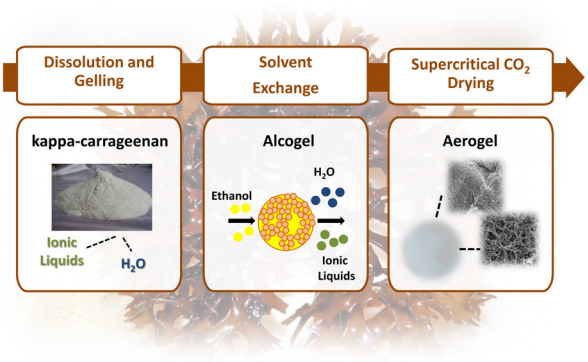
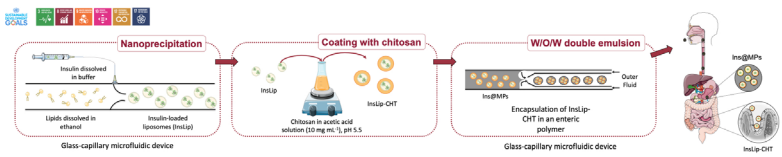
RESEARCH THEMES/
(BIO)MATERIALS ENGINEERING AND PRODUCTION

- **Molecularly imprinted polymers (MIP)** for drug delivery systems and catalytic processes using supercritical fluid technology.
- **Development of plastic antibodies with affinity for biomolecules** under the scope of the ongoing project BioMIPs.
- **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).[9-21]
- **Natural polymers extracted from plants for the production of bioinspired materials** with high biocompatibility for tailored drug delivery.[22,23]



- **Nano-in-micro dry powder formulations** based on polyurea dendrimers, PLGA and cholesterol with excellent biocompatibility prepared using super supercritical fluid technology.[24]
- **Continuous microfluidic assembly of insulin-loaded pH responsive nano-in-microparticles** for efficient encapsulation of insulin into PEGylated liposomes.[25]



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RESEARCH THEMES/ SUSTAINABLE ENVIRONMENT

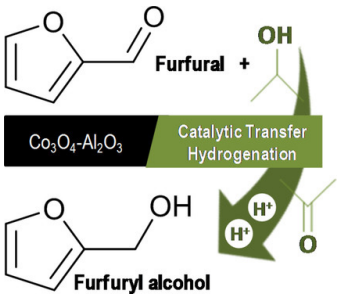
CATALYSIS FOR A SUSTAINABLE ENVIRONMENT

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.

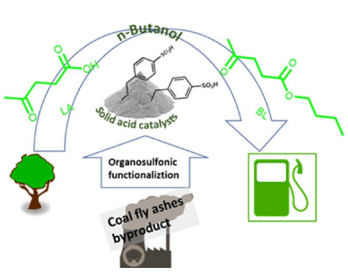
Selective homogeneous and heterogeneous chemical catalysis

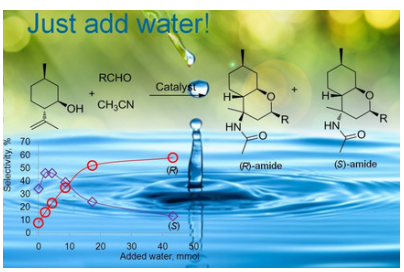
- **Nitroaromatics reduction** including 4-nitrophenol (a prevalent pollutant found in wastewater) to 4-aminophenol with great industrial interest for the synthesis of bulk and fine chemicals using recyclable nanocatalysts: carbon-based materials hybridized with metal oxides or magnetic ferrite nanoparticles.
- **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.[26]

Conversion of biomass derivatives into value-added products



- 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.
- Catalytic transfer hydrogenation (CTH) of furfural to produce valuable furfuryl alcohol over 3*d*-transition metal-based catalysts.[27]
- HSO_3-functionalized derived catalysts based on naturally occurring mineral resources (K10, HNT and cloisite Na+ clays) and coal fly ashes as a new strategy to produce solid acid catalysts for industrial catalytic applications: i) biodiesel and biofuels production and ii) highly valuable chromenols.[28-30]





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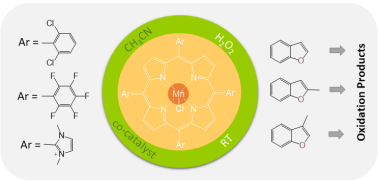
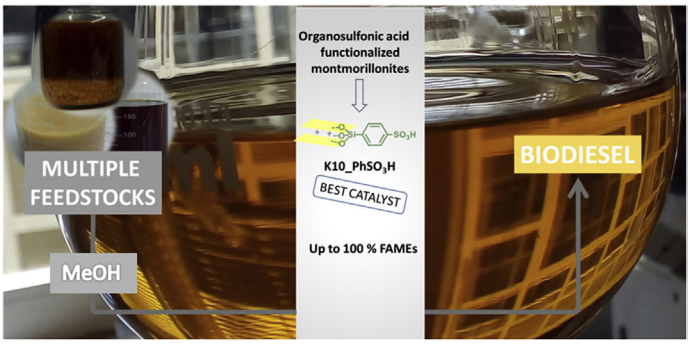
RESEARCH THEMES/ SUSTAINABLE ENVIRONMENT

- **Environmentally friendly oxidation reactions** for the eco-sustainable valorization of renewable raw materials.[31]



- **Desulfurization of real fuels** based on active heterogeneous catalysts having polyoxometalates as active centres, in collaboration with Galp Energia company.[32]
- **Biodiesel production** using waste shells derived catalysts;[33] using sulfonic-acid montmorillonites as catalysts (real feedstocks, *e.g.* waste oils); using membrane reactors for sustainable production.[34]



- **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;[35,36] selective oxidized carbon nanotubes and graphene flakes carbocatalysts for the mild oxidation of cis-cyclooctene.

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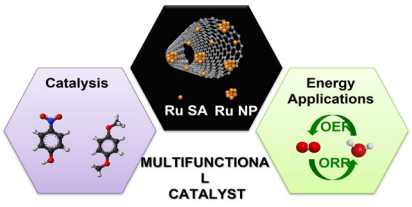
RESEARCH THEMES/ SUSTAINABLE ENVIRONMENT

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. 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 and mixed-valence Co and Mn oxides@doped-graphene nanocomposites for application in electrochemical energy-related reactions – hydrogen evolution reaction (HER), oxygen evolution reaction (OER), and oxygen reduction reaction (ORR).[37-43]



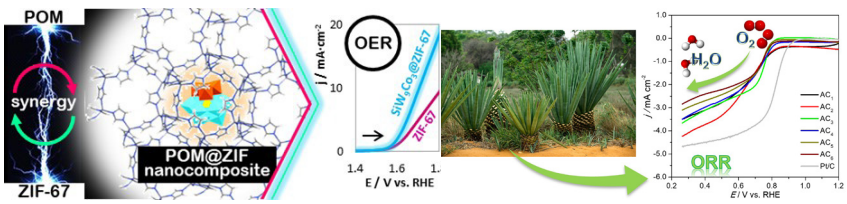
- **CO_2 conversion and valorization:**

  We are interested on 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.[44]

RENEWABLE ENERGY & CLIMATE CHANGE MITIGATION

MatSusWell is committed in advancing green and sustainable chemistry, therefore research work has focused the development of metrics and scoring tools to analyse and quantify activated carbons from biomass, mixed-valence Co and Mn oxides@doped-graphene nanocomposites and composites of metal nanoparticles (e.g., Cu, Pd) with carbon-based materials.

- **Quantitative framework for measuring greenness and/or sustainability** of chemical products and processes.[45]



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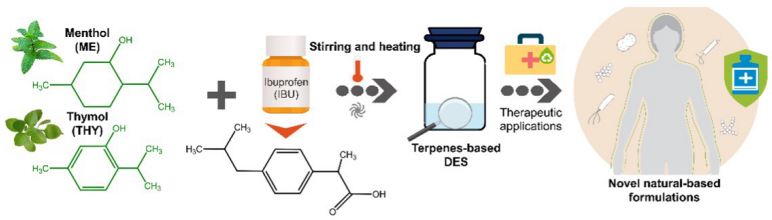
RESEARCH THEMES/
DRUG DELIVERY AND TISSUE REGENERATION

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 CO_2-assisted spray drying (SASD) enabled the design and production of effective systems for pulmonary delivery of siRNA.[46]
- **Cyclodextrin host-guest complexation by SASD for HIV drug delivery.**[47]
- **Therapeutic deep eutectic systems (THEDES) based on natural terpenes and anti-inflammatory agents explored as anticancer therapeutic** pharmaceutical ingredients.[48,49]



- **Tetracycline-releasing biospace maintainer materials** for craniofacial tissue healing engineering to control tissue infection and prime the healing of both soft and hard tissues of the craniofacial region, highlighting the adequacy to a multitude of clinical applications.[50-52]

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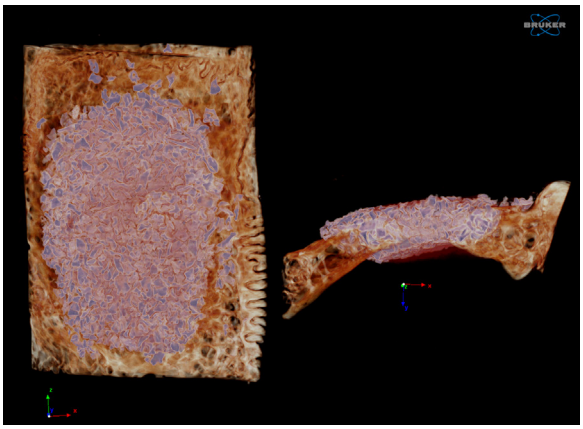
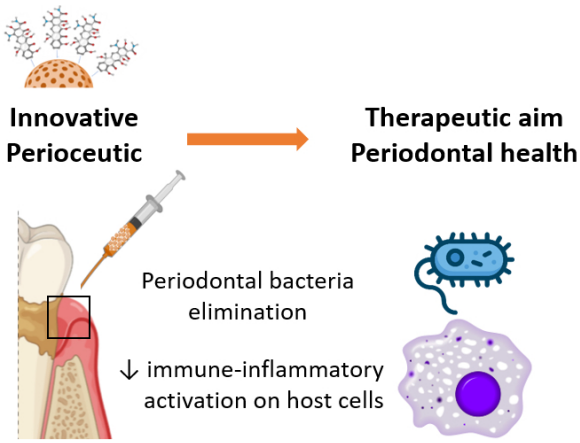
doi:10.1016/j.ceramint.2019.09.101

RESEARCH THEMES/
DRUG DELIVERY AND TISSUE REGENERATION

- **Innovative biomimetic biomaterials** for enhanced bone regeneration able to modulate cell response and enhance regenerative outcome.[53-60]



- **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.
- **Development of customized 3D structures for bone regeneration by additive manufacturing** using Computer Assisted Design (CAD) models.
- **Innovative perioceutics targeting the two key issues in the etiology/progression of Periodontal Diseases**, *i.e.* the immune inflammatory host response and the local polymicrobial synergy and dysbiosis.



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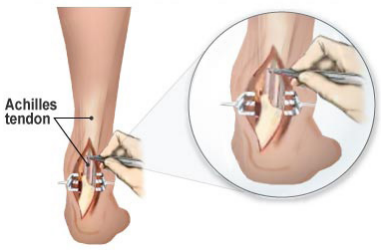
55 H. Sooraj, et al., Materials Letters, 2020, 273, 127935. doi.org/10.1016/j.matlet.2020.127935
56 N. Cruz, et al., Materials, 2020, 13, 2177. doi:10.3390/ma13092177
57 I. Pereira, et al., Regenerative Biomaterials, 2020, 8, 1-10. doi:10.1093/rb/rbaa036
58 S. Teixeira, et al., Pharmaceutics, 2020, 293. doi:10.3390/pharmaceutics12030293
59 D. Morais, et al. Polymer Testing, 2020, 106507. doi:10.1016/j.polymertesting.2020.106507
60 A. Pinho, et al., Materials Science & Engineering C, 2020, 107, 110243. doi:10.1016/j.msec.2019.110243

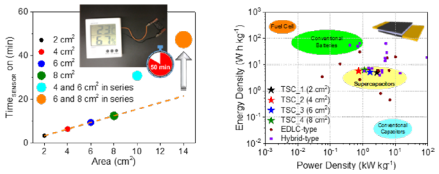
RESEARCH THEMES/
WEARABLE TECHNOLOGIES AND DEVICES

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,[61] namely:

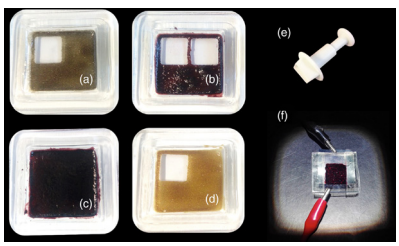
- **Healthcare and medical devices:** 3D Textile-based structures for tendon/ligament repair with improved mechanical performance using innovative textile technology. A worldwide patent application (PCT) has been published and multinational companies that operate in the medical sector have demonstrated a great interest in these developments.[62-65]



- **Smart wearable & flexible energy storage & harvesting technologies for IoT applications:** Energy storage/harvesting textiles and flexible devices based on hybrid carbon/metal oxide electrode nanomaterials to power miniaturized electronic sensors and devices integrated on clothes for IoT applications.[66] An international patent application under EU evaluation has been published.[67]



- **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.
- **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.
- **A New class of donor-acceptor dedrimers with photodiode-like behavior** was developed.[68]



SELECTED PUBLICATIONS

61 I. Pereira, et al., in Handbook of Functionalized Nanomaterials for Industrial Applications, Chaudhery Mustansar Hussain Editor, Chapter 21, pp. 611-714, Elsevier, 2020. **doi:10.1016/B978-0-12-816787-8.00021-1**

62 A. Pinho, et al., Biomater. Sci., 2020, 8, 798-811. **doi:10.1039/c9bm00901a**

63 T. Peixoto, et al., Adv. Eng. Mater., 2020, 22, 2000492. **doi:10.1002/adem.202000492**

64 D. Morais, et al., J. Mech. Behav Biomed Mater, 2020, 106, 103734. **doi:10.1016/j.jmbbm.2020.103734**

65 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**

66 R. S. Costa, et al., J. Mater. Sci., 2020, 55, 10121-10141. **doi:10.1007/s10853-020-04709-0**

67 Thermionic Capacitor Chargeable By Soret Effect Using a Temperature Gradient. **WO/2020/065533. International Patent Application. Publication Date: April 2, 2020. International filed patent under EU evaluation**

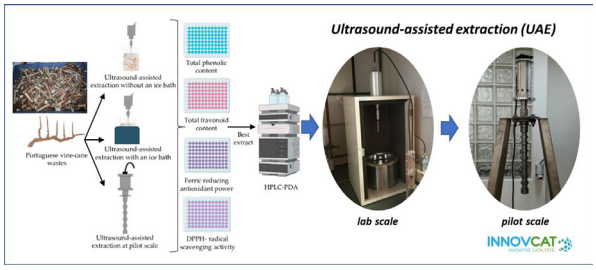
66 R. F. Pires, et al., J. Applied Polymer Sci, 2020, 137, 48635. **doi:10.1002/app.48635**

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.

i) Collaboration with companies and technological centres

- **Porous functionalized carbons derived from spent tire rubber** - INOV.AÇÃO 2018 promoted by Valorpneu, the Portuguese Management Company of Used Tires, awarded first prize to "ROBUST" project. This project proposes tire recycling through the chemical and energetic valorization of spent tire in the context of the circular economy, since new products (nanoporous carbon materials) for innovative applications (recovery of critical rare earth elements) were produced.
- **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).
- **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.[69-72]
- **Scale-up of catalysts and functional materials production and natural compounds extraction using advanced technologies**[73], in collaboration with INNOVCAT company.



- **CATALVALOR**[74] **and WEStoreOnTEX**[75] projects were awarded with 20,000 euros to support proofs of concept under the BIP Proof - Business Ignition Programme, promoted by U.Norte Inova, University of Porto, 2018.

INNOVCAT
INNOVATIVE CATALYSTS

SELECTED PUBLICATIONS

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

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

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

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

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

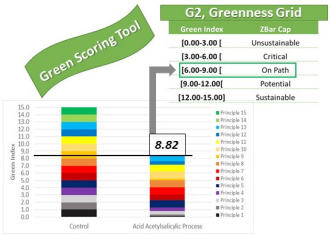
74 https://upin.up.pt/pt-pt/content/catalysinggreener-future

75 https://upin.up.pt/pt-pt/tecnologias/flexiblethermoelectric-supercapacitors

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.

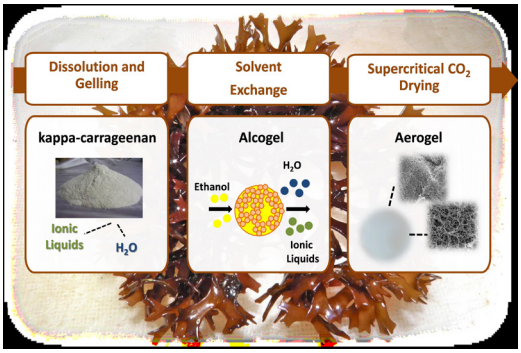


Towards a new, green and dynamic scoring tool, G2, to evaluate products and processes.

J Clean. Prod. 2020, 276, 123079

PROPERTIES OF κ-CARRAGEENAN AEROGELS PREPARED BY USING DIFFERENT DISSOLUTION MEDIA AND THEIR APPLICATION AS DRUG DELIVERY SYSTEMS

Kappa-carrageenan aerogels were synthesized using different dissolution and crosslinking media in order to evaluate their effects on the textural properties of the matrixes and further on the drug loading and release performance. The different aerogel samples were produced through the dissolution of the biopolymer in water with addition of potassium salts as crosslinking agents and, in two different ionic liquids derived from imidazolium ion, being further dried with supercritical CO_2. Tetracycline was used as a model drug and loaded in two of the prepared aerogels samples. With a higher macroporosity, the kappa-carrageenan aerogel prepared by dissolution into ionic liquid showed higher loading capacity than the one prepared by dissolution into water and a slightly higher release rate. The matrixes were considered to present a good potential to be used as biocompatible carriers on drug controlled delivery.

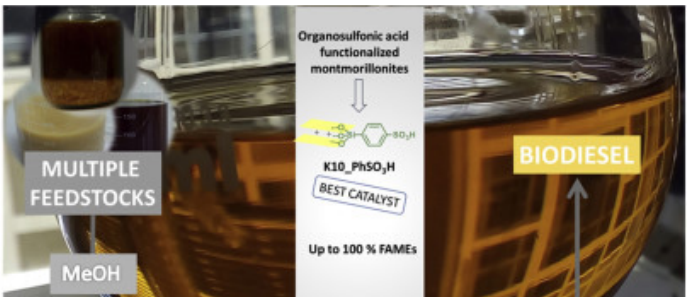


Properties of k-carrageenan aerogels prepared by using different dissolution media and its application as drug delivery systems.

Materials Chemistry and Physics, 2020, 253,123290

HIGHLIGHTS

SOLID ACID CATALYSTS FOR BIODIESEL PRODUCTION USING LOW-GRADE AND HYBRID FEEDSTOCKS

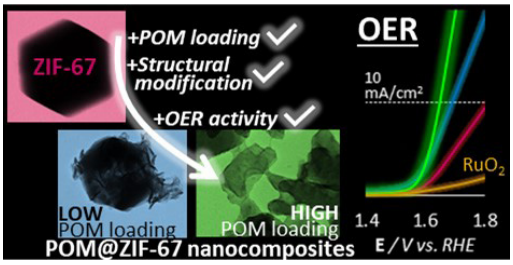


Organosulfonic acid functionalized montmorillonites as solid catalysts for (trans) esterification of free fatty acids and (waste) oils.

Renew. Energy 2020, 146, 2416-2429

HSO_3-functionalized MMTs were prepared using a naturally occurring low-cost mineral material by different methodologies including one-pot organosilylation or direct sulfonation and two-step organosilylation followed by sulfonation or oxidation as new strategies to prepare efficient organosulfonic acid functionalized catalysts. K10_$PhSO_3H$ showed to be active as solid acid catalyst to a simultaneous esterification and transesterification of different feedstocks and combination of feedstocks (hybrid feedstocks) with conversions up to 100% using moderate conditions. These results highlighted the potential of this catalyst as solid acid catalyst for biodiesel production using low-grade and hybrid feedstocks. The proof-of-concept economic viability of the catalyst to produce biodiesel from multiple feedstocks was also evaluated. This work was awarded by some national entrepreneurship competitions and led to the creation of INNOVCAT company.

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



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

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

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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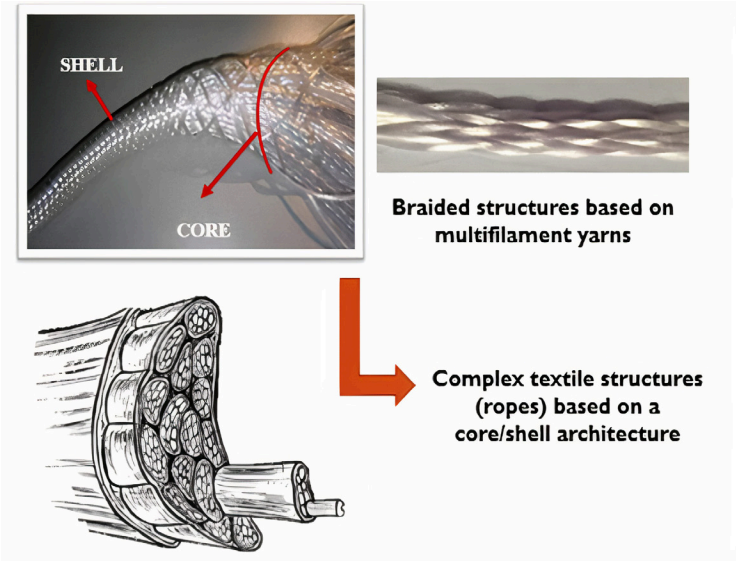
HIGHLIGHTS

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 attained 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.

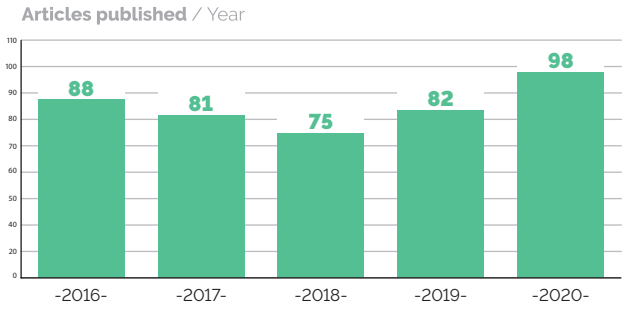
PCT/IB2020/053014, International Application No. WO/2020/194280, Publication Date 01.10.2020.

Dextran-based tube-guides for the regeneration of the rat sciatic nerve after neurotmesis injury.

Biomaterials Science, 2020, 8, 798-811

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION



H-index: **82**

424 articles*
41583 citations

*2016-2020
From WOS core collection

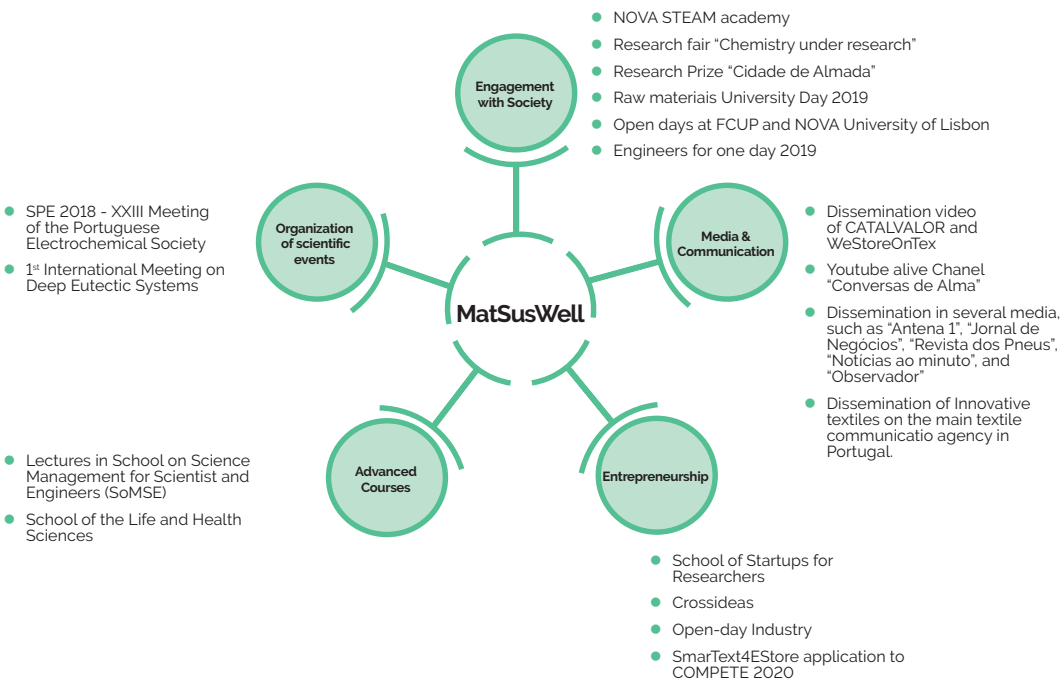
FUNDED PROJECTS *(Representative projects)*

- **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
- **NANOGUARD2AR – Nanomaterials-based innovative engineering solution to ensure sustainable safeguard to indoor air**
  H2020 - MSCA-RISE-2015 – 690968. Svitlana Lyubchyk (PI). Funding: € 351,000.00
  Total Funding: € 1,386,000.00
- **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

INTERNATIONAL COOPERATION AND NETWORKING

- COST Action EsSENce - High-performance Carbon-based composites with Smart properties for Advanced Sensing Applications CA19118 - Member of Management Committee
- COST Action CA18224, "Greenering - Green Chemical Engineering Network Towards Upscaling Sustainable Processes", LAQV role: coordinator, 2019–2023
- COST Action CA17107, "CONTEXT - European Network to connect research and innovation efforts on advanced Smart Textiles", LAQV role: Participation as National Management Committee Member, 2018-2022
- SERP+ - International SERP-Chem master with Laboratoire de Chimie Physique, Université Paris-Sud, Paris, France
- Collaborations: Catalysis: Finland, Spain, Czech Republic, Chile; Drug delivery: Finland; Imprinting materials: United Kingdom; Algeria. Energy conversion: France, Germany, Spain.

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.

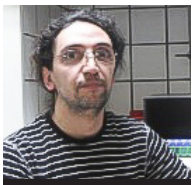
RESEARCH OBJECTIVES [2020-2023]

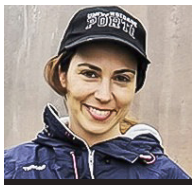
The research activity of the Nanoplatforms group has attracted significant attention to the optimization of innovative nanoplatforms to overcome several clinical, chemical, environmental, and food quality challenges. The main research objectives are the:

- 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

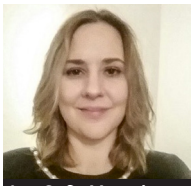
SENIOR RESEARCHERS

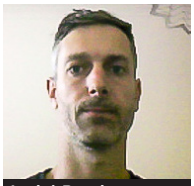

Abel Duarte

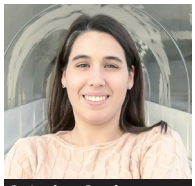

Alexandra Plácido


Ana Cláudia Santos


Ana Figueiras

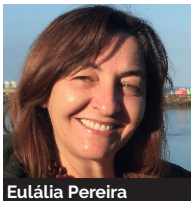

Ana Sofia Macedo


André Pereira


Catarina Seabra


Cláudia Nunes


David Ribeiro


Eulália Pereira


Filipa Melo


Francisco Veiga


Helena Gonçalves

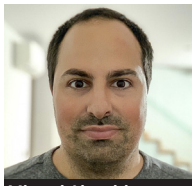

João Santos


Lúcia Saraiva

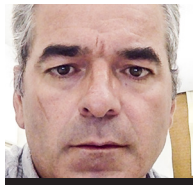

Lucinda Bessa


Luis Ribeiro


Marieta Passos

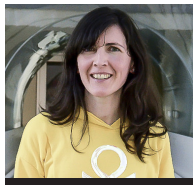

Miguel Almeida


Paula Gameiro


Rui Carvalho


Salette Reis


Sofia Lima


Sofia Rodigues


Susana Sousa


Tânia Moniz

 Group coordinator

RESEARCH TEAM

OTHER DOCTORATE RESEARCHERS
Ana Sofia Macedo
Catarina P. Leite
Luís Almeida
Paula Pinto
Peter Eaton

POST-DOCTORAL FELLOWS
Mariana Ferreira
Sarmento Mazivila

PhD STUDENTS
Ana Isabel Barbosa
Ana Marta Azevedo
Ana Rita Pinto
Andreia Granja
Andreia Marinho
Fábio Costa
Irina Pereira
Joana Sequeira
João Costa
José Soares
Laura Ferreira
Maria Enea
Miguel P. Silva
Raquel Costa
Sarah Pereira

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André Vilaranda
Andreia Guimarães
Iago Soares
Filipa Serrasqueiro
Svitlana Prots
Diana Rodrigues
Pedro Costa
Carla Sofia Pereira
Nuno Costa
Ana Beatriz Ferreira
Tiago Azevedo

RESEARCH GRANTEES
Ana Filipa Neves
Ana Isabel Martins
Diana Costa
Diana Peixoto
Fátima Mota
Filipa Soares
Rafael Castro
Raquel Andrade
Susana Neves
Tiago Azevedo

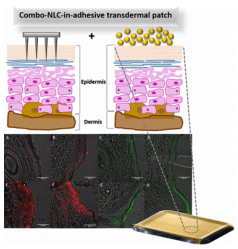
OTHER RESEARCHERS
Cátia Domingues

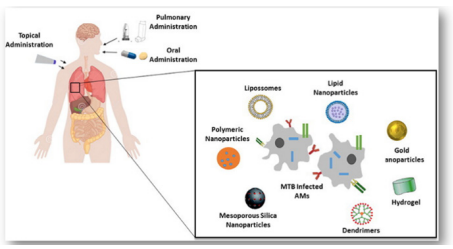
RESEARCH THEMES/ DELIVERY SYSTEMS

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.
- 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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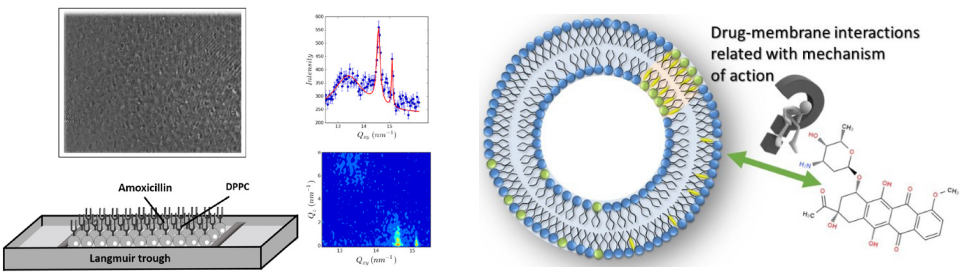


RESEARCH THEMES/ BIOMIMETIC MODELS

MULTIFUNCTIONAL (BIO)SENSORS FOR MOLECULAR IMAGING, TARGETING AND DIAGNOSIS

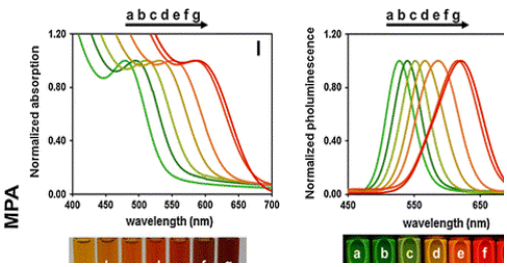
The NanoPlatform group seeks to provide a strong contribution to the development of distinct types of (bio)sensors and analytical devices that exploit the remarkable physical-chemical properties of different nanomaterials, including metallic nanoparticles, semiconductor, and graphene quantum dots, carbon 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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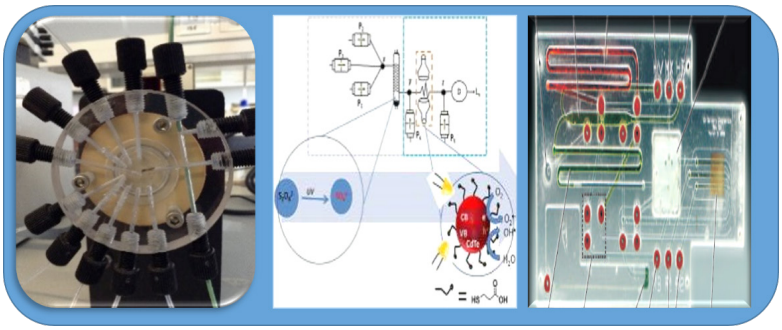
RESEARCH THEMES/
(BIO)SENSORS AND ANALYTICAL AUTOMATION TOOLS

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 with different types of nanomaterials such as multi-colored quantum dots, lateral flow assays, and microfluidic platforms for different (bio)assays. 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 a generic tool, based on a battery of miniaturized (bio)assays, for rapid screening of the (eco)toxicity and of chemicals and materials 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 particular structural elements and to guide their modification to reduce their hazardous potential. So, the evaluation of toxicity is 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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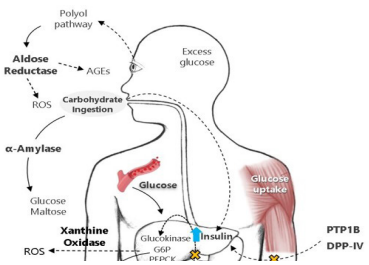
RESEARCH THEMES/
(BIO)SENSORS AND ANALYTICAL AUTOMATION TOOLS

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 watere.

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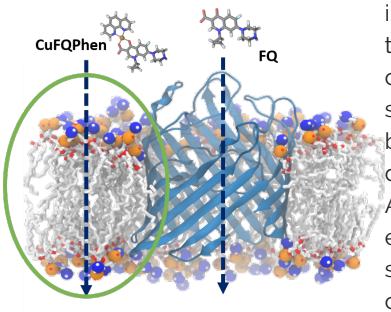
HIGHLIGHTS

BIOPHYSICAL SUPPORTED STRATEGIES TO BYPASS THE BACTERIAL RESISTANCE

Over the last years several studies have been performed, showing the stability of copper (II) complexes and that copper complexes with 1,10-phenanthroline possess nuclease. These findings gave rise to the synthesis and characterization of ternary complexes of copper(II), 1,10- phenanthroline and fluoroquinolones These compounds are highly stable under physiological conditions, pH and temperature and exhibit antibacterial activity (comparable or improved to pure FQs).



The permeation of FQs and its metalloantibiotics in E. coli was studied, evaluating the role of OmpF, the major porin involved in the uptake of FQs in E. coli, for its influx. The results corroborate previous studies that propose that metalloantibiotics may be a promising substitute to FQs against E. coli, due to its presumable ability to circumvent the AMR mechanism based on the reduction of the expression of porins. Furthermore, toxicological data show that metalloantibiotics are non-toxic at MIC concentrations.

Fluoroquinolone Metalloantibiotics to Bypass Antimicrobial Resistance Mechanisms: Decreased Permeation through Porins.

Membranes, 2021, 11, 3

The binding of free and copper-complexed fluoroquinolones to OmpF porins: an experimental and molecular docking study.

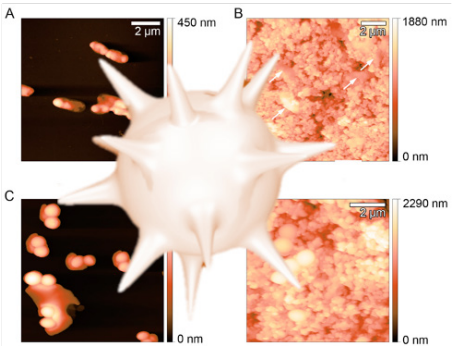
RSC Adv., 2017, 7, 10009

Passive Diffusion of Ciprofloxacin and its Metalloantibiotic: A Computational and Experimental study.

Journal of Molecular Biology, 2021, 433, 166911

SILVER NANOSTARS-COATED SURFACES WITH POTENT BIOCIDAL PROPERTIES

The bactericidal effects of silver nanospheres (AgNPs) and silver nanostars (AgNSs) against P. aeruginosa ATCC 27853 and of S. aureus ATCC 25923 were compared. Although AgNPs are more effective than AgNSs in inhibiting bacterial growth, AgNSs were found to be very effective as coatings for anti-bacterial surfaces. The bactericidal effect of the AgNSs-coated surfaces was apparent 6 h after contact with inoculated bacteria, that were unable to proliferate and were totally dead after 24 h. AgNSs can be a promising agent to engineered biocidal surfaces with applications in the biomedical and food industry sectors.



AFM images of P. aeruginosa ATCC 27853 (A,B) and of S. aureus ATCC 25923 (C,D) deposited on non-coated (A,C) and AgNSs-coated surfaces (B,D) after 24 h. Arrows point to the P. aeruginosa cells, clearly damaged.

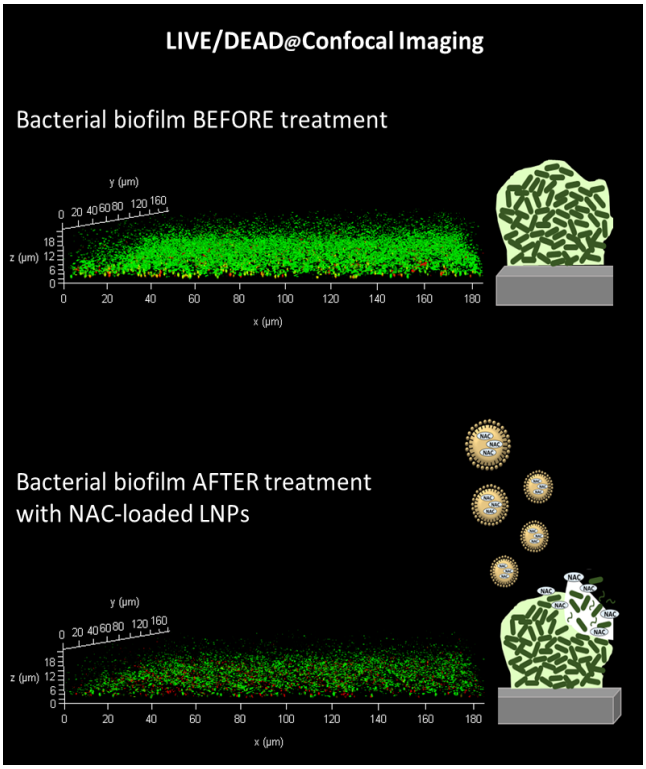
Silver Nanostars-Coated Surfaces with Potent Biocidal Properties

Int. J. Environ. Res. Public Health 2020, 17, 7891

HIGHLIGHTS

TOWARDS THE ERADICATION OF BACTERIAL BIOFILMS

Bacterial biofilms are a major health concern, mainly due to their contribution to increased bacterial resistance to well-known antibiotics. The conventional treatment of implant-associated biofilms represents a challenge and frequently, eradication is not achieved. Although the search for effective and innovative treatments is a growing research field, no solutions to prevent implant removal surgeries have yet been discovered. In this context, an innovative therapeutic approach that is focused on the encapsulation of N-acetyl-L-cysteine (NAC) into lipid nanoparticles (LNPs) functionalized with -amino acids is proposed to target and disrupt bacterial biofilms. In vitro biocompatibility studies showed a low cytotoxicity effect in fibroblasts and a low hemolytic activity in human red blood cells. The in vitro antibiofilm efficacy of the developed formulations showed that the NAC-loaded LNPs had a significant reduction of biofilm biomass and bacterial viability in Pseudomonas aeruginosa biofilms. In a more complex therapeutic approach, the LNPs were further combined with moxifloxacin, revealing a beneficial effect between the LNPs and the antibiotic. Overall, the developed formulations present a potential therapeutic approach against Pseudomonas aeruginosa biofilms, alone or in combination with antibiotics.



Impact of nanosystems in Staphylococcus aureus biofilms treatment.
FEMS Microbiology Reviews, 2019, 43 (6), 622.

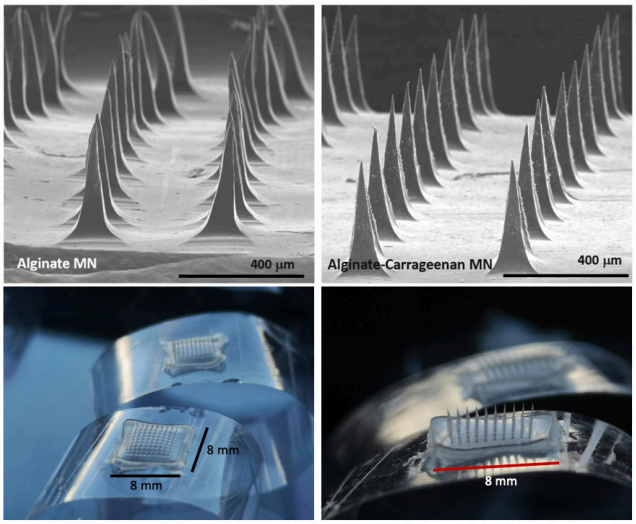
Innovative Strategies Toward the Disassembly of the EPS Matrix in Bacterial Biofilms.
Frontiers Microbiology, 2020, 11, 952

N-Acetyl-L-cysteine-Loaded nanosystems as a promising therapeutic approach toward the eradication of Pseudomonas aeruginosa Biofilms.
Applied Materials and Interfaces, 2021

HIGHLIGHTS

OVERCOMING THE SKIN BARRIER: NANOSTRATEGIES TO ENHANCE DRUG ABSORPTION

SApproaches to overcome the stratum corneum skin layer and allow entry into the skin involves physical and chemical methods, including colloidal formulations based in nanotechnology. Hydrogels have been explored in the field of cutaneous application and have proven to be a good solution as a topical vehicle, due to their high-water content, biocompatibility, improved drug delivery, responsiveness to stimuli and versatility in terms of preparation and drug-loading. Research work establishes the sodium alginate-poly(vinyl) alcohol (SA-PVA) hybrid hydrogels as effective delivery systems for bioactive polyphenols intended for pharmaceutical applications. Blends of different ratios of SA and PVA polymers successfully produced three types of hybrid hydrogels, able to incorporate quercetin within the polymeric network. The permeability of quercetin through the skin showed different penetration/ permeation profiles according to the hydrogel's blend. Distinct behaviours allow the selection of SA-PVA at 2/1 ratio for a local and prolonged skin effect, making the use of these hydrogels a good solution for the treatment of skin ageing and local



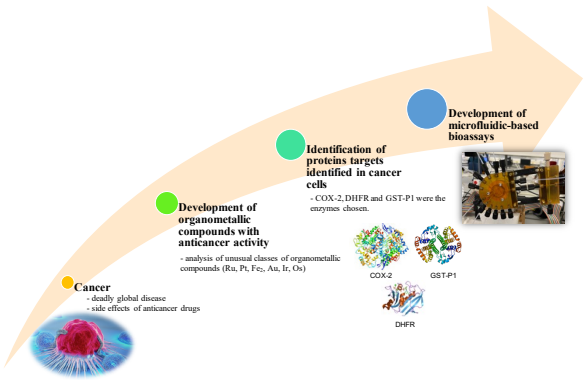
Marine Polymeric Microneedles for Transdermal Drug Delivery.
Carbohydr Polym 2021, 266:118098

Design and Characterization of Sodium Alginate and Poly(vinyl) Alcohol Hydrogels for Enhanced Skin Delivery of Quercetin.
Pharmaceutics 2020, 12, 1149

HIGHLIGHTS

DEVELOPMENT OF NEW ORGANOMETALLIC DRUGS TO INHIBIT ENZYMES INVOLVED IN CANCER BASED ON A RATIONAL APPROACH

New drug families are being studied with the aim of reducing or even eradicate side effects of common anticancer drugs. Unusual classes of organometallic agents, such as ruthenium, platinum, diiron, gold, osmium and iridium compounds are being analysed.



The key protein targets of organometallic compounds have now been identified. These compounds are not completely designed to inhibit these targets, so we expect to obtain much better inhibitors with new ones. A microfluidic-based bioassays for these targets, such as cyclooxygenase-2, dihydrofolate reductase, glutathione S-transferase P1, were developed providing rapid and reliable results and sustainable improved cost-effective easy-to-use methodologies. So putative libraries of compounds are being screened. From the key hits will be designed and synthesized efficient organometallic compounds that will be characterized, and their inhibition validated with in vitro assays.

Recent progress in the development of organometallics for the treatment of cancer.

Current Opinion in Chemical Biology 2020, 56, 28

Bis-conjugation of Bioactive Molecules to Cisplatin-like Complexes through (2,2'-Bipyridine)-4,4'-Dicarboxylic Acid with Optimal Cytotoxicity Profile Provided by the Combination Ethacrynic Acid/Flurbiprofen.

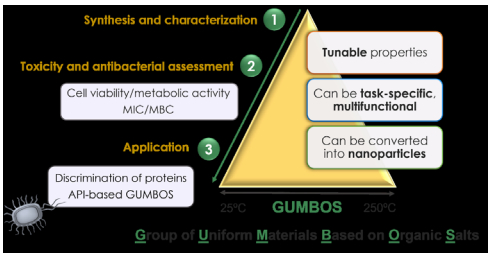
Chemistry—A European Journal, 2020, 26, 1

Automatic evaluation of cyclooxygenase 2 inhibition induced by metal-based anticancer compounds.

Journal of Inorganic Biochemistry, 2021, 218, 111399

XANTHENE-BASED GUMBOS AND NANOGUMBOS: VALUABLE MATERIALS FOR DISCRIMINATING PROTEINS AND FIGHTING AGAINST BACTERIAL INFECTIONS

GUMBOS is a novel class of materials that exhibits similar features to those of ionic liquids but have melting points between 25 and 250 °C. Due to the huge number of possible cation-anion combinations, these materials can be designed for a specific task and be multifunctional. Additionally, GUMBOS can be easily converted into nanoparticles (nanoGUMBOS), with the advantages of working at the nanoscale.



This work includes three main steps: the synthesis and characterization of GUMBOS/nanoGUMBOS (1), assessment of their toxicity and antibacterial activity (2) as well as the study of their application as materials for discriminating protein biomarkers and fighting against bacterial infections (3). The toxicity and antibacterial activity of developed compounds were evaluated by use of an automated yeast-based spectrophotometric assay, MIC, and MBC tests. It is intended to improve the sensitivity and simplicity of the analytical methods for the discrimination of proteins and provide novel alternatives for combating bacterial infections

Development of an automated yeast-based spectrophotometric method for toxicity screening: Application to ionic liquids, GUMBOS, and deep eutectic solvents

Chemosphere 2021, 277, 130227

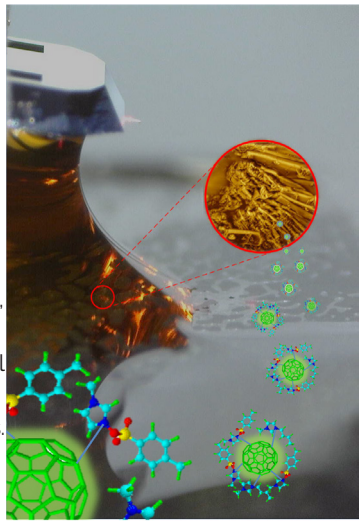
GUMBOS and nanoGUMBOS in chemical and biological analysis: A review.

Analytica Chimica Acta 2020, 1133, 180-198, 1

HIGHLIGHTS

NON-NEWTONIAN THERMOSENSITIVE NANOFLUID BASED ON CARBON DOTS FUNCTIONALIZED WITH IONIC LIQUIDS

This work focused to implement sensor schemes based on fluorescence resonance energy transfer (FRET) processes involving the use of semiconductor quantum dots, carbon dots, and organic molecules as energy donor and/or acceptor elements. The work contemplated the evaluation of distinct strategies for the simultaneous use of multiple energy transfer processes, which provided multiple sensor/analyte interactions, originating multiple analytical signals that reinforced the discriminating capacity of the developed sensor devices. The use of chemometric techniques facilitated the processing of analytical signals obtained in the implemented multi-detection schemes.

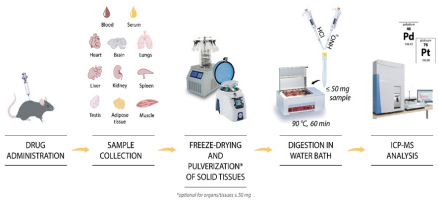


Non-Newtonian Thermosensitive Nanofluid Based on Carbon Dots Functionalized with Ionic Liquids.

Small 2020, 16, 1907661

VISUAL DETECTION USING QUANTUM DOTS SENSING PLATFORMS

Ln recent years visual detection has acquired a renovated relevance as research has been focused on the development of fast, expeditious, cost-effective, and easy to handle analytical methodologies, for on-site monitoring of distinct analytes, from pollutants to food contaminants, pharmaceuticals, biomarkers, pathogens, etc.



The developed work examines fluorescence-based visual detection methods resorting to quantum dots, either alone or in combination with other molecules and nanoparticles, discussing the formats employed to implement sensing platforms, including strategies for enhanced sensitivity and selectivity, multi-analyte determinations, detection modes, sensors assembly, readout acquisition and processing, etc.

The different types of quantum dots used, from binary to ternary nanocrystals, the tailoring of their surface chemistry with appropriate molecules for target recognition, the implementation of multi-detection schemes and the panoply of analytes determined, are also comprehensively investigated.

Visual detection using quantum dots sensing platforms.

Coordination Chemistry Reviews, 429 (2021) 213637

Determination of Atenolol Based on the Reversion of the Fluorescence Resonance Energy Transfer Between AgInS2 Quantum Dots and Au Nanoparticles.

Analyst, 146 (2021) 1004-1015

Label-Free Quantum Dot Conjugates for Human Protein Il-2 Based on Molecularly Imprinted Polymers.

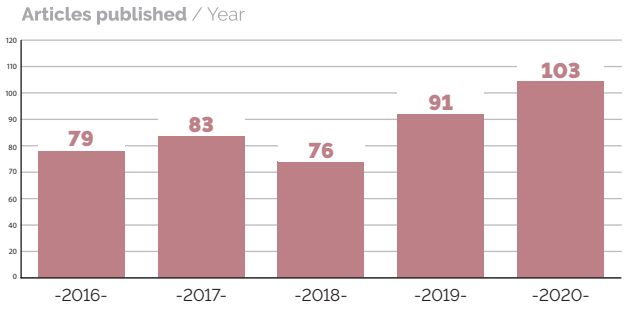
Sensors And Actuators B-Chemical, 304 (2020) 127343

Photocatalytic Activity of AgInS2 Quantum Dots upon Visible Light Irradiation for Melatonin Determination Through Its Reactive Oxygen Species Scavenging Effect.

Microchemical Journal, 155 (2020) 104728 (9)

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION



H-index: **80**

432 articles*
34478 citations

*2016-2020
From WOS core collection

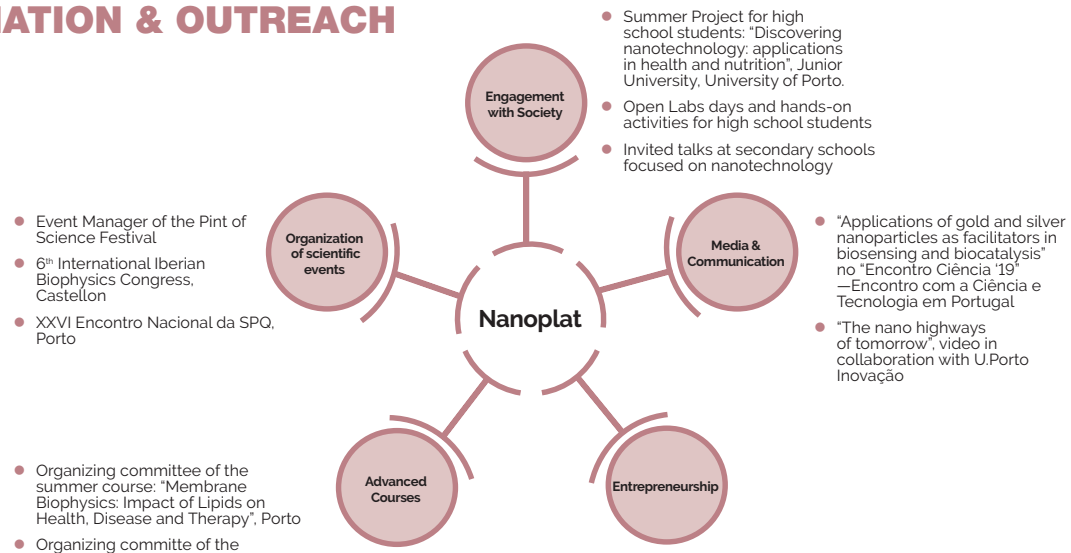
FUNDED PROJECTS *(Representative projects)*

- **MAGNAMED – Novel magnetic nanostructures for medical applications**
  H2020-MSCA-RISE-2016, Cláudia Nunes (local PI)
  Total funding: € 67,500.00
- **Nano2prevent – Nanoparticles to prevent SARS-CoV-2 transmission**
  Funded by the Portuguese Foundation for Science and Technology – FCT under "Research4Covid", nº 427, Salette Reis (PI)
  Total Funding: € 40,000.00
- **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 – FCT (PTDC/BTM-MAT/4738/2020), Ana Cláudia Santos (co-PI),
  Total Funding: € 248,432.29
- **AMAZING: toxinas de serpentes da AMAZónia: INvestiGação na valorização de biorrecursos**
  Funded by the Portuguese Foundation for Science and Technology – FCT CIRCNA/BRB/0281/2019 Paula Gameiro (Co-PI),
  Total Funding:
- **FOODSENS – "Transferência de Tecnologias para reduzir riscos alimentares"**
  INTERREG POCTEP, 0591_FOODSENS_1_E,
  João Santos (participant),
  Total Funding: € 171,890.00
- **Novel therapeutic strategy for osteosarcoma combining polyplexes and polymeric micelles**
  Funded by the Portuguese Foundation for Science and Technology – FCT (PTDC/BTM-MAT/30255/2017),Ana Rita Figueiras (PI),
  Total Funding: € 231,417.37
- **NANOMODE – Gold nanoparticle-based molecular detection of metabolic diseases**
  Funded by the Portuguese Foundation for Science and Technology – FCT (PTDC/NAN-MAT/30589/2017), Eulália Pereira (co-PI)
  Total Funding: € 232,148.66
- **Tailored NanoGumbos: The green key to wound infections chemsensing**
  Funded by the Portuguese Foundation for Science and Technology – FCT (PTDC/QUI_QAN/30163/2017), Lúcia Saraiva (PI)
  Total Funding: € 239,893.12
- **3DS - Administração Transdérmica de Fármacos**
  Funded by the Portuguese Foundation for Science and Technology – FCT (POCI-01-0145-FEDER-030834), Sofia Costa Lima (PI)
  Total Funding: € 237,466.89
- **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
- **Valorização de Moléculas Isoladas de Anfíbios Aquáticos Portugueses**
  Funded by the Portuguese Foundation for Science and Technology – FCT (PTDC/BII-BIO/31158/2017), Paula Gameiro (participant)
  Total Funding: € 180,749.94

INTERNATIONAL COOPERATION AND NETWORKING

- COST Action CA16124, "Brillouin Light Scattering Microspectroscopy for Biological and Biomedical Research and Applications", 2017-2020 (Working Group Leader).
- COST Action CA26205, "European Network on Understanding Gastrointestinal Absorption-related Processes", 2017 -2020 (Management Committee).
- COST Action TD1402, "Multifunctional Nanoparticles for Magnetic Hyperthermia and Indirect Radiation Therapy (RADIOMAG)", 2014-2018, (Management committee, Working Group Leader and Science Communication Manager)
- Cost Action CA18233, "European Network for Innovative Diagnosis and Treatment of Chronic Neutropenias".

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 novel foods and processing technologies, control of allergens, additives, chemical contaminants and adulterants, promoting sustainable foods with enhanced health and sensorial properties. Chromatographic and spectroscopic methods for evaluation of nutrients, bioactive compounds, contaminants and DNA-based methods for species identification and 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 technology 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; and extraction of bioactive compounds from industrial by-products and agricultural wastes for novel technological applications.

RESEARCH OBJECTIVES [2020-2023]

Main research objectives include:

- Search for new sources of food and feed proteins and lipids with increased nutritional properties, higher bioactivity, and safety;
- Deploying innovative technologies and processes to increase the production of sustainable and healthy foods;
- Exploit new food preservation methodologies, namely active and intelligent food packaging and hyperbaric storage to extent shelf-life;
- Develop nutritious and safe processed products;
- Explore the agricultural biodiversity to uncover neglected highly-bioactive varieties;
- Use agricultural wastes and food industry by-products as sources of valuable compounds to be included in novel matrices, providing new sensations of flavors, texture, and health properties, under a circular economy;
- Determine trace levels of food allergens;
- Implement fast and high-throughput DNA-based methods for species/varieties and their respective adulterants traceability in the food chain;
- Assess food contamination from natural toxins, environmental pollutants, agrochemicals, veterinary drugs, packaging materials and formed during processing, and exploit innovative mitigation strategies;
- Estimate the bioaccessibility and intestinal transport *in vitro* of nutrients, bioactives, and contaminants;
- Evaluate new endocrine disruptors on human reproduction;
- Develop human cells based assays for testing the effects of food bioactive/toxic compounds;
- Develop omic strategies to test the effects of food bioactive/toxic compounds in 3D human cell models using advanced data analysis approaches.

The abovementioned research objectives follow the general strategy of establishing the linkages between basic food science and consumers' well-being, and are anchored to work programs of the Horizon 2020 societal challenges SC1, SC2, and SC5. Thus, it will contribute to strengthening the analytical capacity on Food Quality & Technology, to improve the monitoring of food composition, and to find integrated approaches to effectively control the incidence of hazardous compounds and reduce contamination throughout the food chain.

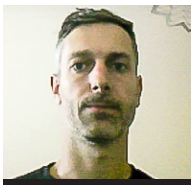
RESEARCH TEAM

SENIOR RESEARCHERS

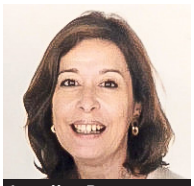

Ana Fernandes

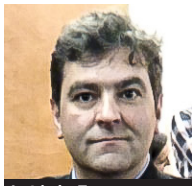

Ana Reis


Ana Rita Cabrita

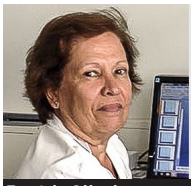

André Pereira

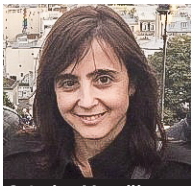

Luís Cruz

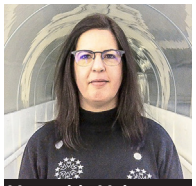

Angelina Pena


António Fonseca

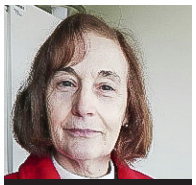

Armindo Melo

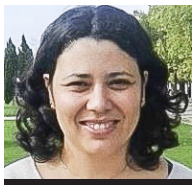

Beatriz Oliveira


Catarina Mansilha


Margarida Maia


Catarina Pereira

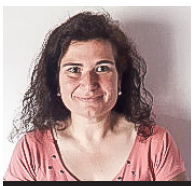

Celeste Lino


Cláudia Passos


Daniel Carvalho

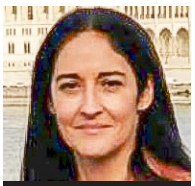

Edgar Pinto


Natércia Teixeira


Elisabete Alexandre


Elisabete Coelho


Elsa Brandão


Fátima Martins


Fernando Ramos


Olívia Pinho


Filipe Coreta-Gomes


Hélder Oliveira

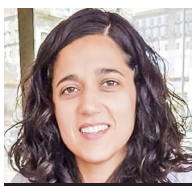

Helena Costa


Hileia Souza


Isabel Ferreira


Sara Cunha


Isabel Mafra


Iva Fernandes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Jorge Barbosa


Susana Soares


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José Fernandes


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RESEARCH TEAM


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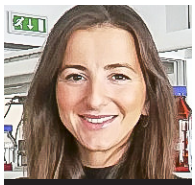
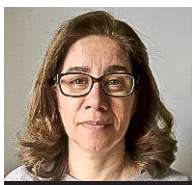
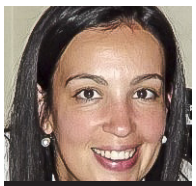

Olga Viegas


Rita Alves


Rosa Perez-Gregorio


Sílvia Rocha


Susana Casal


Tânia Albuquerque


Victor Freitas


Sofia F. Reis

OTHER DOCTORATE RESEARCHERS

Ada Rocha
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Andreia Freitas
Bela Franchini
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Dulcineia Wessel
Idalina Gonçalves
Joana Amaral
João Rocha
João Rosa
Liliana Fidalgo
Luana Fernandes
Lúcia Ferraz
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Nélson Andrade
Pilar Gonçalves
Ricardo Dias
Sara Ferreira
Sofia Duarte
Sonia Losada-Barreiro
Susana Fonseca
Tânia Dias
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POST-DOCTORAL FELLOWS

Bárbara Teixeira
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Carlos Guerreiro
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Joana Fernandes
Joana Lopes
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Liliana Grazina
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Ricardo Duarte
Ricardo Ferreira
Rita Bastos
Sandra Chemane
Sara Pardilhó
Sónia Ferreira
Susana Pinho
Tassadit Benhammouche
Telmo Fernandes
Vânia Gomes
Vasco Lima
Vitor Silva
Zita Avelar

MSc STUDENTS

Adriana Pais
Alan Gomes
Alexandra Borges
Ana Carolina Amaral
Ana Lopes
Ana Pires
Ana Valadão
Andreia Moreira
Bernardo Ferreira
Bruna Gomes
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Carolina Ribeiro
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Diana Pimenta
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João Santos
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Mireia Masoler
Patricia Oliveira
Pedro Nicola
Roberto Chighine
Sara Rocha
Sérgio Viduêdo

RESEARCH GRANTEES

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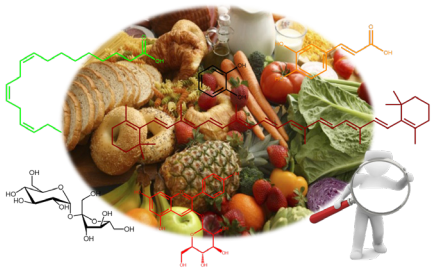
OTHER RESEARCHERS

Anabela Costa
Dulce Teixeira
Eulália Mendes
Margarida Martins
Marisa Castro
Sílvia Dias
Zélia Azevedo

RESEARCH THEMES/
FOOD COMPOSITION, SENSORY PROPERTIES, AND FOOD AUTHENTICITY

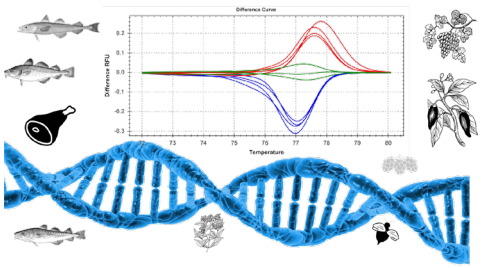
FOOD COMPOSITION AND SENSORY PROPERTIES



- Chemical characterization of food components for selection of new or enhanced food plant varieties and for general quality assessment (*e.g.* coffee, grapes, olive oil, strawberries, pomegranate, licuri, moringa, milk);
- Launch of a relationship between food composition and quality parameters, such as aroma, colour, and flavour (astringency and bitterness);
- Evaluation of nutritional composition and quality features of agricultural products and foodstuffs registered with EU quality schemes (PDO, PGI, and TSG).
- Chemical characterization of food components for selection of new or enhanced food plant varieties and for general quality assessment.
- Screening of new compounds toward modulation of quality parameters.
- Application of dynamic sensory analysis and consumer preferences to understand market trends & consumer choices

GENETICALLY MODIFIED ORGANISMS, FOOD AUTHENTICITY, AND FRAUD FIGHT

- Advanced methods to detect genetically modified organisms in foods;
- Authentication of foods from animal and plant origin based on molecular makers;
- 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 for species identification in foods, herbal medicines, and plant food supplements;
- Botanical and entomological authentication of honey.



SELECTED PUBLICATIONS

1 S. Petronilho, et al., Molecules 2020, 25, 272. doi:10.1016/j.carbpol.2019.115525

2 V. Gomes, et al., Synlett 2020, 31 (04), 334. doi: 10.1055/s-0039-1690744

3 S. Boukandoul, et al., J. Food Process. Preserv. 2020, 44(9), e14693. doi:10.1111/jfpp.14693

4 L. Cruz, et al., Dyes Pigm. 2020, 181, 108592. doi: 10.1016/j.dyepig.2020.108592

5 V. Belchior, et al., Food Anal. Methods. 2020, 13(1), 275-283. doi:10.1007/s12161-019-01619-z

6 A. Pinto, et al., Solar Energy 2020, 206, 188. doi: 10.1016/j.solener.2020.05.101

7 H. Souza, et al., ACS Sustain. Chem. Eng. 2020, 8 (43), 16184. doi: 10.1021/acssuschemeng.0c04839

8 A. Fernandes, et al., Food Hydrocoll. 2020, 102, 105625. doi: 10.1016/j.foodhyd.2019.105625

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13 R. Pérez-Gregorio et al., Molecules. 2020, 25 (15), 3443. doi: 10.3390/molecules25153443

15 J. Azevedo, et al., Foods. 2020, 9 (12), 1867. doi: 10.3390/foods9121867

16 A. Reis et al., Critical Reviews in Food Science and Nutrition, 2020, pp. 1–24. doi:10.1080/10408398.2018.1503155

17 A. Reis et al., Food Chem, 2020, 333, 127509. doi: 10.1016/j.foodchem.2020.127509

18 Z Martins, et al., J. Chemometrics. 2020, 34(9), e3285. doi.org/10.1002/cem.3285;

19 N. Rodrigues, et al., Food Res, Int. 2020, 128, 108759. doi.org/10.1016/j.foodres.2019.108759

20 J. Machado, et al., J Agric. Food. Chem. 2020, 68(7), pp. 2155–2163. doi.org/10.1021/acs.jafc.9b06139

21 C. Martins, et al., Foods, 2020, 9, 1276, 1-22. doi:10.3390/foods9091276

RESEARCH THEMES/
IMPROVEMENT OF ANIMAL FEEDING AND NUTRITION

- Evaluation and valorisation of underexploited feeds towards increased sustainability of livestock and pet sectors, and improved circular economy;
- Modulation of feeding strategies to increase animals' nutrient efficiency use, health, welfare and safety;
- Understanding rumen function to improve ruminant nutrition and production;
- Identification of new biomarkers of the rumen function in non-invasive biological samples (e.g. urine, faeces, milk) to identify metabolic dysbiosis in dairy cows prior to clinical symptoms;
- Mitigation of ruminant methane emissions and nitrogen excretion.

22 G. Albuquerque, et al., Nutr. Food Sci.. 2020, 8(10), 5309-5320. **doi.org/10.1002/fsn3.1753**

23 R.N. Pereira, et al., Food Funct. 2020, 11: 4002-4013. **doi.org/10.1039/C9FO02834J**

24 S. S. Ferreira et al., Food Res. Int. 2020, 132, 109055. **doi:10.1016/j.foodres.2020.109055**

25 A.M. Pereira, et al., FEMS Micro. 2020, 10, 3, 400. **doi: 10.1093/femsle/fnaa085**

26 A.R.F. Rodrigues, et al., PeerJ 2020, 8:e9488. **doi: 10.7717/peerj.9488**

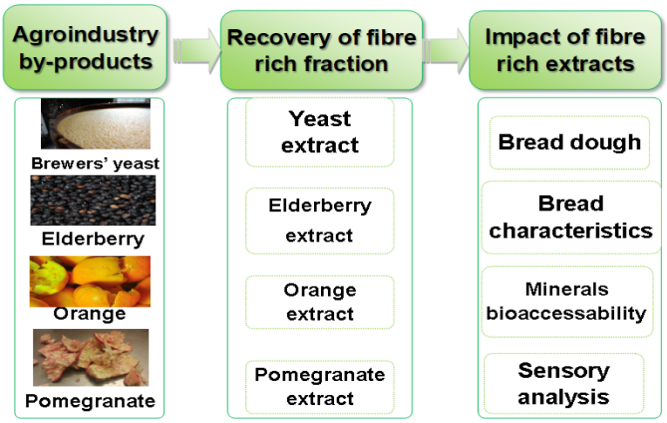
27 R.S. Inácio, et al., Sci. Food Agric. 2020, 1-6. **doi.org/10.1002/jsfa.11023**

28 A.C. Ribeiro, et al., Foods. 2020, 9 (8), 1133. **doi.org/10.3390/foods9081133**

29 L. Fernandes, et al., Food Res. Int. 2020, 132, 109070. **doi.org/10.1016/j.foodres.2020.109070**

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, potato fried chips and 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 agro-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.



SELECTED PUBLICATIONS

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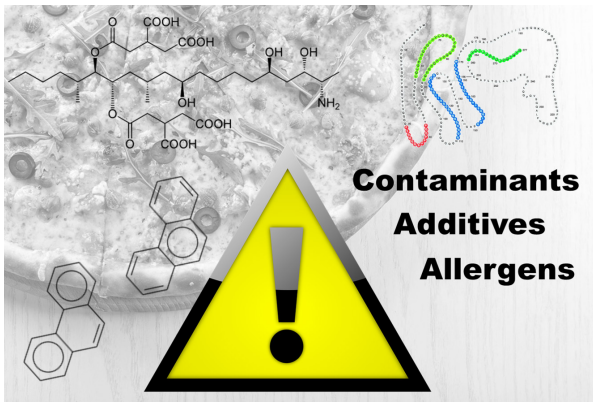
RESEARCH THEMES/ FOOD AND HEALTH

ALLERGENS, ADDITIVES, AND CONTAMINANTS

- Assessment of food allergens from plant and animal origin at trace levels by DNA markers and immunochemical approaches;
- Assessment of the allergenicity of foods as affected by food processing and food matrix; find new strategies that reduce allergenicity
- 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) and mycotoxins;
  - "emerging pollutants", such as flame retardants, disinfection by-products, pharmaceuticals, personal care products and biosolids as fertilizers;
  - packaging materials (*e.g.* bisphenols);
  - heat generated compounds (*e.g.* acrylamide, 4-methylimidazole, furans, heterocyclic aromatic amines) in foods or water.
- Estimate contaminants bioaccessibility and intestinal transport *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) 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.

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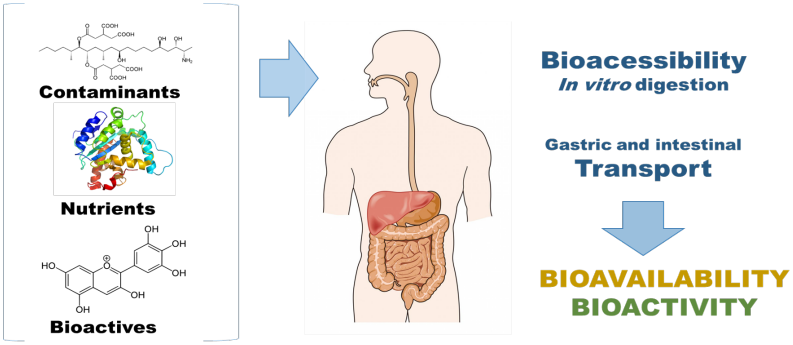
RESEARCH THEMES/ FOOD AND HEALTH

BIOAVAILABILITY AND FUNCTIONAL MECHANISMS

- Digestion, bioavailability, 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 activity; hypocholesterolemic ingredients);
- 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;
- 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 microbiota-polyphenol interactions and health;
- Synthesis of bluish flavylium and pyranoflavylium compounds towards topical photodynamic therapy (PDT).



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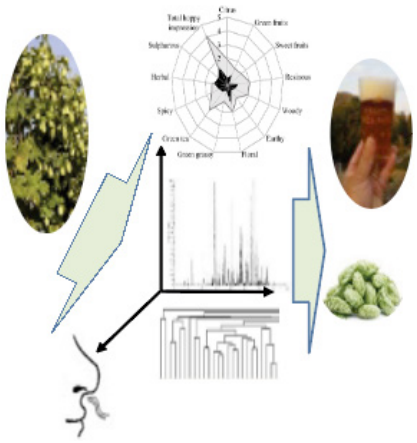
HIGHLIGHTS

UNEXPLORED PORTUGUESE WILD HOPS PROVIDE NEW FLAVORS TO BEER

Modern beer industry reclaims new hop varieties following the worldwide demand for beer flavor diversity. Unexplored wild hop genotypes are an interesting alternative, but surveys from wild populations or breeding are time consuming and dispendious to evaluate hop characteristics and impact on beer.
Sensory and Olfactometry Chemometrics provide an innovative approach to predict the spiciness and fruitiness that Portuguese wild hops impart to beer and establish comparisons with commercial hops.



A chemometric approach to compare Portuguese native hops with worldwide commercial varieties.

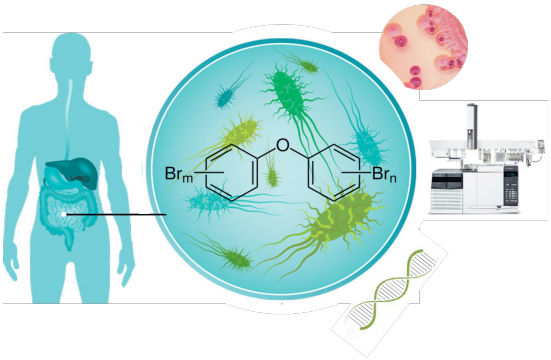
Journal of Chemometrics. 2020;34:e3285

Sensory and Olfactometry Chemometrics as Valuable Tools for Assessing Hops' Aroma Impact on Dry-Hopped Beers: A Study with Wild Portuguese Genotypes.

Foods 2020, 10, 6,1397.

PIONEER STUDY EVALUATES THE EFFECT OF PLASTIC ADDITIVES ON GUT MICROBIOTA

Brominated flame retardants are plastic additives with recognized endocrine disruptors activity, which are often found in food, thus leading to numerous health issues.
This pioneering study showed significant changes in both volatolome and microbiome structure in a time and dose-dependent manner. It revealed noteworthy modifications in the human gut microbiome with serious health implications even at oral exposure doses considered as safe by worldwide regulatory entities.



Multidisciplinary approach to determine the effect of polybrominated diphenyl ethers on gut microbiota.

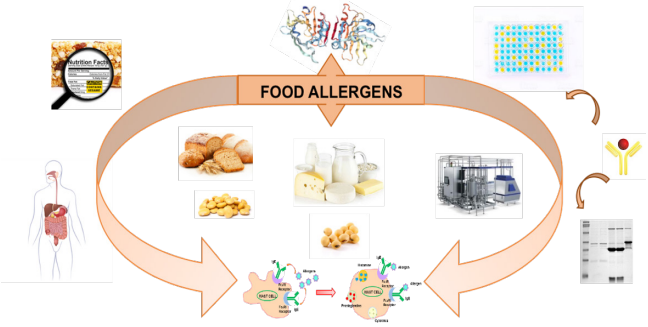
Environmental Pollution, 2020, 260, 113920

HIGHLIGHTS

TOWARDS ALLERGEN RISK ASSESSMENT OF FOODS

The allergenic potential of foods is affected by processing and matrix, understanding and predicting food allergenicity is a hot topic nowadays.

The immunoreactivity of lupine and soybean proteins was reduced by thermal treatment. Ohmic heating showed potential at reducing the allergenic potential of ß-lactoglobulin. Additionally, a novel real-time PCR targeting the 12S rRNA gene was proposed to detect milk ingredients.



Immunoreactivity of lupine and soybean allergens in foods as affected by thermal processing.

Foods, 2020, 9, 254

Effects of ohmic heating on the immunoreactivity of ß-lactoglobulin – a relationship towards structural aspects.

Food & Function, 2020, 11, 4002-4013

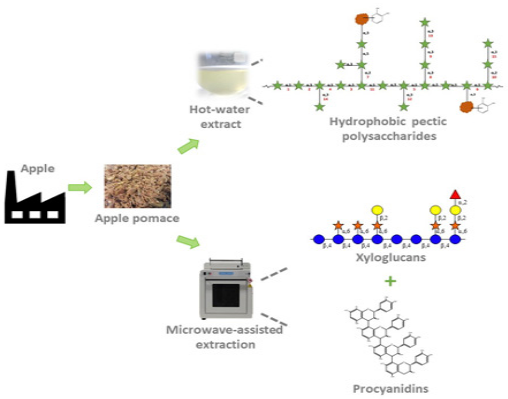
Cow's milk allergens: Screening gene markers for the detection of milk ingredients in complex meat products.

Food Control, 2020, 108, 106823

VALUATION OF FRUIT BY-PRODUCTS: NEW INSIGHTS ON FRUIT WASTES POLYSACCHARIDES

The increasing environmental concerns have led industries to revisit their main by-products aiming to find new applications and implement a circular economy model.

Besides the hydrophilic pectic polysaccharides, apple pomace contains water soluble hydrophobic polysaccharides, some behaving hydrophobically at neutral pH, others in acidic conditions. Despite pectic polysaccharide charge have a relevant role, this feature is mostly attributed to phenolic compounds attached to the arabinans, constituent of pectic polysaccharides. Microwave-assisted extraction has also shown that xyloglucans might also possess linked phenolic compounds, mostly oxidized derivatives. All these polysaccharides, co-extracted with phenolic compounds and their oxidized derivatives can be used as coloring and antioxidant ingredients to promote a circular economy.



Revisiting the chemistry of apple pomace polyphenols.

Food Chemistry, 2019, 294, 9-18

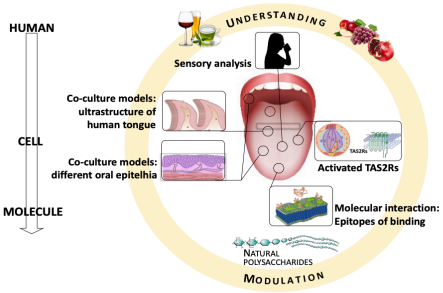
The hydrophobic polysaccharides of apple pomace.

Carbohydrate Polymers, 2019, 223, 115132

HIGHLIGHTS

PLANT-BASED BIOACTIVE COMPOUNDS AND TASTE PROPERTIES: LINKING HEALTHY AND TASTY COMPOUNDS

Plant-based products are highly related to health benefits and well-being, in particular the ones rich in polyphenols. However, these compounds can induce unpleasant taste properties, namely astringency and bitterness, which can impair consumer intake. New models including salivary proteins, oral mucosal pellicle, oral cells, and bitter taste receptors have been developed to study the molecular onset of these taste properties directly in food matrices. This knowledge has been applied both for unravelling the molecular onset of these properties as well as to for the screening of compounds isolated from food matrices or food byproducts to find new compounds to modulate these properties toward consumer acceptance. This research-line aims an integrative and comprehensive approach covering from sensory assays to cell-based and molecular assays.
The effect of pectic polysaccharides from grape skins on salivary protein – procyanidin interactions.

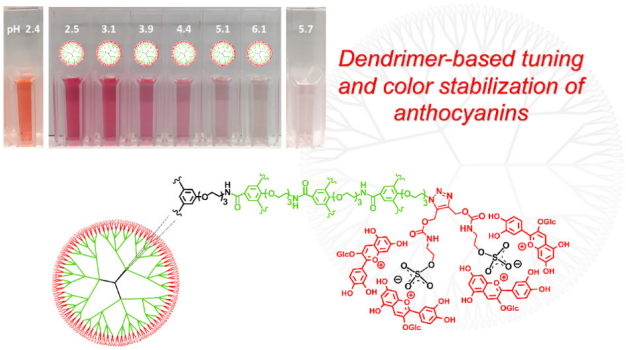


The effect of pectic polysaccharides from grape skins on salivary protein – procyanidin interactions.

Scientific Reports, 2020, 10, 12638

IMPACT OF A WATER-SOLUBLE GALLIC ACID-BASED DENDRIMER ON THE COLOR-STABILIZING MECHANISMS OF ANTHOCYANINS

A high red color intensification and stabilization was obtained for cyanidin-3-glucoside at a wide pH range as a result of the strong interaction with a polyanionic gallic acid-based dendrimer through the formation of ionic pairs. The interaction parameters ($K \sim 700\ M^{-1}$, $n \sim 295$) indicated the binding of approximately two anthocyanin molecules by each peripheral sulfate group of the dendrimer.



Impact of a Water-Soluble Gallic Acid-Based Dendrimer on the Color-Stabilizing Mechanisms of Anthocyanins.

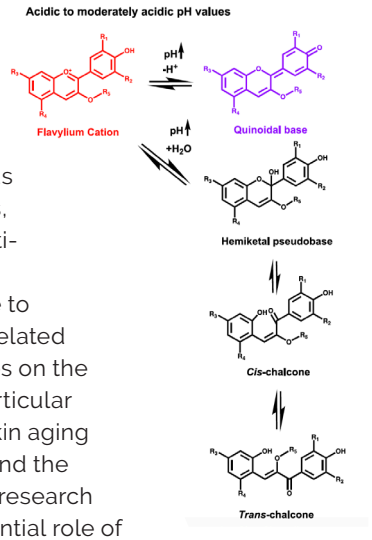
Chemistry – A European Journal, 2019, 25, 11696-11706

HIGHLIGHTS

ANTHOCYANINS AS PHOTOPROTECTIVES AGENTS IN DIFFERENT BIOLOGICAL SYSTEMS

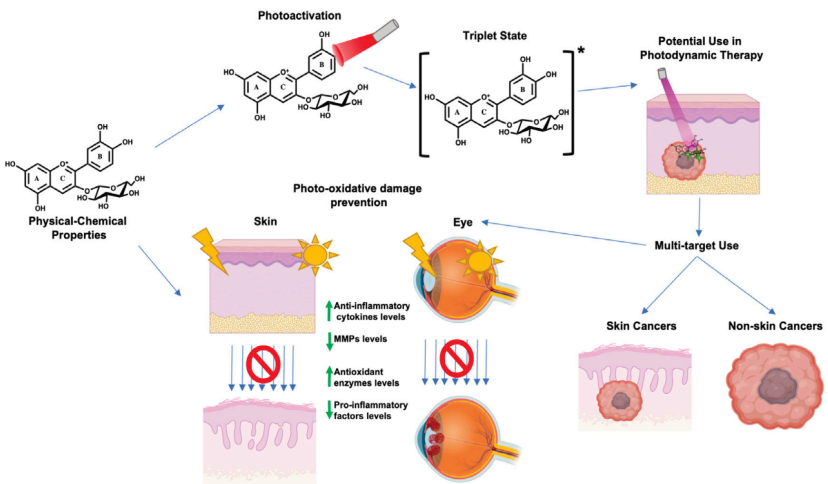
Due to their physical and chemical characteristics, anthocyanins are amongst the most versatile groups of natural compounds. Such unique signature makes these compounds a focus in several dierent areas of research. Anthocyanins have well been reported as bioactive compounds in a myriad of health disorders 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.

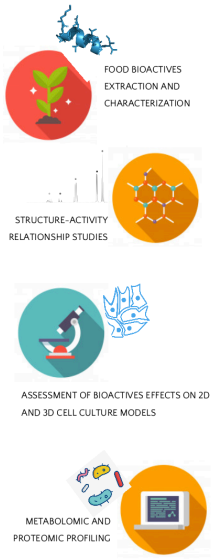
International Journal of Molecular Sciences, 2020, 21, 7464



HIGHLIGHTS

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

CAFFEINE-ENRICHED CAPSULES USING COFFEE SILVERSKIN EXTRACTS: THE U2SCOFFEE PROJECT

Silverskin is the main by-product of the coffee roasting industry. Unitary doses for espresso coffee preparation enriched with silverskin extracts (containing controlled doses of caffeine, and other bioactive compounds) are being developed in collaboration with the coffee industry, in order to answer to specific market needs. The new product will be produced through a green and sustainable ultrasound technology, (avoiding the use of organic solvents), reusing and valuing a waste based on the principles of circular economy (POCI-01-0247-FEDER-033351).

COMPETE 2020 PORTUGAL 2020 UNIÃO EUROPEIA Fundo Europeu de Desenvolvimento Regional

Coffea canephora silverskin from different geographical origins: A comparative study.

Science of the Total Environment, 2018, 645, 1021–1028

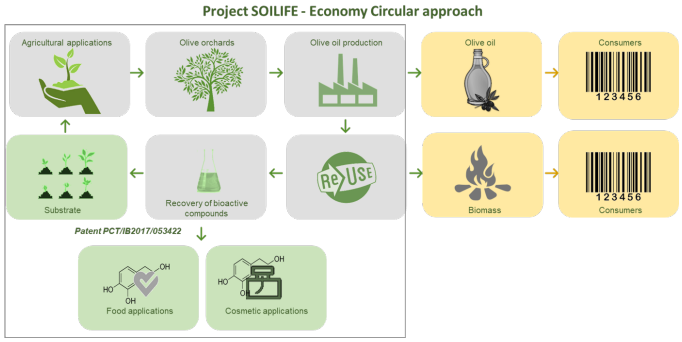
A study on the protein fraction of coffee silverskin: Protein/non-protein nitrogen and free and total amino acid profiles.

Food Chemistry, 2020, 326, 126940

HIGHLIGHTS

SOILIFE – A SUSTAINABLE OLIVE POMACE PROCESSING INTENDING THE PRODUCTION OF A SUBSTRATE FOR AGRICULTURAL APPLICATIONS AND THE RECOVERY OF BIOACTIVE COMPOUNDS FOR FOOD AND COSMETIC APPLICATIONS

Over the last years, olive oil production increased significantly. Along with the growth of this agro-industry sector, high rates of residues as olive pomace are produced. Olive pomace has high phytotoxicity causing environmental problems if discarded without any previous treatment. Usually, olive mills transfer and discharge olive pomace in large open-air containers where it is kept stored through long periods until it is further transformed into olive pomace oil and the correspondingly remaining solid residue – extracted olive pomace.



Patent PCT/IB2017/053422.

Oliveira, M.B.P.P., Costa, A.S.G., Nunes, M.A., and Pimentel, F.B., Olive pomace products, method of production and their uses (2017).

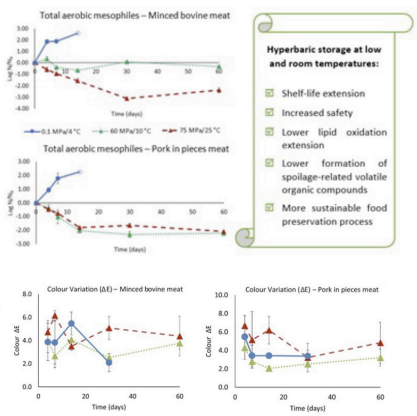
SOILIFE is an eco-friendly process that converts extracted olive pomace, the above-mentioned phytotoxic by-product of olive oil production, into an ecological product. By using this patented simple, low-cost, and clean methodology, it is possible to obtain a substrate for soilless agriculture with reduced phytotoxicity and recover bioactive compounds with high commercial/market value.

QUALITY IMPROVEMENT OF RAW BOVINE AND PORK MEAT WITH EXTENDED SHELF-LIFE USING HYPERBARIC STORAGE AT LOW TEMPERATURE

Hyperbaric storage at low temperature (HS/LT, 60 MPa/10 ˚C) was efficient to slowdown microbial growth, with additional inactivation after 30 days, which resulted in a shelf-life extension and enhanced microbial safety of both meats compared to refrigeration (RF).

Moreover, HS/LT resulted in lower lipid oxidation degrees, when compared to RF and avoided the formation of volatile organic compounds related to meat-spoilage. General quality parameters as color were also well maintained by HS.

HS represents a promising more sustainable methodology for fresh meat preservation, increasing meat shelf-life with good quality for at least 30 days, compared to 7 days for RF.



Quality Evolution of Raw Meat under Hyperbaric Storage– Fatty Acids, Volatile Organic Compounds and Lipid Oxidation Profiles.

Food Bioscience, 2020, 42, 101108

HIGHLIGHTS

SELENIUM AND ZINC DOG FOODS SUPPLEMENTS

The influence of sources of supplemental selenium and zinc (organic vs inorganic) for dog foods was evaluated in vivo with Beagle puppies and young adults, respectively. Organic selenium (enriched Saccharomyces cerevisiae) was associated with a higher faecal concentration of total volatile fatty acids, propionate, and butyrate, a higher number of DNA copies of Lactobacillus, and a trend to lower DNA copies of Escherichia coli. Results suggests benefits of organic selenium over inorganic (sodium selenite) due to the positive modulation of the gut microbiome observed in puppies. Feeding young adult Beagle dogs with organic zinc (proteinate) improved the bioavailability of phosphorus and immune function comparatively to inorganic zinc (sulfate). Overall, results show that mineral source should be considered to define strategies to support the nutritional needs and improve the value of pet foods.

Effect of zinc source and exogenous enzymes supplementation on zinc status in dogs fed high phytate diets.

Animals, 2020, 10 (3): 400

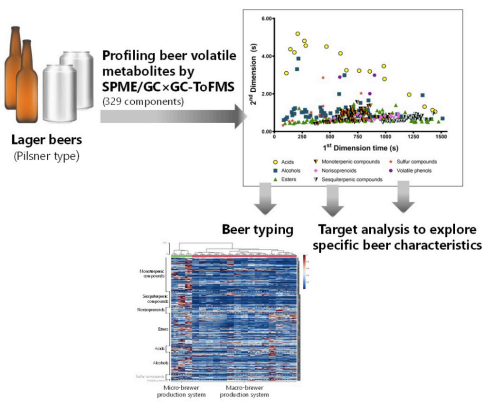
Supplemental selenium source on gut health: Insights on fecal microbiome and fermentation products of growing puppies.

FEMS Microbiology Ecology, 2020., fiaa212

ENLARGING KNOWLEDGE ON LAGER BEER VOLATILE METABOLITES: THE ROLE OF THE PRODUCTION SYSTEM

A comprehensive study of lager beer volatile composition was provided by profiling 329 metabolites. Clustering analysis allowed a beer typing according to production system: macro- and microbrewer beers. Monoterpenic and sesquiterpenic compounds were the chemical families that showed wide range of chemical structures, which may contribute for beers' peculiar aroma characteristics.

This study presents the most in-depth volatile profiling of lager beer, which knowledge can be further applied and exploited to obtain relevant information in various contexts, such as beer quality control, monitoring brewing steps, raw materials composition, among others.

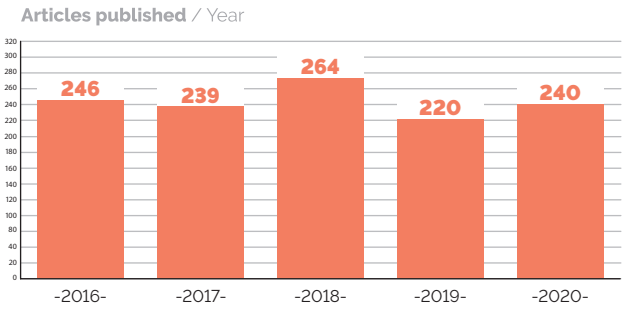


Enlarging knowledge on lager beer volatile metabolites using multidimensional gas chromatography.

Foods, 2020, 9, 1276, 1-22.

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION



H-index: **100**

1209 articles*
71245 citations

*2016-2020
From WOS core collection

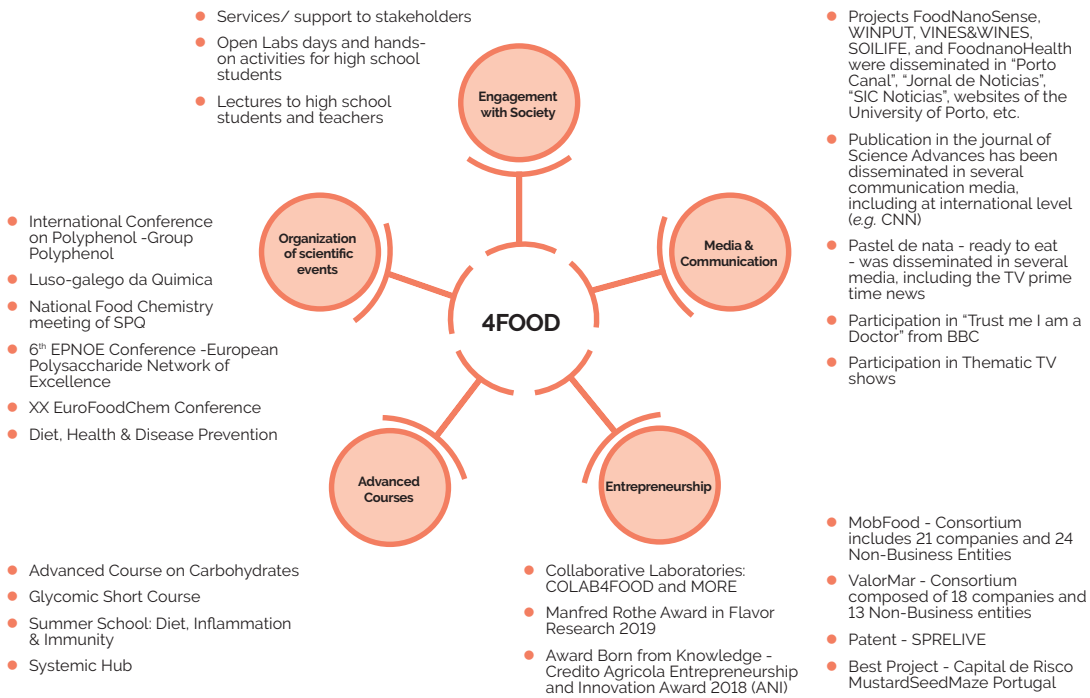
FUNDED PROJECTS *(Representative projects)*

- SEAFOODTOMORROW
  Horizon 2020, GA 773400, Sara Cunha (local PI)
  Funding: € 209,325.00. Total funding: € 7,520,196.91
- DIETimpact – Diet impact on the prevention of chronic diseases: a foodohmics approach
  PTDC/SAU-NUT/30322-2017, Isabel Ferreira (PI)
  Total funding: € 239.839,53
- AlleRiskAssess – Towards allergen risk assessment of foods: structural and immunogenic changes induced by novel processing technologies and alternative protein sources
  PTDC/BAA-AGR/31720/2017, Isabel Mafra (PI)
  Total funding: € 239.374,46
- MOR2020 – Valorization of the protein fraction from Moringa oleifera
  PTDC/OCE-ETA/32567/2017, Miguel Faria
  Total funding: € 239.421,21
- EDCs-Seafood
  POCI-01-0145-FEDER-028708, Sara Cunha
  Funding: € 230.268,13
- US2Coffee - Cápsulas de cafeína
  FEDER (POCI/01/0247/FEDER/033351),
  Beatriz Oliveira (PI - FFUP), Rita Alves (PI - ICETA)
  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
- WINPUT – Wine-inspired synthesis of blue pyranoflavyliums for topical Photodynamic Therapy
  Funded by Portuguese Foundation for Science and Technology – FCT (PTDC/QUI-OUT/29013/2017). Joana Oliveira (PI).
  Total funding: € 219,806.53
- NUTRALLERPHEN – Dietary polyphenols as prophylactic agents in food allergies
  Funded by Portuguese Foundation for Science and Technology – FCT (PTDC/SAU-NUT/30448/2017). Maria Gregório (PI).
  Total funding: € 232,891.63
- POLY4CD - Natural Polyphenol´s Role in Prevention of Celiac Disease
  Funded by Portuguese Foundation for Science and Technology – FCT (PTDC/OCE-ETA/32287/2017). Victor Freitas (PI).
  Total funding: € 229,354.66
- FoodSmarTag – Novel Anthocyanin-Based Smart Sensors for Food Packaging
  Funded by Portuguese Foundation for Science and Technology – FCT (PTDC/OCE-ETA/31250/2017). Luís Cruz (PI).
  Total funding: € 228,235.90
- Polyphenols in Art- chemistry and biology hand in hand with conservation of cultural heritage"
  Funded by Portuguese Foundation for Science and Technology – FCT (PTDC/QUI-OUT/29925/2017).
  Total Funding: € 239,061.88
- Development of a dry yeast protein extracts for white and red wine finning"
  Funded by Agency National for Research (ANI) FCOMP 017687 - Project in collaboration with Proenol – Industria Biotecnológica, S.A.
- CorkPlus – Chemical contribution of cork stoppers for the chemical composition and sensorial properties of wines
  Funded by Agency National for Research (ANI) QREN/I & DT / 2016 - Project in collaboration with AMORIM & IRMÃOS, S.A.
- 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 €

INTERNATIONAL COOPERATION AND NETWORKING

- COST Action FA1402, "ImpARAS: Improving Allergy Risk Assessment Strategy for New Food Proteins", 2014-2018
- INFOGEST - international network gathers more than 380 research scientists from 40 countries.
- COST Action CA18227, "COMFA - The Core Outcome Measures for Food Allergy", 2019-2023
- COST Action CA18127, "International Nucleome Consortium", 2019-2023
- COST Action CA18111, "PlantEd – Genome editing in plants - a technology with transformative potential", 2019-2023
- COST Action CA18101, "SOURDOMICS - SOURDOugh biotechnology network towards novel, healthier and sustainable food and bloproCesseS", 2019-2023
- 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)

DISSEMINATION & OUTREACH




LABORATÓRIO ASSOCIADO
PARA A QUÍMICA VERDE

Computing

HIGH PERFORMANCE COMPUTING IN MOLECULAR MODELLING

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

Group Coordinator:

Maria João Ramos

The High Performance Computing in Molecular Modelling uses high-performance supercomputing to simulate chemical and biochemical systems of great interest with atomic and sub-atomic detail. These systems encompass proteins, enzymes, DNA, RNA, biomembranes, and small biomolecules (such as medicinal drugs), all in an aqueous physiologic environment. We are also devoted to the computational study of novel functional materials. Our main goal is to provide a better understanding of how their physicochemical properties can be fine-tuned to specific applications. The association between new materials (nanotubes, graphene) with biomolecules is also an area we work on.

We study reaction mechanisms for heterogeneous and homogeneous catalysed reactions, using both enzymes and novel catalytic materials. Our endeavour also encompasses studying the formation of nanostructured materials. These include molecularly imprinted and grafted polymers, carbon-based materials, deep eutectic solvents, ionic liquids, and self-assembled monolayers. Our studies provide valuable insights for targeting the application of these materials in different fields. These include catalysis, sensors, drug-delivery systems and biomedical devices. We also develop appropriate quantitative structure-activity relationship models, for accessing the biological activity and potential toxicity of these materials. Studies of protein structure, protein:protein interactions, and structure-based drug discovery are also an important focus of our research.

The molecular simulations and molecular modelling we perform are mostly based on the rigorous principles of physics (both classical and quantum mechanics), allowing us to simulate, understand, and predict the behaviour of (bio)chemical systems with accuracy and reliability. The simulations methods we use the most are molecular dynamics - in the purely classic and hybrid quantum mechanics/molecular mechanics flavours - and electronic structure calculations. We also perform molecular docking/virtual screening and homology modelling calculations. Additionally, we also use purely mathematical models to derive Quantitative Structure-Activity Relationships.

RESEARCH OBJECTIVES [2020-2023]

One of the main objective of the High Performance Computing in Molecular Modelling is to understand the chemical machinery of living systems. Within this vast chemical universe, our major objectives 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, production of biofuels or plastic recycling), (iii) to understand and predict the small-molecule drug diffusion process across cell membranes, to increase the success rate in drug delivery, (iv) to discover small-molecule competitive inhibitors of therapeutic enzymes to be developed into new drugs towards unmet clinical needs, and to (v) to construct supramolecular biosystems coupling engineered enzymes to new-material solid surfaces that can replace industrial catalysts for more efficient and greener alternatives.

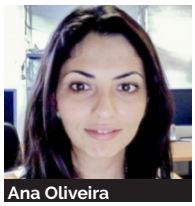
Our group also focus on the rational design of advanced novel functional materials within the green chemistry paradigm. These materials will thus be optimised towards a high performance during their application and an easy degradability in further stages of their life cycle. Our theoretical survey should then enable a whole life cycle assessment for these materials. For this purpose, these macromolecular systems will be modelled according to two different approaches: On the one hand, the insights provided by our work will bring a deeper understanding of the structure and properties of these materials at a molecular level. We will use Density Functional Theory (DFT) methods to study catalytic reaction mechanisms and molecular simulations to provide crucial information on structural organisation and dynamics of complex systems at a microscopic level. These studies will contribute to design new effective solutions for frontier fields and to identify the waste produced during the life cycle of these materials. On the other hand, we will use Quantitative Structure-Activity Relationship (QSAR) and Machine Learning (ML) models for accessing the potential ecotoxicity of both original materials and waste products.

RESEARCH TEAM

SENIOR RESEARCHERS


Alexandre Magalhães


Ana Moura


Ana Oliveira


André Melo


Daniel Santos


Elisabete Ferreira


Filipe Teixeira


Iulia Voroshylova


João Coimbra


J. Luís Fajin


Krzysztof Biernacki

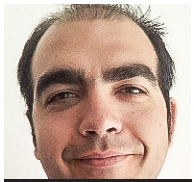

Maria João Ramos

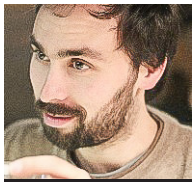

Michael Durruthy


Natália Cordeiro


Natércia Brás


Pedro Fernandes


Riccardo Concu


Rui Neves

 Group coordinator

RESEARCH TEAM

OTHER DOCTORATE RESEARCHERS
Ana Silva
Elizabeth Vieira

POST-DOCTORAL FELLOWS
Amit Kumar Halder
Ivan Veloso

PhD STUDENTS
João Sousa
Matilde Viegas
Nádia Figueiredo
Pedro Paiva
Pedro Ferreira

MSc STUDENTS
Bruno Oliveira
Edgar Santos
Filipa Miranda
José Lopes
Juliana Amorim
Mariana Contreiras

RESEARCH GRANTEES
Alexandre Pinto
José Caetano

OTHER RESEARCHERS
Óscar Passos

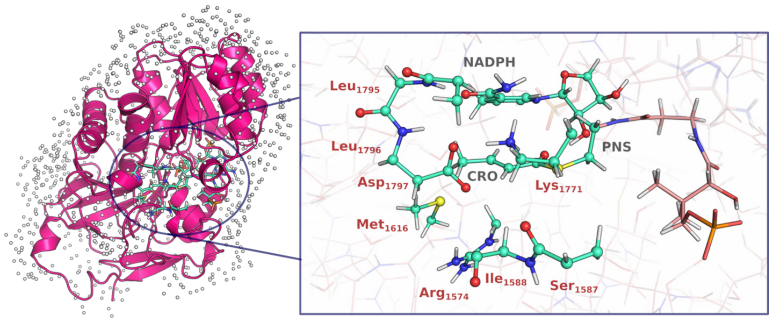
RESEARCH THEMES/ ENZYMES

ENZYME CATALYTIC MECHANISMS

Enzymes are the most perfect catalysers ever created. They combine very high reaction rates with insuperable chemo- and stereoselectivity. They act at room temperature, use water as a solvent, and are fully biodegradable. Unsurprisingly, the way they achieve this amazing feat is still poorly understood and we try to shed light on this issue.

We perform high level calculations using hybrid quantum mechanics/molecular mechanics methods to represent the enzymatic systems and test every reaction mechanism that is plausible, by calculating the structure and free energy of the reactants, transition states, intermediates, and products of the tested reaction pathways.

We identify the correct mechanism through the most favourable kinetic profile (besides the reproduction of all available experimental information). Clarifying the mechanism of an enzyme does not only enlighten a prodigy of catalytic chemistry developed during millions of years of natural evolution but also provides the perfect templates for transition-state-analogue drug discovery towards the studied enzyme.



The enoylreductase domain of the mammalian fatty acid synthase enzyme, simulated with hybrid quantum mechanics/molecular mechanics methods. Most of the enzyme (purple ribbons) and water (white spheres) are represented at the molecular mechanics level. The quantum mechanics region encompasses the active site and substrate and is represented atomistically in the RHS of the figure.

SELECTED PUBLICATIONS

1 P. Ferreira, et al., ACS Catal. 2020, 10, 9276. **doi:10.1021/acscatal.0c02627**

2 M. Prejanò, et al., ACS Catal. 2020, 10, 2872. **doi:10.1002/chem.201901763**

3 M. Prejanò, et al., ACS Catal. 2020, 10, 5372. **doi:10.1021/acscatal.0c01697**

4 S. F. Sousa, et al., ACS Catal. 2020, 10, 8444. **doi:10.1021/acscatal.0c01947**

7 M. Prejanò, et al., ChemPhysChem 2020, 20, 2881. **doi:10.1002/cphc.201900650**

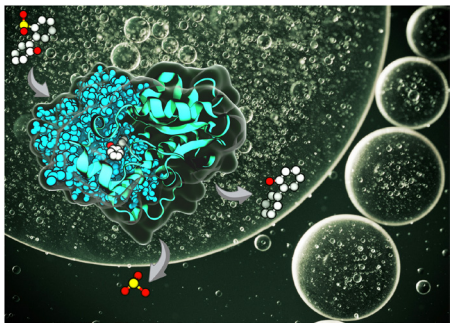
8 P. Paiva, et al., ChemCatChem 2020, 11, 3853. **doi:10.1002/cctc.201900548**

RESEARCH THEMES/ ENZYMES

ENZYME REACTIVITY AND ENGINEERING

We want to understand the physical origin of the extraordinary reaction rate of enzymes so that we can rationally engineer them for the purposes we need. For that, we study in detail the electrostatic interactions the enzyme scaffold does with the reactant state and the transition state and try to understand exactly how the enzyme can lower the free energy barrier of the transition state. The role of specific long-range interactions and of the enzyme conformational diversity have been a subject of particular attention in our studies. We have devised strategies for rational enzyme engineering that take advantage of the computational insights we gain with the simulations. A concrete example we are working on is the biodesulphurization of crude oil.

We are engineering a whole metabolic pathway of the bacterium Rhodococcus erythropolis so that it can remove sulphur from recalcitrant compounds in a much greener way than chemical methods actually do. The purpose is to accelerate the bacteria sulphur-removing pathway to a point that it becomes attractive and competitive with current, highly polluting chemical methods within oil refining facilities. The first set of computationally rate-enhancing mutations are now at the stage of experimental testing and validation.



The enzyme DszB, seen at the centre of the figure, is one of the four enzymes that constitute the "4S pathway", a metabolic pathway of the bacterium Rhodococcus erythropolis that is able to remove sulphur from the most recalcitrant organosulphur compounds of the diesel fraction of crude oil. The bacterium is stable is small water droplets within crude oil and captures the organosulphur compounds at the water-oil interface. Removing these compounds with harsh chemical methods is very polluting, albeit mandatory due to the acid rains that burning organosulphur compounds causes.

SELECTED PUBLICATIONS

9 J. P. M. Sousa, et al., Green Chemistry, 2020, 22, 7604. **doi:10.1039/D0GC02055A**

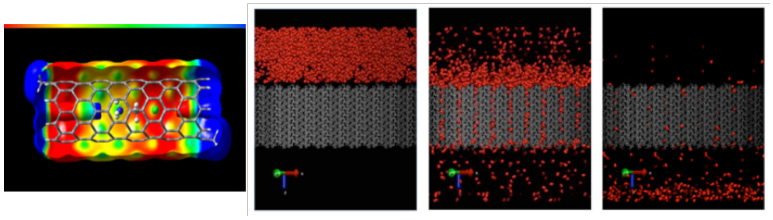
10 J. P. M. Sousa, et al., ACS Catal. 2020, 10, 9545. **doi:10.1021/acscatal.0c03122**

11 P. Paiva, et al., J. Comput. Chem., 2020, 41, 2459. **doi:10.1002/jcc.26188**

RESEARCH THEMES/
MODELLING CHEMICAL SPECIES AND NANOSTRUCTURED MATERIALS

MODELLING CHEMICAL SPECIES UNDER CONFINEMENT

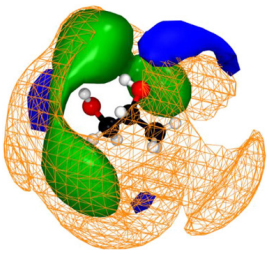
Chemical species under spatial and chemical confinement may show dramatic changes in their physical and chemical properties when compared to gas phase conditions. A large variety of computational methods are employed to study single molecules, simple chemical reactions, metal complexes or small aggregates trapped into a wide range of surrounding media, with special emphasis on zeolites, porous dipeptide crystals, and carbon nanotubes. The theoretical approach is meant to get enhanced features at the molecular level in important areas such as catalysis, bioinorganic chemistry, gas storage, and nanotechnology.[23,24]



Left: Reaction Mechanism of the S_N2 reaction between ammonia and chloromethane inside a pristine carbon nanotube. Right: Simulation of the diffusion of O_2 molecules through nanopores of LS-dipeptide crystals.

ATOMISTIC MOLECULAR SIMULATIONS OF NEOTERIC SOLVENTS

Nowadays, one of the most demanding societal challenges is to conciliate the industrial development with the environment. The selection of appropriate solvents for industrial processes is of special importance, because they usually generate an enormous amount of toxic wastes. The neoteric solvents are usually a more sustainable alternative to conventional ones, due to their specific properties. These include low volatility, non-flammability and low toxicity. However, the low biodegradability of some of these solvents also originates serious environmental problems. This means it is necessary to fine-tune their structure and properties, to obtain real green solvents. For this purpose, we performed atomistic molecular simulations of neoteric solvents. These include ionic liquids (ILs),[25-30] deep eutectic solvents (DESs),[31] and dipolar aprotic solvents (DASs).[32]



SELECTED PUBLICATIONS

12 A. V. Pinto, et al., J. Phys. Chem. A 2020, 124, 9542. **doi: 10.1021/acs.jpca.0c03710**

13 K. Biernacki, et al., ACS Sustainable Chem. Eng. 2020, 8, 18712. **doi: 10.1021/acssuschemeng.0c08288**

14 I. V. Voroshylova, et al., J. Phys. Chem. Lett. 2020, 11, 10408. **doi: 10.1021/acs.jpclett.0c03212**

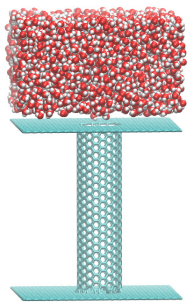
15 E. S. C. Ferreira, et al., J. Mol. Liq. 2020, 298, 111978. **doi: 10.1016/j.molliq.2019.1**

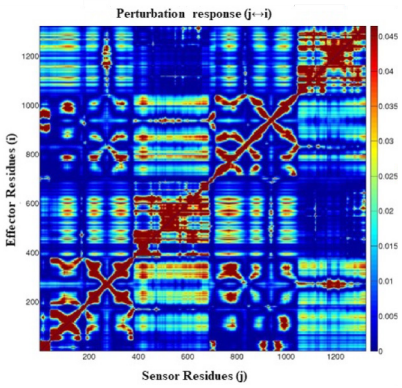
16 E. S. C. Ferreira, et al., J. Mol. Liq. 2020, 298, 111978. **doi:10.1016/j.molliq.2019.111978**

RESEARCH THEMES/
MODELLING CHEMICAL SPECIES AND NANOSTRUCTURED MATERIALS

THEORETICAL MODELLING OF NANOSTRUCTURED MATERIALS

Over the last decade, the nanostructured materials (NSMs) have gained considerable attention due to their extraordinary properties that made them attractive for a variety of applications. We use high-level theoretical methods, for providing new insights about the structure and properties of these materials. Both quantum calculations and molecular simulations are used in these studies. We simulate the application of these materials in important processes, such as: water desalination,[33] drug delivery,[34,35] water pumps,[36] gas adsorption,[37] and molecular imprinting sensing.[38,39] Different MSNs are used in our research. These include carbon nanotubes,[33-36] copper-doped circumcoronene[37] and electrochemical molecularly imprinted polymers.[38,39]





SELECTED PUBLICATIONS

17 M. González-Durruthy,et al., Nano Today 2020, 34, 100913. **doi: 10.1016/j.nantod.2020.100913**

18 M. Gosika, et al., ACS Appl. Polym. Mat. 2020, 2, 3587. **doi: 10.1021/acsapm.0c00596**

19 P. Rebelo, et al., Anal. Methods 2020, 12, 1486. **doi:10.1039/c9ay02566a**

20 P. Rebelo, et al., Biosens. Bioelectron. 2021, 172, 129112. **doi:10.1016/j.snb.2020.129112**

RESEARCH THEMES/
QUANTITATIVE STRUCTURE-ACTIVITY MODELLING

Nowadays, due to the increased risk of exposure to novel functional materials (NFMs), serious concerns about their safety for human health and the environment have also been raised. Toxicity testing is the first essential step for assessing the potential risks of the NFMs, but the experimental assays are often very expensive and usually too slow to flag the number nanoparticles that may cause adverse effects. *In silico* models for toxicity prediction, such as Quantitative Structure-Activity Relationship (QSAR) methods, are alternative approaches that are becoming increasingly important to support risk assessment of NFMs. Therefore, a strong emphasis is always set on the conjugation between effectiveness and safety for the new modelled materials. For this purpose, we develop appropriate QSAR models to predict both the biological activity[40-45] and the toxicity[46-49] of NFMs under diverse experimental conditions.

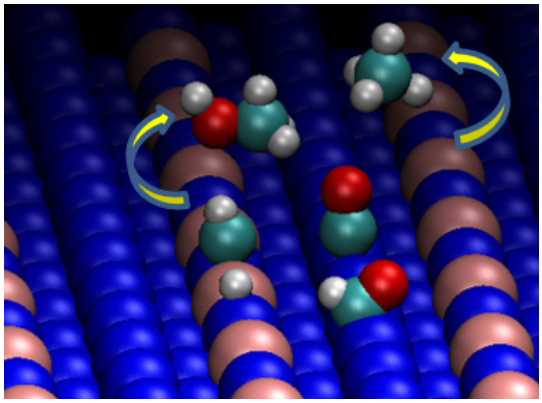
SELECTED PUBLICATIONS

21 A. K. Halder, et al., Chemosphere 2020, 244, 125489. **doi:10.1016/j.chemosphere.2019.125489**

RESEARCH THEMES/
HETEROGENEOUS-CATALYSED REACTIONS

HIGH-LEVEL QUANTUM METHODS FOR STUDYING 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 also predict the catalytic activity of new materials. These studies are mainly based in periodic plane-wave DFT methods. Both metallic surfaces[50-53] and metallic nanotubes[54,55] are used in our research. Reaction descriptors are also derived, from the data obtained, to predict the catalyst activity.[50-55] These descriptors are useful tools for the rational design of novel more efficient catalysts. One of our main goals is the selection of reaction descriptors for the Water Gas Shift (WGS) reaction. This reaction is crucial for eliminating or balancing the carbon monoxide in the methanol and ammonia synthesis; in cleaning the hydrogen used in fuel cells and in the hydrogen production from steam reforming of alcohols.



SELECTED PUBLICATIONS

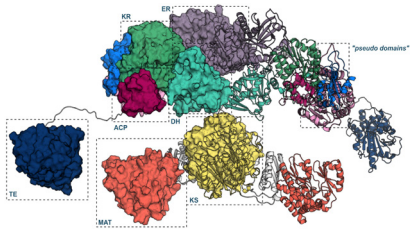
22 J. L.C. Fajín, M. N. D. S. Cordeiro Renew. Sust. Energ. Rev. 2020, 110523.
doi: 0.1016/j.rser.2020.110523

23 J. L.C. Fajín, M. N. D. S. Cordeiro Appl. Catal. B Env. 2020, 263, 118301.
doi:10.1016/j.apcatb.2019.11830

HIGHLIGHTS

ANIMAL FATTY ACID SYNTHASE: AN AMAZING CHEMICAL NANOFACTORY

Fatty acids are crucial molecules for most living beings, very well spread and conserved across species. These molecules play a role in energy storage, cell membrane architecture and cell signalling, the latter through their derivative metabolites. De novo synthesis of fatty acids is a complex chemical process that can be achieved either by a metabolic pathway built by a sequence of individual enzymes, such as in most bacteria, or by a single, large multienzyme, which incorporates all the chemical capabilities of the metabolic pathway, such as in animals and fungi, and in some bacteria. Here we focus on the multienzymes, specifically in the animal FAS. We start by providing a historical overview of this vast field of research. We follow by describing the extraordinary architecture of animal FAS, a homodimeric multienzyme with seven different active sites per dimmer, including a transport domain that carries the intermediates from one active site to the next. We then delve into this multienzyme's detailed chemistry and critically discuss the current knowledge on the chemical mechanism of each of the tenths of steps necessary to synthesize a single fatty acid molecule with atomic detail. In line with this, we discuss the potential and achieved FAS applications in biotechnology, as biosynthetic machines, and compare them with their homologue polyketide synthases, which are also finding wide applications in the same field. Finally, we discuss some open questions on the architecture of FAS, such as their peculiar substrate-shuttling arm, and describe possible reasons for the emergence of large megasynthases during evolution, questions that have fascinated biochemists from long ago but are still far from answered and understood..



Animal Fatty Acid Synthase: A Chemical Nanofactory

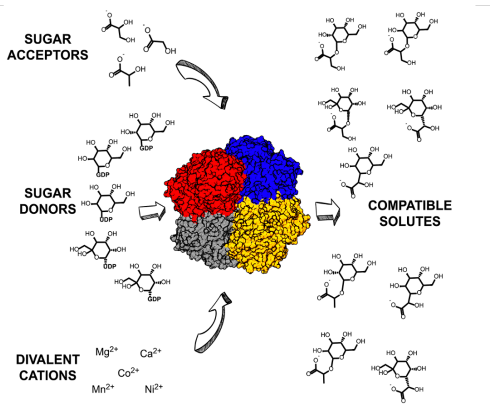
Chemical Reviews 2021, 121 (15), 9502

ENZYME CATALYTIC MECHANISMS

Enzymes are perfect catalysts. They combine very high reaction rates with insuperable chemo- and stereoselectivity. They act at room temperature, albeit some at extreme temperatures, use water as solvent, and are fully biodegradable. We clarify the way in which they achieve this amazing feat by establishing their catalytic mechanisms.

We perform high level calculations using hybrid quantum mechanics/molecular mechanics methods to represent the enzymatic systems and test every reaction mechanism that is plausible, by calculating the structure and free energy of the reactants, transition states, intermediates, and products of the tested reaction pathways.

We identify the correct mechanism through the most favourable kinetic profile (besides the reproduction of all available experimental information). Clarifying the mechanism of an enzyme does not only enlighten a prodigy of catalytic chemistry developed during millions of years of natural evolution but also provides the perfect templates for transition-state-analogue drug discovery towards the studied enzyme.



How the Destabilization of a Reaction Intermediate Affects Enzymatic Efficiency: The Case of Human Transketolase

ACS Catalysis, 2020, 10, 5372

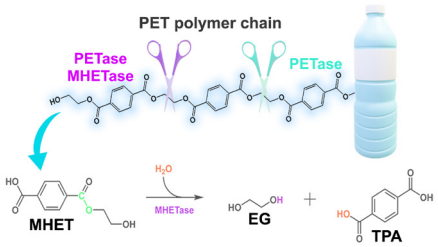
Activation Free Energy, Substrate Binding Free Energy, and Enzyme Efficiency Fall in a Very Narrow Range of Values for Most Enzymes

ACS Catalysis, 2020, 10, 15, 8444-8453

HIGHLIGHTS

NEW STRATEGY TO RECYCLE PLASTIC PET

Over the last half century, the unregulated massive production of plastics provoked an environmental problem at the planetary scale and, consequently, there is today an urgent need for technologies aiming at sustainable and circular economy. The PETase and MHETase enzymes, produced by the Ideonella sakaiensis 201-F6 bacterium, are known to act sequentially in the degradation of PET-polyethylene terephthalate, which is a type of plastic used extensively worldwide. The complete characterization of the whole reaction mechanism, at the molecular scale, is of paramount importance for engineering methods to improve these enzymes efficiencies. The study has been done using state-of-the-art hybrid QM/MM MD computational techniques, which combine high theoretical methods and extensive sampling molecular dynamics simulations. The results revealed that PETase and MHETase act via a two-step mechanism, with a rate-limiting step activation barrier of 20.0 kcal·mol–1 and 19.35 kcal·mol–1, respectively. The catalytic reaction ends with the formation of ethylene glycol (EG) and terephthalic acid (TPA), which are actually the precursors used in PET production.



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.

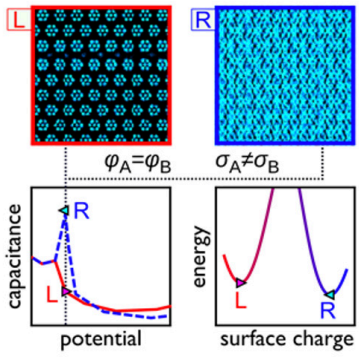
ACS Catalysis 2021, 11, 18, 11626–11638

Novel PetDegrading Enzymes: StructureFunction from a Computational Perspective.

ChemBioChem, 2021, 22,12, 2032-2050

POTENTIAL HYSTERESIS AT THE IONIC LIQUID–GOLD INTERFACE

Understanding the origin of the hysteresis is key to taking full advantage of ionic liquid (IL) | electrode interfaces, ensuring further progress in developing IL-based actuators, transistors, supercapacitors, and other innovative technological devices. We report the first observation of the capacitance–potential hysteresis at IL | electrode interfaces by atomistic molecular dynamics simulations. While modelling the differential capacitance dependence on the potential scan direction, we detected two long-living types of interfacial structure for the BMImPF6 ionic liquid at specific charge densities of the gold Au(111) surface. These structures differ in how counterions over-screen the surface charge. The high barrier for the transition from one structure to another slows down the interfacial restructuring process and leads to the marked capacitance–potential hysteresis



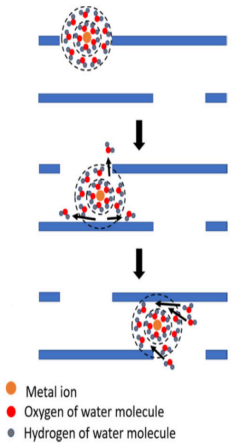
Differential capacitance dependence on the potential scan direction, showing the two long-living types of interfacial structures (L and R).

J. Phys. Chem. Lett., 2020, 11, 10408–10413

HIGHLIGHTS

HEAVY METAL ION SEPARATION FROM INDUSTRIAL WASTEWATER USING STAKED GRAPHENE MEMBRANES

In recent years, fluid transport through stacked graphene membranes has gained special attention due to its potential applications in water decontamination. Here, we are resorting to molecular dynamics (MD) simulations to elucidate the metal ion separation efficiency and mechanism of ion transport in stacked graphene membranes of varying interlayer spacing (d). Our results show that metal ions, like Cd2+, Cu2+, Hg2+, and Pb2+, can permeate through wide membranes (d = 1.0 nm) but metal ion rejection is close to complete for the narrower channels, irrespectively of the metal ion type. Further, steered MD simulations reveal that the free energy profile of a metal atom in wider channels is almost the same and always higher compared to that for water. To sum up, our results suggest that stacked graphene membranes have a high potential for metal ion separation and with marked efficient selectivity

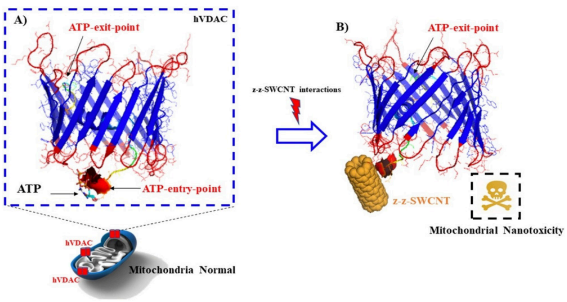


Molecular structure of the GO membrane grafted with hydroxyl groups. Red and white balls represent oxygen and hydrogen atoms in hydroxyl.

Desalination, 2019, 460, 1–14

COMPUTATIONAL MODELLING ON MITOCHONDRIAL CHANNEL NANOTOXICITY

The interactions between the zig-zag-single-walled carbon nanotube (z-z-SWCNT(8.0)) and the ATP-entry-point of the human mitochondrial voltage-dependent anion-selective channel (hVDAC1) were analysed in detail, by using molecular docking and molecular dynamics simulations. The results obtained provided a molecular basis for the mitochondrial channel nanotoxicity mechanism generated by carbon nanotubes. These results also open new opportunities towards the rational design of new carbon-based nanomaterials and in silico mitotarget drug-discovery.

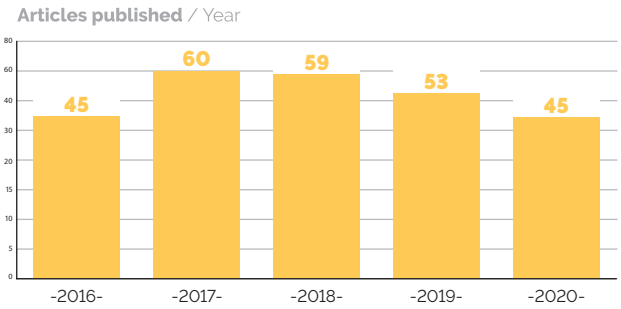


Three-dimensional representation of A) ATP/hVDAC1 and B) z-z-SWCNT/hVDAC1 complexes.

Nano Today, 2020, 34, 100913.

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION



H-index: **60**

254 articles*
20974 citations

***2016-2020**
From WOS core collection

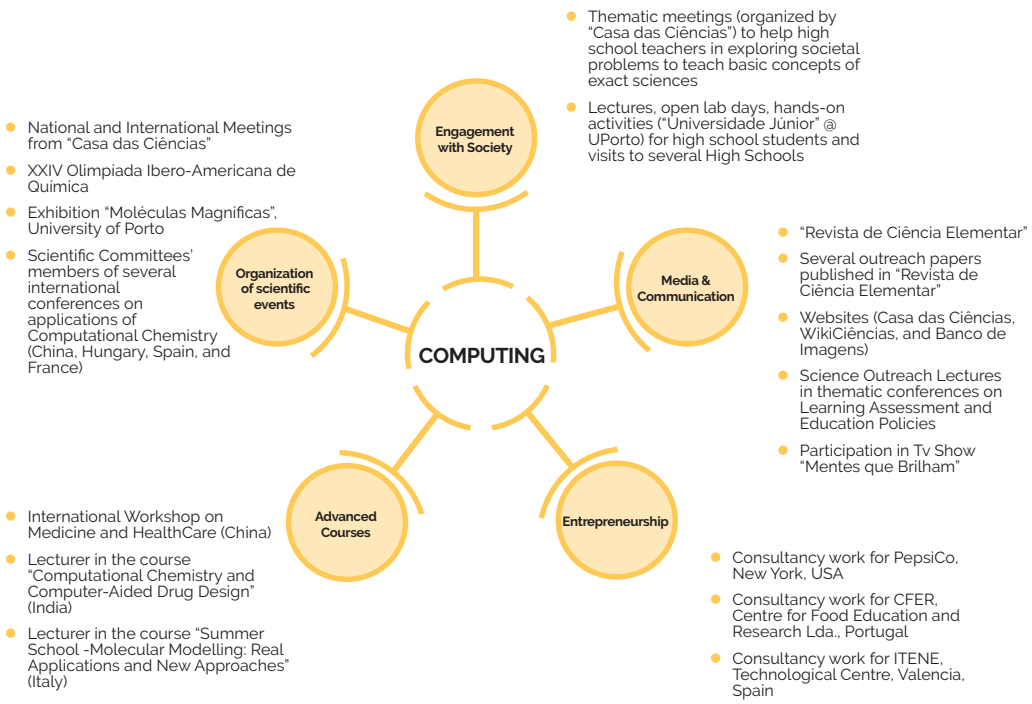
FUNDED PROJECTS *(Representative projects)*

- **REALM – Reactive Learning Machines**
  Funded by the Portuguese Foundation for Science and Technology - FCT (PTDC/QUI-QIN/30649/2017). Natália Cordeiro (PI).
  Total Funding: € 223,269.00
- **NanoDESK – Advanced web-based tools to promote the application of nanotechnology and safe use of nanomaterials in the plastic industry**
  Funded by Interreg Sudoe. Natália Cordeiro (Local PI).
  Total Funding: € 599,531.89
- **New Biocatalysts for Green Crude Oil Desulfurization**
  Funded by the Portuguese Foundation for Science and Technology – FCT (PTDC/QUI-QFI/28714/2017). Pedro Fernandes (PI).
  Total Funding: € 239,819.58
- **Enzyme Instantaneous Disorder as a Key Player in the Catalytic Power of Enzymes; CHM151**
  Pedro Fernandes (PI); Funding: 10 million CPU hours in Cray Titan and IBM Summit (the fastest supercomputer in the world), funded by the Oak Rigde National Laboratory, U.S.A.
  Corresponds to circa 1 million €
- **Local and Collective Motions as a Gateway to the Catalytic Power of Enzymes; CHM150**
  Maria João Ramos (PI); Funding: 10 million CPU hours in Cray Titan and IBM Summit (the fastest supercomputer in the world), funded by the Oak Rigde National Laboratory, U.S.A.
  Corresponds to circa 1 million €
- **Dipeptide Crystals as Biomaterials for Gas Purification**
  Funded by the Portuguese Foundation for Science and Technology – FCT (PTDC/QUI-QFI/29914/2017). Alexandre Magalhães (PI).
  Total Funding: € 238,067.13
- **European Joint Doctorate TCCM - Theoretical Chemistry and Computational Modelling**
  European Project (H2020) ITN-EJD-642294 – Maria João Ramos (PI)
  Local funding: € 362,000
- **Biodegrading plastic", Maria João Ramos (PI)**
  Funding: 45 million CPU hours in the BSC. Funded by EU PRACE Project no. 2018184467.
  Corresponds to circa 4.5 million €

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).

DISSEMINATION & OUTREACH




LABORATÓRIO ASSOCIADO
PARA A QUÍMICA VERDE

MolSyn
MOLECULAR SYNTHESIS

NATPRO
NATURAL PRODUCTS CHEMISTRY AND BIOACTIVITY

AnalytDev
ANALYTICAL DEVELOPMENT

BCO
(BIO)CHEMISTRY & OMICS

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

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LABORATÓRIO ASSOCIADO PARA A QUÍMICA VERDE

2020
ACTIVITY REPORT
& HIGHLIGHTS

04

Post-Graduation

MASTER PROGRAMS | MSC

Biochemistry
FCUP

DIRECTOR:
Paulo Correia de Sá (ICBAS-UP)

LOCAL COORDINATOR:
Paula Gameiro (LAQV)

Biochemistry
U.Aveiro

DIRECTOR:
Rita Ferreira (LAQV)

Bioorganic Chemistry
FCT NOVA (Lisbon)

COORDINATOR:
Paula Branco (LAQV)

Biotechnology
FCT NOVA (Lisbon)

COORDINATOR:
Susana Barreiros (LAQV)

Chemistry
U.Aveiro

DIRECTOR:
Helena Nogueira (U.Aveiro)

LOCAL COORDINATOR:
Diana Pinto (LAQV)

Conservation and Restoration
FCT NOVA (Lisbon)

DIRECTOR:
Joana Lia Ferreira (LAQV)

Food Science and Technology
FCUP

DIRECTOR:
Victor Freitas (LAQV)

Gastronomic Sciences
FCT NOVA (Lisbon)

COORDINATOR:
Paulina Mata (LAQV)

Integrated Master Programme in Chemical and Biochemical Engineering
FCT NOVA (Lisbon)

COORDINATOR:
Rui Freitas Oliveira (LAQV)

Membrane Engineering (Erasmus Mundus)
FCT NOVA (Lisbon)

COORDINATOR:
Isabel Coelhoso (LAQV)

Quality Control
FFUP

DIRECTOR:
Beatriz Oliveira (LAQV)

DOCTORAL PROGRAMS | PHD

Sustainable Chemistry

DIRECTOR:
Ana Aguiar Ricardo (LAQV),

CO-DIRECTORS:
Artur Silva (LAQV),
Baltazar de Castro (LAQV)

Conservation and Restoration of Cultural Heritage

CORES

DIRECTOR:
Maria João Melo (LAQV)

Bioengineering Systems

BIO-E, MIT-Portugal

DIRECTOR:
João Crespo (LAQV)

Molecular and Cellular Biotechnology Applied to Health Sciences

BiotechHealth

DIRECTOR:
Manuel Vilanova (ICBAS-UP)

CO-DIRECTOR:
Salette Reis (LAQV)

Medicines and Pharmaceutical Innovation

i3DU

DIRECTOR:
Cecília Rodrigues (FF/ULisboa)

LOCAL COORDINATORS:
José Costa Lima & Maria Beatriz Oliveira (LAQV)

Refining, Petrochemical and Chemical Engineering

EngIQ

DIRECTOR:
Fernando Gomes Martins (FEUP)

LOCAL COORDINATOR:
João Crespo (LAQV)

Erasmus Mundus Doctorate in Membrane Engineering

EUDIME

DIRECTOR:
Enrico Drioli (Univ. Calabria, Italy)

LOCAL COORDINATOR:
João Crespo (LAQV)

Animal Science

SANFEED

DIRECTOR:
António Mira da Fonseca (LAQV)

Materials Chemistry

ChemMat

DIRECTOR:
Manuel Leite de Almeida (IST/ULisboa)

LOCAL COORDINATOR:
Cristina Freire (LAQV)

Bioengineering Systems

BIO-E, MIT-Portugal

DIRECTOR:
João Crespo (LAQV)

Medical Biochemistry and Biophysics

M2B-PhD

DIRECTOR:
Miguel Castanho (FM/ULisboa)

LOCAL COORDINATOR:
Victor Freitas (LAQV)

Biochemistry

U.Aveiro

COORDINATOR:
Maria do Rosário Domingues

LOCAL COORDINATOR:
Francisco Amado (LAQV)

Chemical and Biochemical Engineering

PDEQB

COORDINATOR:
José Paulo Mota (LAQV)

Chemistry

U.Aveiro

COORDINATOR:
Augusto Tomé (LAQV)

Chemistry

FCT NOVA (Lisbon)

COORDINATOR:
Marco Gomes da Silva (LAQV)

Chemistry

U.Porto

DIRECTOR:
Victor Freitas (LAQV)

Food Sciences

DPFD

COORDINATOR:
Marco Gomes da Silva (LAQV)

Food Consumption and Nutrition Sciences

DIRECTOR:
Olívia Pinho (LAQV)

LAQV requimte
LABORATÓRIO ASSOCIADO PARA A QUÍMICA VERDE

2020
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/

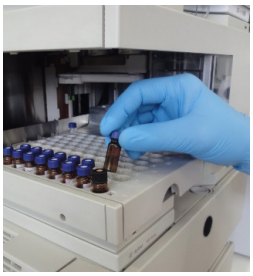
EQUIPMENT – U. PORTO

- 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

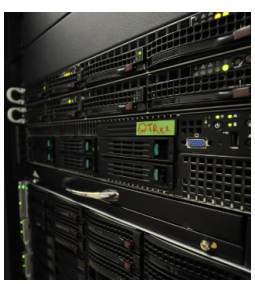
For more information:
https://sites.fct.unl.pt/labanalises

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

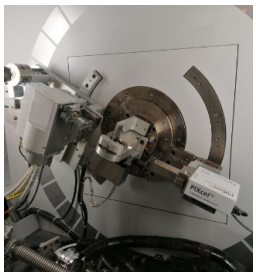
- 5 AISI 316 Extractors (up to 500 bar and 80 °C; Volume capacity: 4 with 1800 cm^3 + 1 with 3800 cm^3)
- 2 AISI 316 Cyclones (up to 450 bar; Volume capacity: ca. 200 cm^3)
- Countercurrent packed column (4 m high; 4 cm of internal diameter; Sulzer structured gauze packing; up to 300 bar and 100 °C; 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° (2θ) Scanning speed: 0,01~ +100°/min (2θ) Minimum step width: 0,01° (2θ).

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 ACTIVITY REPORT & HIGHLIGHTS

PORTO
Setembro 2021