LAQV
requimte
LABORATÓRIO ASSOCIADO
PARA A **QUÍMICA VERDE**

2013/2018
ACTIVITY REPORT
& HIGHLIGHTS

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

LAQV
2013-2018 ACTIVITY REPORT & HIGHLIGHTS

EDIÇÃO
LAQV – Laboratório Associado para a Química Verde
Porto · Setembro 2018

LABORATÓRIO ASSOCIADO
PARA A **QUÍMICA VERDE**

Universidade do Porto
R. D. Manuel II, Apartado 55142, 4051-401 Porto, Portugal
Tel: +351 226 069 420 / Fax: +351 226 066 097
E-mail: mpcunha@fc.up.pt

Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa
Campus de Caparica
2829-516 Caparica, Portugal
Tel: +351 212 948 575 / Fax: +351 212 948 550
E-mail: mimrc@fct.unl.pt

Universidade de Aveiro
Campus Universitário de Santiago
3810-193 Aveiro, Portugal
Tel: +351 234 370 200 / Fax +351 234 370 985
E-mail: geral@ua.pt

requimte
rede de química e tecnologia

U.PORTO

UNIVERSIDADE NOVA DE LISBOA

universidade de aveiro

01. ABOUT LAQV

02. THEMATIC LINES

03. RESEARCH GROUPS

04. POST-GRADUATION

05. SCIENTIFIC PLATFORMS

LAQV requimte
LABORATÓRIO ASSOCIADO PARA A QUÍMICA VERDE

2013/2018
ACTIVITY REPORT
& HIGHLIGHTS

01

About LAQV

DESCRIPTION & MISSION

REQUIMTE, the Network of Chemistry and Technology, was created in 1996 and merged two Research Centers from University of Porto and Nova University of Lisbon. In 2001 the Network obtained the status of Laboratório Associado para a Química Verde (LAQV) committing itself to promote the principles of Sustainable Chemistry through research, networking, training and outreaching activities. At present, LAQV configuration spreads out from the metropolitan areas of Porto and Lisbon to Aveiro, with small sites in Coimbra, Évora and Vila Real.

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. The need of a Sustainable Development to achieve the social, economic and environmental challenges of modern society is well accepted by governments, industry and general public. As modern society relies on chemicals and chemical processes for its way of living and Sustainable Development is mandatory to preserve life, 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.

To achieve these goals LAQV focuses its activity in six Thematic Lines aligned with SUSCHEM Research Agenda, EU Horizon 2020 and UN Sustainable Development Agenda. The complementary proficiencies to stimulate innovation across these Thematic Lines are provided by ten Research Groups which aggregate scientists who share similar backgrounds.

Through 2018-2022, 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 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 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. Its main general goal is to enhance contributions to Science, and to increase the impact of publications, especially onto the international Green Chemistry community. As an University-based research center, improving training at PhD level is a second key goal, and intimately linked to the previous one. Fulfilling these two core objectives will also allow LAQV to pursue: a) collaboration with industry/ technology transfer; b) start-up launching, c) participation in public awareness activities.

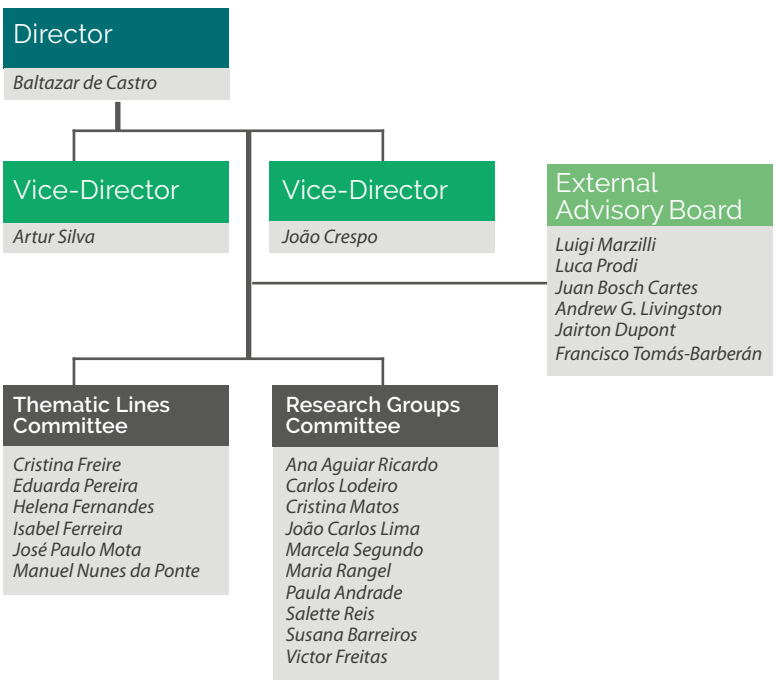
GOVERNANCE

The executive management of LAQV is assured by a Director (University of Porto) and two Vice-Directors (Universities of Aveiro and Nova University of Lisbon), which are elected by the Scientific Council.

The Scientific Council comprises all integrated members holding a PhD degree, which normally operates in two smaller committees: the Thematic Lines Committee and the Research Groups Committee.

The Thematic Lines Committee and the Research Groups Committee are composed of the coordinators of each Thematic Line and Research Group (respectively), which are nominated by the board of directors.

The Board of Directors are also supported by the External Advisory Board, constituted of 6 renowned specialists in Sustainable Chemistry.



SCIENTIFIC ORGANIZATION

The research activity of LAQV is organized in six Thematic Lines, vectors in which Chemistry and Chemical Engineering play a crucial role and that are aligned with SUSCHEM Research Agenda, EU Horizon 2020 and UN Sustainable Development Agenda:

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 ten 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. Cultural heritage and responsive materials
7. (Bio)Chemical process engineering
8. Materials for sustainability and wellbeing
9. Nanoplatforms
10. Food quality and technology

LAQV requimte
LABORATÓRIO ASSOCIADO PARA A QUÍMICA VERDE

2013/2018
ACTIVITY REPORT
& HIGHLIGHTS

02

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 Wellbeing

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

In order to maximize these concepts, effective integrated approaches and interventions, addressing major health challenges are conducted through interdisciplinary and multidisciplinary research approaches by a team with background in Chemistry, Biochemistry, Materials Science & Engineering, Biomedical Sciences, Clinical Sciences and Entrepreneurship & Business Development. Distinct LAQV research groups put their efforts on creating strategic frameworks that, by embracing Sustainable & Green Chemistry design principles, interdependently create supportive environments for health, through a sustainable and flexible path.

Acknowledging the interconnectedness of the agents, actions and challenges, groundbreaking research and development is accomplished through a unity of approach and the adoption of a common outcome-focused framework, setting a global focus on:

- The design, advancement and upscaling of efficient and sustainable ways to remove hazardous chemicals from the environment, further reducing and potentially eliminating air, water and soil pollutants and contaminants;
- 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 and management;
- The validation of the efficacy and biosafety of new bioactive compounds and medicines, targeting specific markers for communicable and non-communicable 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, with an improved efficiency and sustainability for heightened tissue healing and regeneration;
- Entrepreneurship & Business Development

The multidisciplinary research team contributing to the Health & Wellbeing thematic line shares a common vision of a challenge-driven concept of "excellence", stem from the need to achieve progressive structural changes in order

HEALTH & WELLBEING (CONT.)

to flow valued scientific knowledge into all societal processes, aligned with the Global Challenges for sustainable development. Excellence is envisaged as a dynamic process encompassing:

- valued breakthrough scientific knowledge in strict alignment with existing societal demands and needs;
- unity in the interdisciplinary scientific background; and
- anticipation of new societal needs and challenges to foster ahead scientific knowledge.

In this scenario, the ultimate goal is scientific knowledge transfer and technological valorization to generate beneficial and scalable outcomes and solutions in the provision of treatment and care to deliver safer, more effective and inclusive strategies for improved health and wellbeing. Accordingly, achieved innovative products and services must be showcased adequately, throughout sustainable pipelining strategies that allow an effective scaling up, substantiating a rapid and effective technology transfer.

The team benefits from the solid background and experience of researches in entrepreneurship & business development, fostered within the intersection between of environmental and social sustainability with economic sustainability, in order to produce innovative business models. Regular activities include a bottom-up approach with 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, further inspiring new mental attitude to societal sustainability, inclusiveness and healthiness.

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 Wellbeing

The main goal of the Line Environment Monitoring and Analysis 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, modeling 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), 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 rapid screening of contaminants; development of innovative products and low carbon technology; use of biotechnology and molecular tools to address cell cascades signaling the impact of contaminants; 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 for monitoring purposes. 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 REQUIMTE; aim to support, among others, the Water Framework directive and the Integrated Coastal Management; and are developed in close cooperation with the economic sector, environmental policy-making authorities at regional, national and international level, and with other stakeholders. This Line also contributes to REQUIMTE 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 Wellbeing

We are strongly committed over the next years to help find sustainable solutions for energy conversion, storage, distribution, and recycling, jointly using 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, and the use of the LAQV strategic scientific employment plan to hire at least one senior researcher and two junior ones with adequate expertise. The scientific program of this Thematic Line will focus on 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; and new membranes incorporating ionic liquids and MOFs, as well as novel cyclic adsorption processes, for purification of industrial gaseous streams; 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 and simultaneously incorporated in line with enzymatic cascade bioreactors aiming at the production of biofuels as secondary products. We shall continue studying new nanostructured materials, such as metal organic frameworks (MOFs) and clathrates, to investigate 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, 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 us 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, as well as biomass hydrolysis/fractionation using subcritical water.

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

The core activities of Food & Nutrition thematic line are the improvement of food quality, authenticity, control of allergens, additives, and chemical contaminants, optimization of advanced food processing methods and formulation of new processed products, which will enhance food nutritional and sensorial characteristics, ensure high levels of food safety and traceability and help consumers to make informed choices. Moreover, research activities are focused in conserving natural resources, promote sustainable procedures/technologies that minimize food losses and waste, implement circular economy principles across the whole food system, while reducing its environmental footprint. Thus, contributing to climate change mitigation, increase the quality of products, by adding commercial value to them. Understand the mechanisms that underlie protective effects of nutrients and bioactive compounds and reduce the incidence of non-communicable diet-related diseases are also a relevant area of research. Therefore, Food & Nutrition thematic line is anchored to work programs of the Horizon 2020 societal challenges SC1, SC2 and SC5 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 joins 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, contaminants;
- 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 human cells in vitro and tissues;
- use of non-invasive techniques to study animal metabolism and 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, which is expected to provide new insights into complex regulatory networks and identification of genes relevant to new biological processes.

RESOURCE EFFICIENCY – SUSTAINABLE PROCESSING

Thematic Line Coordinator:
Manuel Nunes da Ponte

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 Wellbeing

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 CO2 utilization, design of new smart materials and effective recovery of non- renewables. 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 web-conferences. 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 agro-industrial wastes (such as brewer spent grain and yeast, fruit peels and pomace, spent coffee, olive pomace, eggshell and canned fish wastes) 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 extensive expertise on supercritical carbon dioxide as solvent to venture into its chemical and electrochemical transformation. Apart from the power-to-gas and CO_2 capture schemes developed under the Thematic Line Clean and Renewable Energy, 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, 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 bio-medical, 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 Wellbeing

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 with the development of new high-performance functional and smart (nano)(bio)materials through eco-sustainable, cost-effective and scalable processes, to boost innovation on 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 (nano)materials with high-efficiency energy storage and/or responsive properties to be integrated in textiles/flexible substrates 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 will be implemented in applications 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, dyes).
- In cultural heritage field: we will contribute to history of plastics, to preservation of historic photographic collections and to creation of an online access to Winsor & Newton artist materials supplier database.

LAQV requimte
LABORATÓRIO ASSOCIADO PARA A QUÍMICA VERDE

2013/2018
ACTIVITY REPORT
& HIGHLIGHTS

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 WELLBEING

NanoPlat
NANOPLATFORMS

4FOOD
FOOD QUALITY AND TECHNOLOGY

MolSyn

MOLECULAR SYNTHESIS

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

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, 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 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 [2018-2022]

The Molecular Synthesis group will continue to pursue work aiming 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.

Development of innovative methods for chemical synthesis or computational design, and study of relevant target molecules will be pursued. 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 will benefit from the incorporation of new members upcoming from the University of Aveiro. This circumstance will reinforce 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 chemosensing, photodynamic therapy of tumors, or the photodynamic inactivation of 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


Amparo Faustino


Ana Fernandes


Ana Lourenço


Ana Silva


André Silva


Anthony Burke


Artur Silva


Augusto Tomé


Baltazar de Castro


Carolina Marques


Cátia Teixeira


Elisabete Carreiro


Galya Ivanova


J. Aires de Sousa


J. Rodríguez-Borges


José Cavaleiro


Krasimira Petrova


Luísa Ferreira


★ Maria Rangel


M. Graça Neves


M. Luísa do Vale


M. Manuel Marques


Mário Simões


Paula Branco


Paula Gomes

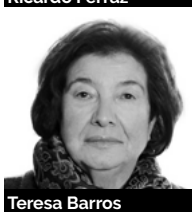

Paulo Mendes


Ricardo Ferraz


Samuel Guieu


Susana Braga


Teresa Avilés


Teresa Barros


Vera Silva

★ Group coordinator

RESEARCH TEAM

OTHER DOCTORATE RESEARCHERS
Ana Cláudia Nunes
Maria João Araújo

POST-DOCTORAL FELLOWS
Ana T. Gomes
Andreia Leite
Catarina Ramos
Cátia Esteves
Luísa Carvalho
Daniela Peixoto
Diogo A.R.S. Latino
Hélio Albuquerque
Joana Lia Sousa
Patrícia Máximo
M. Florbela Pereira
M. Isabel Pinto
Miglena Georgieva
Nuno Moura
Vitor Rosa
Raquel Seixas
Sandra G. F. Silva
Tânia Moniz
Vasco Bonifácio
Yuri Binev
Zeljko Petrovski

PhD STUDENTS
Alexandre Borges
Ana S. M. Gomes
Carina I. Crucho
Carla Queirós
Cátia V. A. Santos
Cláudia D. Raposo
Diogo L. Poeira
Fausto D. Queda
Ivo E. Sampaio-Dias
Luísa Aguiar Silva
Mani Hosseinzade
Maria A. Medeiros
Marina D. Pires
Pedro Salgueiro
Regiane G. Lima
Ricardo Chagas

MSc STUDENTS
Alexandra Loupas
Ana Sofia Santos
Ana Teresa T. Silva
André Jorge
Carlos R. Gonçalves
Cátia V. A. Santos
Diogo L. Poeira
Edgar H. Teixeira
Fausto D. Queda
Ian Rodrigues
Joana R.V.P. Costa
João Macara
Margarida G. Figueiredo
Mélanie F. Fonte
Mónica Lopes
Natália Fagundes
Rafael A. Rippel
Rafael M. Mamede
Sara C. Silva Reis
Sara I. Purificação
Sandro Belchior
Vanessa Fadista
Vanessa Sabino

RESEARCH GRANTEES
Ana Laura R. Silva
André O. Sequeira
Ana Sofia S. Sousa
Rodrigo Monteiro
Carlos F. P. Branco
Catarina Pereira
Francisco Faísca
José Almeida
Luís M. G. Sousa
Mariama Djalo
Tomé Silva

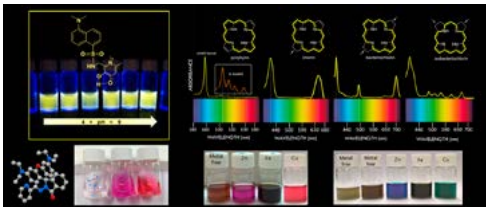
OTHER RESEARCHERS
Ana R. S. Dias
Beatriz B. A. Pinto
Hélio Martins Gil
Mariana Barbosa
Sílvia S. P. Vinhas

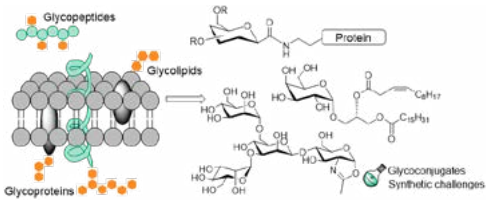
RESEARCH THEMES / MOLECULES

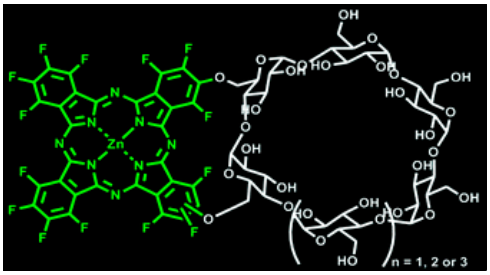
Chemical synthesis of a wide diversity of molecules for:

BIOMEDICAL APPLICATIONS

- chelates and chelators to address iron imbalance-related diseases[1,2]
- membrane-active peptides as novel antimicrobial agents[3,4]
- modification of classical anti-malarials to bypass parasite resistance[5,6]
- bioactive ionic liquids derived from anti-infective drugs[7,8]
- synthetic analogues of vitamin D3 precursors[9]
- peptidomimetics to address neurodegenerative disorders[10]
- benzimidazole-based compounds as cyclooxygenase-inhibitors[11]
- nature-inspired molecules, from marine compounds,[12] and xenobiotic metabolites, to bacterial cell wall disaccharide components,[13] and sugar-based compounds with bactericidal and cytotoxic activities[14]
- oxygen heterocycles as potential antioxidant,[15] anticancer[16] and anti-diabetic[17] agents
- porphyrin derivatives as potential anticancer[18] and antimicrobial agents[19]







SELECTED PUBLICATIONS

1 T. Moniz, et al. Medicinal Chemistry Communications, 2015, 6, 2194. doi:10.1039/C5MD00456J

2 J.T.S. Coimbra, et al. Journal of Physical Chemistry B 2014, 118, 14590-14601 doi:10.1021/jp509491p7

3 C. Monteiro, et al. Molecular Pharmaceutics 2015, 12, 2904. doi:10.1021/acs

4 S. Almeida Dias, et al. Front Microbiol. 2017, 8: 775. doi:10.3389/fmicb.2017.0077

5 A. Gomes, et al. ChemMedChem 2015, 10, 1344. doi:10.1002/cmdc.201500164

6 E. Moles, et al. Biomaterials 2017, 145, 178. doi:10.1016/j. biomaterials.2017.08.020

7 R. Ferraz, et al. ChemMedChem 2015, 10, 1480. doi:10.1002/cmdc.201500142

8 R. Ferraz, et al. RSC Adv. 2016, 6, 56134. doi:10.1039/C6RA10759A

9 S. Vinhas, et al. J. Steroid Biochem. Mol. Biol. 2017, 173, 83. doi:10.1016/j.jsbmb.2016.07.015

10 I. Sampaio-Dias, et al. Org. Biomol. Chem. 2016, 14, 11065. doi:10.1039/C6OB02248K

11 L. C. Carvalho, et al. RSC Adv. 2015, 5, 49098. doi:10.1039/c5ra04984a

12 P. Máximo, et al. Marine Drugs 2016, 14:139. doi:10.3390/md14080139

13 R. Enugala, et al. Carbohydr. Res. 2014, 384, 112. doi:10.1016/j.carres.2013.12.007

14 K. T. Petrova, et al. Carbohydr. Res. 2015, 417, 66. doi:10.1016/j.carres.2015.09.003

15 A. M. Oliveira et al. Neurochem. Int., 2015, 91, 1. doi:10.1016/j.neuint.2015.10.004

16 O. Talhi, et al. Eur. J. Org. Chem., 2016, 965. doi:10.1002/ejoc.201501278

17 C. Proença, et al. J. Enz. Inhib. Med. Chem., 2017, 32, 1216. doi:10.1080/14756366.2017.1368503

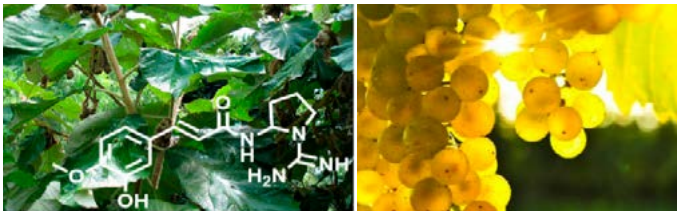
18 L. M. O. Lourenço, et al. Chem. Commun. 2014, 50, 8363. doi:10.1039/c4cc02226b

19 J. F.B. Barata, et al. Biomacromolecules. 2016, 17, 1395. doi:10.1021/acs.biomac.6b00006

RESEARCH THEMES / MOLECULES

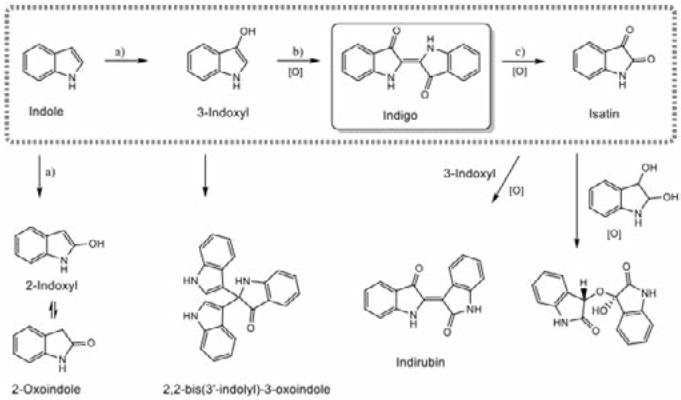
AGRICULTURAL, ENVIRONMENTAL AND FOOD APPLICATIONS

- chelators for regulation of iron uptake and storage in plants[20]
- pyridinone chelators for iron speciation in waters[21,22]
- peptides and proteins of relevance in wine properties[23,24]
- ferrocene-based imine ligands as selective sensors for mercury(II)
- organometallic molecules as catalysts for CO_2 functionalization,[25] and other chemical reactions[26]
- porphyrin derivatives as potential antimicrobial agents[27]
- porphyrin derivatives and analogues as chemosensors for anions[28] and metal ions[29]



CATALYSIS

- Homogeneous and heterogeneous oxidation of alkenes, alkanes, catechol, organosulfur compounds[30-39]
- Homogeneous oxidation of indole to afford indigo dye[40,41]



SELECTED PUBLICATIONS

20 C. Santos, et al. Plant Physiol. Biochem. 2016, 106, 91. doi:10.1016/j.plaphy.2016.04.050

21 J.L. Miranda, et al. Talanta 2016, 148, 633. doi:10.1016/j.talanta.2015.05.062

22 R. Mesquita, et al. Polyhedron, 2015, 101, 171. doi:10.1016/j.poly.2015.09.015

23 R. Ferrer-Gallego, et al. J. Agr. Food Chem. 2017, 65, 6434. doi:10.1021/acs.jafc.6b05414

24 R. Chagas, et al. Food Chem. 2016, 192, 460. doi:10.1016/j.foodchem.2015.07.052

25 D. Specklin, et al. Chem. Eur. J. 2017, 23, 5509. doi:10.1002/chem.201605907

26 C. Fliedel, et al. Dalton Trans. 2015, 44, 12376. doi:10.1039/c5dt00458f

27 E. Alves et al. Dyes Pigments. 2014, 110, 80. doi:10.1016/j.dyepig.2014.05.016

28 F. Figueira, et al. Chem. Commun. 2016, 52, 2181. doi:10.1039/c5cc08128a

29 N. M. M Moura, et al. Chem. Eur. J. 2014, 20, 6684. doi:10.1002/chem.201402270

30 K.A.D.F. Castro, et al. Catal. Sci. Technol. 2014, 4, 129. doi:10.1039/c3cy00472d

31 S.M.G. Pires, et al. Appl. Catal. B: Environ. 2014, 160-161, 80. doi:10.1016/j.apcatb.2014.05.003

32 G. Silva, et al. Catal. Commun. 2014, 56, 68. doi:10.1016/j.catcom.2014.06.032

33 K.A.D.F. Castro, et al. Appl. Catal. A: General. 2015, 503, 9. doi:10.1016/j.apcata.2014.12.048

34 K.A.D.F. Castro, et al. J. Colloid Interface Sci. 2015, 450, 339. doi:10.1016/j.jcis.2015.03.028

35 K.A.D.F. Castro, et al. Inorg. Chem. 2015, 54, 4382. doi:10.1021/acs.inorgchem.5b00196

36 R. de Paula, et al. J. Mol. Catal. A: Chem. 2015, 404, 156. doi:10.1016/j.molcata.2015.04.021

37 K.A.D.F. Castro, et al. J. Catal. 2016, 344, 303. doi:10.1016/j.jcat.2016.09.010

38 K.A.D.F. Castro, et al. Inorg. Chim. Acta. 2017, 455, 575. doi:10.1016/j.ica.2016.05.038

39 K.A.D.F. Castro, et al. ChemCatChem. 2017, 9, 2939. doi:10.1002/cctc.201700484

40 M. Linhares, et al Appl. Catal. A: General. 2014, 470, 427. doi:10.1016/j.apcata.2013.11.023

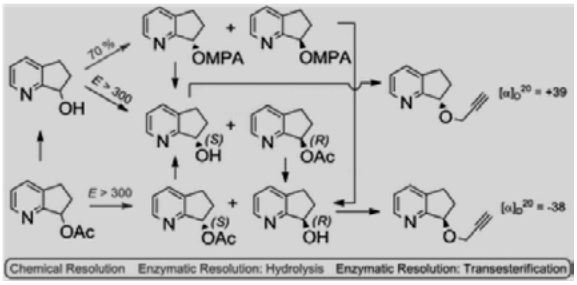
41 S.L.H. Rebelo, et al. J. Catal. 2014, 315, 33. doi:10.1016/j.jcat.2014.04.012

RESEARCH THEMES / METHODS

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

SYNTHETIC APPROACHES

- innovative approaches for one-pot synthesis of oligopeptides,[42] and heterocycles of interest in medicinal and process chemistry[43,44]
- solid-phase synthesis and grafting of peptides onto biomaterials[43]
- new routes for enantioselective synthesis of chiral compounds with potential pharmaceutical interest[46,47,48]
- ohmic heating as an emerging concept in organic synthesis and their application in the synthesis of bioactive compounds[49,50]
- design and synthesis of efficient solid fluorophores with potential application in luminescent materials[51,52]
- cycloaddition reactions for creating improved porphyrin-based photosensitizers[53]
- aza-Michael addition reactions – unprecedented sapphyrin derivatives[54]
- Design and synthesis of porphyrins[55] and phthalocyanines[56] for supramolecular systems



COMPUTATIONAL APPROACHES

- tools for accurate prediction of reaction conditions[57]
- models for frontier orbitals energies[58] and partial atomic charges[59]
- improved NavMol molecular editor for blind users[60]

SELECTED PUBLICATIONS

42 I. Sampaio-Dias, et al. Org. Biomol. Chem. 2017, 15, 7533. doi:10.1039/c7ob01544e

43 S.I. Purificação et al. Org. Lett. 2017, 19, 5118. doi:10.1021/acs.orglett.7b02403

44 M.J.D. Pires, et al. Org. Lett. 2016, 18, 3250. doi:10.1021/acs.orglett.6b01500

45 M. Barbosa et al. Carbohydr. Polym. 2017, 165, 384. doi:10.1016/j.carbpol.2017.02.050

46 C. A. D. Sousa, et al. RSC Adv. 2015, 5, 104509. doi:10.1039/C5RA24868J

47 R. G. Soengas, et al. J. Org. Chem., 2013, 78, 12831. doi:10.1021/jo4021634

48 O. Talhi, et al. New J. Chem., 2017, 41, 10790. doi:10.1039/C7NJ02168B

49 J. Pinto, et al. Green Chem., 2013, 15, 970. doi10.1039/C3GC36881E

50 V. L. M. Silva, et al. Chem. Eur. J., 2017, 23, 7853. doi:10.1002/chem.201700307

51 P. A. A. M. Vaz, et al. New J. Chem., 2016, 40, 8198. doi:10.1039/C6NJ01387B

52 S. Guieu, et al. Eur. J. Org. Chem., 2015, 3423. doi10.1002/ejoc.201500318

53 J. C. J. M. D. S. Menezes, et al. Chem. Eur. J. 2014, 20, 13644. doi:10.1002/chem.201403214

54 F. Figueira, et al. Chem. Eur. J. 2016, 22, 14349. doi:10.1002/chem.201602313

55 J. I. T. Costa, et al. Dyes and Pigments. 2016, 135, 163. doi:10.1016/j.dyepig.2016.02.035

56 L. Wibmer, et al. Nanoscale. 2015, 7, 5674. doi: 10.1039/c4nr05719h

57 G. Marcou et al. J. Chem. Inf. Model. 2015, 55, 239. doi:10.1021/ci500698a

58 F. Pereira et al. J. Chem. Inf. Model. 2017, 57, 11. doi:10.1021/acs.jcim.6b00340

59 Q. Zhang et al. Mol. Inf. 2016, 35, 62. doi:10.1002/minf.201500113

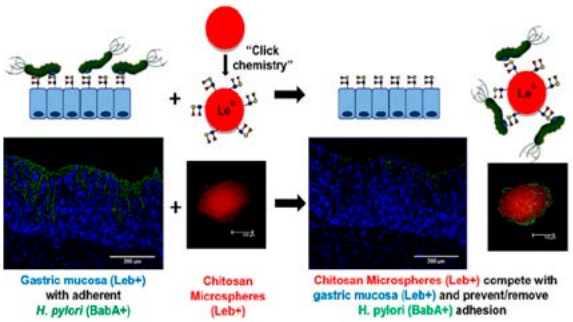
60 Y. Binev et al. Bioinformatics 2017, btx556. doi:10.1093/bioinformatics/btx556

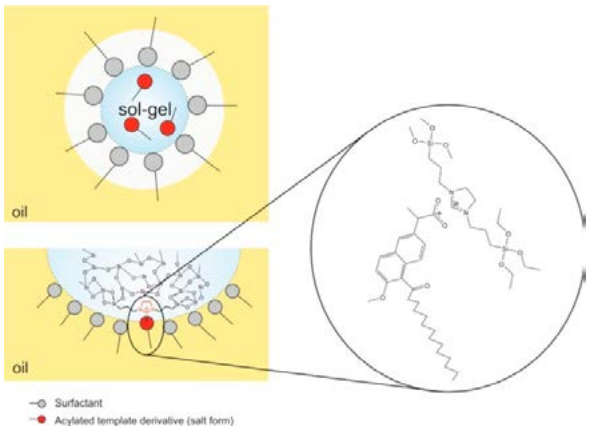
RESEARCH THEMES / MATERIALS

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

- peptide-tethered antimicrobial coatings for bone implants[61]
- "click"-chemistry-coated microspheres for bacterial removal[62]
- sugar-based polymeric nano/microparticles[63,64] and aminoacid-based surfactants[65-67] for drug delivery and gene therapy





SEPARATION AND CLEANER ENERGIES

- drug-imprinted xerogels for chromatographic applications[68,69]
- coumarin-based chromophores for dye-sensitized solar cells[70]

SELECTED PUBLICATIONS

61 F. Costa et al. Biomaterials 2015, 52, 531. doi:10.1016/j.biomaterials.2015.02.049

62 I. C. Gonçalves et al. Acta Biomaterialia 2016, 33, 40. doi:10.1016/j.actbio.2016.01.029

63 C.I.C. Crucho et al. Mat. Sci. Eng. C, 2017, 80, 771. doi:10.1016/j.msec.2017.06.004

64 K.T. Petrova et al. Carbohydr. Polym. 2015, 125, 281. doi:10.1016/j.carbpol.2015.02.052

65 S. G. Silva, et al. Chem. Eur. J. 2015, 21, 4092. doi:10.1002/chem.201406111

66 A. M. Cardoso, et al. Mol. Pharm. 2015, 12, 716. doi:10.1021/mp5005349

67 R. S. Teixeira, et al. Eur. J. Pharm. Biopharm. 2015, 93, 205. doi:10.1016/j.ejpb.2015.02.024

68 P. Kadhirvel et al. J. Chromatogr. A, 2015, 1424, 59. doi:10.1016/j.chroma.2015.10.097

69 M. Ornelas et al. J Chromatogr. A, 2016, 1437, 107. doi:10.1016/j.chroma.2016.01.074

70 S. Martins et al. J. Photochem. Photobiol., 2017, ahead-of-print doi:10.1016/j.jphotochem.2017.12.018

HIGHLIGHTS

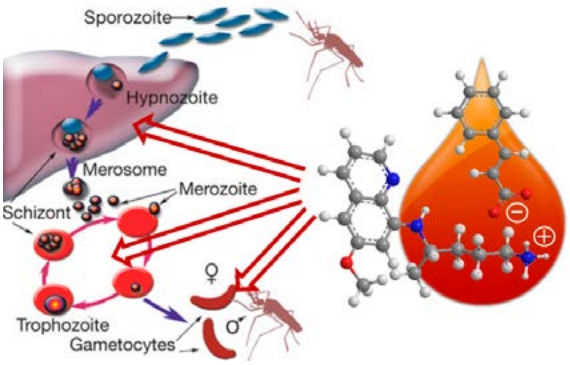
BETTER FE-SHUTTLES TO ADDRESS CROP FE DEFICIENCY

Iron Deficiency Chlorosis (IDC) is a disorder that has consequence not only in plant growth but also in the Fe content of seeds and fruits. To solve the problem, Fe-chelates with properties that allow more efficient pathways for root uptake, root to shoot translocation and maintenance of metal homeostasis are needed. In a pilot study performed in soybean (Glycine max L.) we tested a family of Fe-chelates that permits to design compounds with a variety of chemical properties that can be fine-tuned according to the results obtained on plants. We found that the Fe-chelates have potential as new IDC correctors since plants were significantly greener and had increased biomass when compared to plants supplied with the commercial fertilizers. In particular, plants supplied with one of the compounds, were able to translocate more iron from the roots to the shoots.

Effect of tris(3-hydroxy-4-pyridinonate) iron(III) complexes on iron uptake and storage in soybean *(Glycine max L.)*
Plant Physiology and Biochemistry, 2016, 106, 91-100.

IONIC LIQUIDS DERIVED FROM ACTIVE PHARMACEUTICAL INGREDIENTS

Ionic liquids derived from active pharmaceutical ingredients (API-ILs) may open new perspectives towards greener methods for the rescuing of classical drugs. Following our long track record in the recycling of classical antimalarial drugs currently in decline due to resistance and/or toxicity issues, we have recently unveiled novel ionic liquids derived from the antimalarial drug primaquine as triple-stage antimalarial leads. This unprecedented approach opens a new chapter concerning sustainable development of low-cost drugs, not exclusive to the arena of antiparasitic drug discovery.



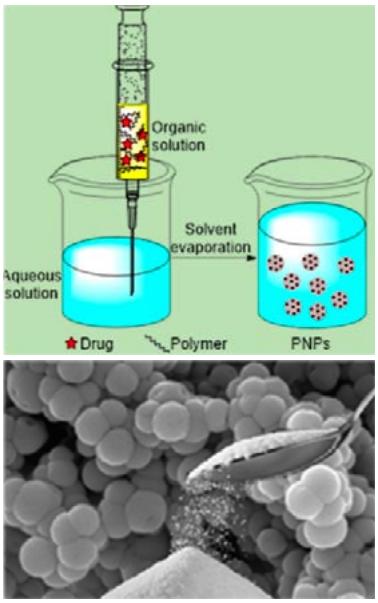
Primaquine-based ionic liquids as a novel class of antimalarial hits
RSC Advances, 2016, 6, 56134-56138.

HIGHLIGHTS

SUGAR-BASED POLYMERIC NANOPARTICLES

Carbohydrates are very important in biology, and excellent targets for the development of therapeutics. Following recent progress in nanoscience, which disclosed the relevance of nanomaterials in healthcare, glycopolymers are gaining prominence for drug delivery, given their high affinity and binding specificity towards targeted receptors.

Our Research Unit has combined nanotechnology and polymer science to develop polymeric nanoparticles (PNPs), based on glycosylation of biocompatible biopolymers. Novel polymer-based materials prepared from monosaccharides obtained by enzyme-catalyzed synthesis, that were homo-polymerized and copolymerized with styrene by a free radical process. Thus, polymer materials with sugar moieties, attached to the polymer backbone via ester linkages were attained where the structural features of the monomers greatly affected the thermal and rheological properties of the polymers. We have further produced novel amphiphilic polymers composed of poly(ethylene glycol) (PEG), cholic acid and sucrose. Owing to their amphiphilic characteristics in aqueous media, these PNPs could be prepared via a greener surfactant-free nanoprecipitation method. The spherical shape and size of the PNPs thus produced were suitable for drug delivery applications.

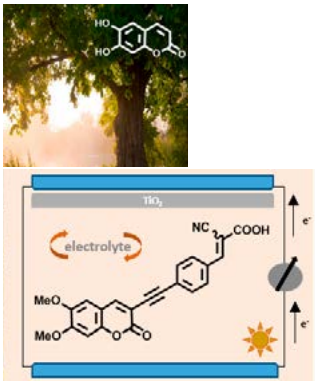


Formation of spherical and core-shell polymeric microparticles from glycopolimers

Carbohydrate Research, 2015, 125, 281-287.

COUMARIN-BASED CHROMOPHORES FOR DYE SENSITIZED SOLAR CELLS

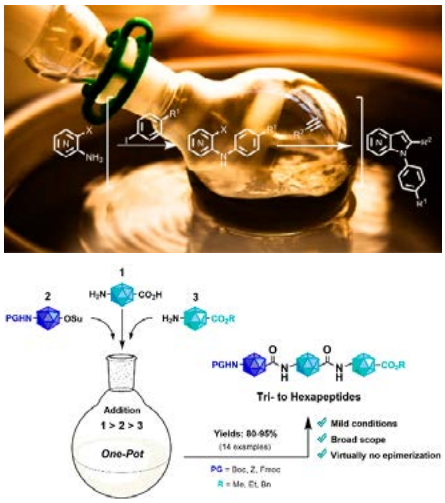
Dye-sensitized solar cells (DSSCs) are low-cost thin film solar cells with many attractive features, such as their ease of preparation and multiple applications, owing to their flexibility and transparency features. Although still less efficient than the best thin-film cells, their price/performance ratio is expected to become good enough to make them competitive with fossil fuels for generation of electricity. Bearing this in mind, and in line with the European Union Photovoltaic Roadmap that targets a significant contribution of DSSCs to renewable electricity generation by 2020, we have produced highly fluorescent coumarin dyes with styryl and phenylethynyl π-bridge moieties, via Sonogashira and regioselective Heck arylation reactions, for application in DSSCs.



Styryl and phenylethynyl based coumarin chromophores for dye sensitized solar cells

Journal of Photochemistry and Photobiology A, 2018, 353, 564-569.

HIGHLIGHTS



Highly efficient one-pot assembly of peptides by double chemoselective coupling

Organic & Biomolecular Chemistry, 2017, 15, 7533-7542.

HIGHLY EFFICIENT ONE-POT SYNTHETIC ROUTES TOWARDS BIOACTIVE COMPOUNDS

The development of new chemical methodologies and greener approaches for the assembly of important scaffolds is one of the main goals of modern organic chemistry. Our Research Unit has been devoted to synthesis of challenging scaffolds, such as azaindoles - a very popular class of compounds for both medicinal and process chemists, and developed a practical and straightforward syntheses of substituted and 1,2-disubstituted azaindoles. Thus, one-pot approaches were developed, involving several Pd-catalyzed cross-coupling reactions, such as Heck, Sonogashira, Buchwald-Hartwig reactions, opening a fast and elegant access to this not always easy to make class of compounds. Equally noteworthy, a methodological advancement in solution-phase peptide synthesis was achieved, through development of a protocol to synthesize oligopeptides in a one-pot three-step cascade method, in which two peptide bonds are introduced chemoselectively. Oligopeptides were obtained in high global yields with no observable epimerization, through a faster, easier and milder approach that operates at equimolar amounts, and is compatible with virtually all protection schemes relevant in the context of peptide synthesis.

OHMIC HEATING: A NEW METHOD IN CHEMICAL SYNTHESIS

Ohmic heating (ΩH) is an advanced thermal processing method. In ΩH, the reaction mixture, which behaves as an electrical ohmic heater, is heated by passing an AC electrical current of high frequency through it. The heat is generated *in situ* and dissipated directly in the reaction, with high-energy efficiency, by Joule effect.

The first ΩH reactor for chemical synthesis was constructed in our group in 2013. This reactor has been used to perform several reactions, including Diels–Alder reactions, nucleophilic substitutions, N-alkylations, C-C cross coupling reactions, sequential Knoevenagel condensations followed by a hetero-Diels–Alder reaction, indium (In)-promoted reductive dehalogenations and reductive eliminations. ΩH allows a rapid and uniform heating of the reaction medium and increases the dynamics/mobility of the charged particles in solution, leading in most cases to better yields, better selectivity and shorter reaction times than classical and microwave heating methods.

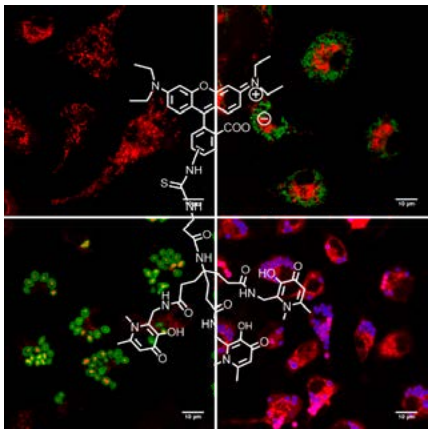
Reactor para síntese química com aquecimento óhmico, método e suas aplicações

PT 105908

HIGHLIGHTS

TUNING ANTIBACTERIAL ACTIVITY OF 3,4-HPO CHELATORS THROUGH FLUOROPHORES

Controlling the sources of Fe available to pathogens is one of the possible strategies that can be successfully targeted by novel antibacterial drugs. By analysing the effect of a variety of 3-Hydroxy-4-Pyridinone Fe chelators in the inhibition of the intramacrophagic growth of Mycobacterium avium, we have gathered information regarding the chemical properties necessary for an efficient antimycobacterial chelator. The results showed that the chelation of Fe is a determinant but not sufficient property for antimicrobial activity. The activity is strongly dependent on the presence of the xanthene fluorophore, its type and on the linker binding the fluorophore and the chelating unit. The more active compound is a rhodamine hexadentate chelator bearing N-ethyl substituents on the rhodamine framework and the thiourea linkage. Such a combination is also responsible for an enhanced uptake by macrophages, thus implying that the efficiency of rhodamine-labelled 3,4-HPO chelators as antimycobacterial agents is strongly determined by the structural features that provide a better permeation through membranes and consequently a superior ability to reach the infection target.

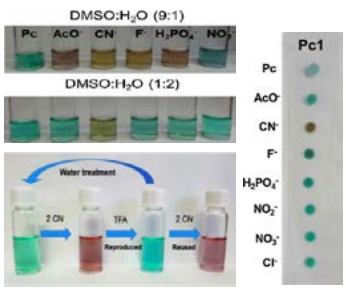


The influence of functional groups on the permeation and distribution of antimycobacterial rhodamine chelators.

Journal of Inorganic Biochemistry, 2017, 175, 138-147.

HIGHLY SELECTIVE OPTICAL CHEMOSENSOR FOR CYANIDE IN AQUEOUS MEDIUM

Starting from commercially available precursors, we developed cyanide selective chromogenic chemosensors based on metallophthalocyanines. The new compounds revealed high sensitivity for several anions (AcO^-, F^-,CN^-, NO_2^-, $H_2PO_4^-$ and OH^-) over other anions, such as Br^-, Cl^-, NO_3^- and HSO_4^-, both in DMSO and THF solutions. Surprisingly, in 1:2 DMSO:water mixtures an extremely high selectivity was observed for CN^- anion. Interestingly, the host:guest complexes formed during the sensing event can be undo by acid treatment without loss of the sensing ability of the chemosensors allowing their reuse. The selectivity of the new phthalocyanines for CN^- anion is preserved when they are adsorbed in filter paper. That allowed the preparation of a simple detection kit for monitoring cyanide anion in contaminated environments.



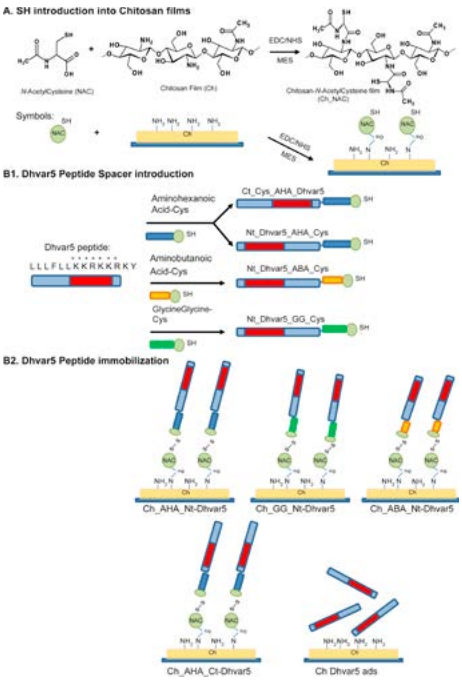
Highly selective optical chemosensor for cyanide in aqueous medium.

Sensors Actuators: B. Chemical. 2016, 224, 81-87.

HIGHLIGHTS

ANTIMICROBIAL PEPTIDE-BASED COATINGS FOR BIOMEDICAL APPLICATION

Implant-associated infection (IAI) and chronic wound infections (CWI) are a considerable burden in medical care. IAI are amongst the most common problems of in vivo implantation of any material and involve bacterial colonization and biofilm formation on the implant surface. CWI occur in individuals with alterations in the complex process of wound healing such as patients with diabetes or poor vascular supply, whose incapacity to fight infection on its onset leads to bacterial growth and subsequent establishment of mixed-species biofilms, resistant to host defenses and existing antibiotics. Also, the growing prevalence of antibiotic-resistant bacteria compromises current antibiotherapy. Antimicrobial peptides (AMP) are well-known components of the innate immune system that can be used to overcome IAI and CWI, as their relevance as alternatives to conventional antibiotics is increasing. Chemical synthesis of AMP and their covalent immobilization onto chitosan-based materials is being addressed by us, with overall results showing that the AMP-tethered surfaces reduce bacterial adhesion, which holds promise towards development of novel antimicrobial coatings for biomedical applications.

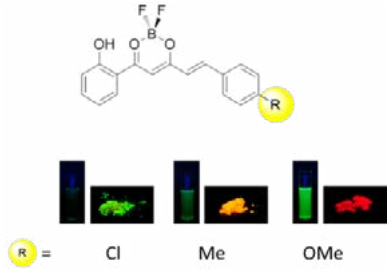


Dhvar5 antimicrobial peptide (AMP) chemoselective covalent immobilization results on higher antiadherence effect than simple physical adsorption.

Biomaterials 2015, 52, 531-538.

ALL-ORGANIC FLUOROPHORES WITH POTENTIAL APPLICATION IN LUMINESCENT MATERIALS

The fluorophores were based on a difluoroboron diketonate core, decorated with peripheral substituents to fine tune the photo-physical properties. The synthesis of the dyes involved the selective complexation of boron in a diketonate pocket and not in another, and were obtained in good yields. The dyes present good photo-physical properties in dilute solutions, and more interestingly they are highly emissive in the solid state, due to their organization into J-dimers, which prevents their self-quenching. With this design, the best dye emits in the solid state at 700 nm with a quantum yield of 12%, this performance being rare for solid state all-organic dyes. These exceptional photo-physical properties make this family of dyes promising building blocks for the preparation of luminescent materials.

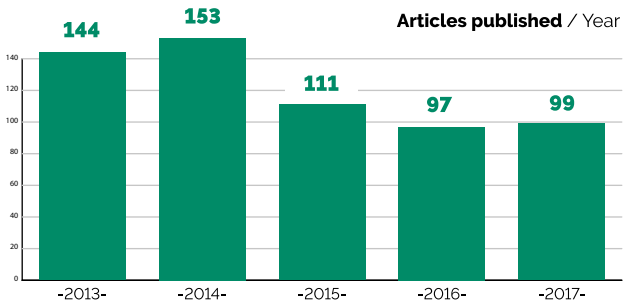


Synthesis, post-modification and fluorescence properties of boron-diketonate complexes.

European Journal of Organic Chemistry, 2015, 16, 3423-3426.

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION 2013-2017*



604 articles
5792 citations**
H-index: **68**

*From WOS core collection
**of the published articles in 2013-2017

FUNDED PROJECTS *(Representative projects)*

- **New Strategies Applied to Neuropathological Disorders**
  CENTRO-07-ST24-FEDER-002034, Artur Silva (PI),
  Total funding: 1,656,081.27 €
- **Chelators for novel therapeutic strategies**
  NORTE-07-0124-FEDER-000066, Maria Rangel (PI),
  Total funding: 972,277.08 €
- **Implementation of the facility for peptide synthesis**
  NORTE-07-0161-FEDER-000111, Paula Gomes (PI),
  Total funding: 512,407.96 €.
- **Rethinking Bacterial Cell Wall: a chemoenzymatic approach**
  FCT, PTDC/QEQ-QOR/2132/2012, Maria Manuel Marques (PI),
  Total funding: 200,000.00 €
- **(Fe)rrying plants to prevent chlorosis**
  FCT, PTDC/AGR-PRO/3515/2014, Maria Rangel (PI),
  Total funding: 199,721.00 €
- **HEDICIN - HEterocycle-DIpeptide-CINnamic acid conjugates to fight malaria**
  FCT, PTDC/QUI-QUI/116864/2010, Paula Gomes (PI),
  Total funding: 68,436.00 €

1 EU project
165 k€

9 national projects
4.17 M€

INTERNATIONAL COOPERATION AND NETWORKING

- COST Action CM1302, European Network on Smart Inorganic Polymers (SIPs), 2013-2018
- 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

OUTREACH

- Ciência Viva: "A Fábrica", "The Kitchen is a Laboratory".
- Open days for high school students.
- Organizing committee of the National Chemistry Olympics.
- Organizing committee of the 3rd European Conference of Smart Inorganic Polymers, September 14-16th 2016, FCUP, Porto.
- Chair of the 15th Iberian Peptide Meeting, February 2016, FCUP, Porto.
- Presidency of the Portuguese Chemical Society (SPQ) (Artur Silva) and the Division of Inorganic and Bioinorganic Chemistry of SPQ (Maria Rangel).
- Executive board member of the European Association for Chemical and Molecular Sciences (EuCheMS).
- Secretary of the European Peptide Society (Paula Gomes) since October 2016.
- National Portuguese representative (Paula Gomes) at Division VII - Chemistry and Human Health of the International Union for Pure and Applied Chemistry (IUPAC), reported in UPORTO news.
- The project iLIQUID has been published in several newspapers, including "Diário de Notícias", "Notícias ao minuto", "Atlas da Saúde", "Sapo", "O Jogo", "Aeiou", "Netfarma", "Sumário Atual", "Acobur", "Jornal da Madeira".
- Participation in radio and TV shows: "Consultório", Porto Canal, concerning the project iLIQUID and "90 segundos de Ciência", Antena 1, regarding the project projeto "PILING".
- Ricardo Chagas was distinguished with the SIVE OENOPPIA 2017 Prize (3rd edition), for the research work developed during his PhD on "Protein haze formation in white wine - The critical involvement of sulfur dioxide in protein aggregation mechanism".
- The journals Synfacts (DOI: 10.1055/s-0036-1591687) and Organic Process and Research Development (DOI: 10.1021/acs.oprd.7b00371) highlighted the article published by Maria Manuel Marques et al. in Organic Chemistry Letters (DOI: 10.1021/acs.orglett.7b02403) concerning an efficient protocol to attain 4-, 5-, 6-, and 7-azaindoles in one pot.
- M. Rangel and M. Vasconcelos. "The future of iron in crops". Communicating Research, December 2017, DOI 10.21820/23987073.2017.11.79. Identical information was published in portuguese newspapers, including "Observador", "Diário de Notícias", "Correiro da manhã", "O Jogo", "Ardina", among others.
- Collaboration with industry: Hovione and Sea4Us.

LABORATÓRIO ASSOCIADO
PARA A **QUÍMICA VERDE**

requimte
rede de química e tecnologia

U.PORTO

UNIVERSIDADE NOVA DE LISBOA

universidade de aveiro

NATPRO

NATURAL PRODUCTS CHEMISTRY AND BIOACTIVITY

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

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 their biological evaluation. Among natural sources, we are particularly interested in plant and animal samples, both from terrestrial and marine origin.

Research activities are focused in 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 [2018-2022]

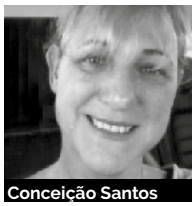
The major research objectives of the Natural Products – Chemistry and Bioactivity group are:

- 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


Carmen Pereira


Conceição Santos


David Pereira


Diana Pinto


Eduarda Fernandes


Jorge Oliveira


Lucília Saraiva

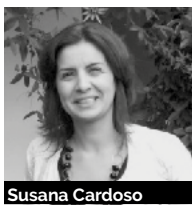

Manuela Morato


Marisa Freitas


Patrícia Valentão


★ Paula B. Andrade


Romeu Videira


Susana Cardoso

★ Group coordinator

RESEARCH TEAM

OTHER DOCTORATE RESEARCHERS
Áurea Carvalho
Mónica Válega

POST-DOCTORAL FELLOWS
Andreia Oliveira
Brígida Pinho
Daniela Ribeiro
Fátima Fernandes
Graciliana Lopes
Joana Soares
Joana Terroso
José Oliveira
Maria Dias
Nelson Gomes

PhD STUDENTS
Ana C. Andrade
Ana Gomes
Andrea Afonso
Carina Proença
Catarina Grande
Cláudia Bessa
Helena Ramos
Joana Loureiro
João Bernardo
José Oliveira
Karen João
Liliana Raimundo
Márcia Araújo
Marcelo Catarino
Maria Rocha
Mariana Barbosa
Pedro Fernandes
Rafael Mendes
Renato Pereira
Rute Nunes
Sara Moreira
Sara Reis
Sofia Domingos
Sofia Soares
Tânia Genebra
Tânia Soares
Vera Ribeiro

MSc STUDENTS
Adelaide Sousa
Ana Circunsisão
Andreia Silva
Beatriz Silva
Catarina Marçal
João Rebelo
Lídia Rocha
Maria Faustino
Miguel Ribeiro
Rafael Vilamarim
Raquel Abreu
Rute Moreira
Sílvia Rocha
Sónia Rocha
Valentina Pinheiro

RESEARCH GRANTEES
Ana Pinto
João Prada
Liliana Almeida
Mário Freitas
Nuno Ponte
Sara Sário
Susana Costa
Tânia Costa

OTHER RESEARCHERS
Rui Gonçalves

RESEARCH THEMES/
METABOLITE PROFILING OF NATURAL MATRICES

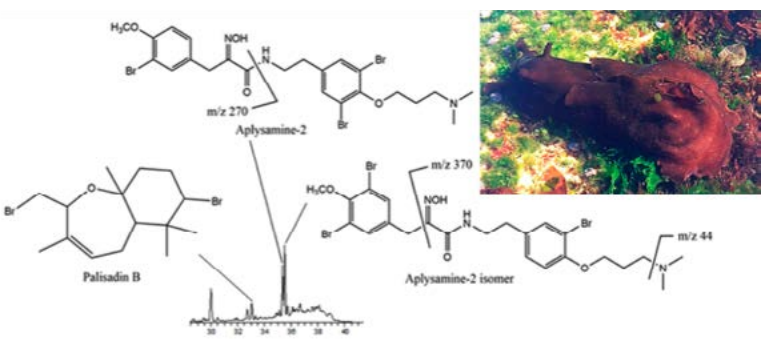
The screening of natural products for the identification of new lead structures, which can be used directly, or as templates for the development of drugs, has been one of the most successful strategies applied in drug discovery programs. Over two-thirds of the drugs placed on the pharmaceutical market are either derived from natural products or structurally similar.

The examination of natural-derived extracts and/or active fractions, to exclude unwanted compounds, is routinely applied in drug discovery, avoiding the costly isolation process. A primary concern is to assure that compounds targeted for full structural characterization are of the highest priority, regarding both structural and/or biological novelty.

In addition, due to their complexity and variability, the most complete characterization of metabolic profiles should also be done to assure the identity, authenticity, quality and safety of natural matrices, particularly of those used in human nutrition and therapeutics.

To address the issues referred above, the group will proceed with the implementation, validation and application of methodologies for the analysis of primary and secondary metabolites in natural matrices (both plants and animals, either from terrestrial and marine origin, including agro-industrial wastes), using chromatographic-based techniques. The development of methodologies to obtain purified extracts or compounds that could be used in nutraceutical industries, with particular focus on green chemistry paradigm, will be also pursued. Emphasis on species found in the Portuguese territory and waters and in Portuguese expression countries will be given.

Research also covers the impact of (a)biotic factors and emerging agents/contaminants (nanoparticles, pesticides, and radiation) in plant cell responses. Additionally, innovative solutions will be developed to modulate crops' signaling cascades, potentiating their use in new emerging sciences and economical fields, like nanoagrotechnology and plant biotechnology. For that end, functional cascades and transcripts of carbon metabolism and oxidative stress are considered.



SELECTED PUBLICATIONS

1 C. Grosso, et al. Talanta. 2014, 130, 128. doi:10.1016/j.talanta.2014.06.043

2 F. Ferreres, et al. Food Chem. 2017, 214, 678. doi:10.1016/j.foodchem.2016.07.129

3 F. Fernandes, et al. Food Chem. 2017, 233, 85. doi:10.1016/j.foodchem.2017.04.068

4 F. Ferreres, et al. Ind. Crops Prod. 2015, 77, 391. doi:10.1016/j.indcrop.2015.09.006

5 R. B. Pereira, et al. J. Funct. Foods. 2017, 37, 164. doi:10.1016/j.jff.2017.07.053

6 R. B. Pereira, et al. RSC Adv. 2015, 5, 8981. doi:10.1039/C4RA14333G

7 V. Ferreira, et al. Food Chem. 2016, 194, 117. doi:10.1016/j.foodchem.2015.07.142

8 F. Fernandes, et al. Arab. J. Chem. 2014, 10, 583. doi:10.1016/j.arabjc.2015.01.012

9 A. B. Ribeiro, et al. Food Chem. 2014, 165, 140. doi:10.1016/j.foodchem.2014.05.079

10 A. Berto, et al. Food Res. Int. 2015, 77, 236. doi:10.1016/j.foodres.2015.06.018

11 J. S. Boeing, et al. Food Chem. 2017, 220, 427. doi:10.1016/j.foodchem.2016.09.188

12 E. O. Barizão, et al. Food Res. Int. 2016, 86, 24. doi:10.1016/j.foodres.2016.05.007

13 F. Machado, et al. Environ. Exp. Bot. 2017, 140, 141. doi:10.1016/j.envexpbot.2017.05.008

14 S. Pereira, et al. Food Chem. 2014, 154, 291. doi:10.1016/j.foodchem.2014.01.019

15 M. Araújo, et al. J Photochem. Photobiol. B Biol. 2016, 162, 278. doi:10.1016/j.jphotobiol.2016.06.048

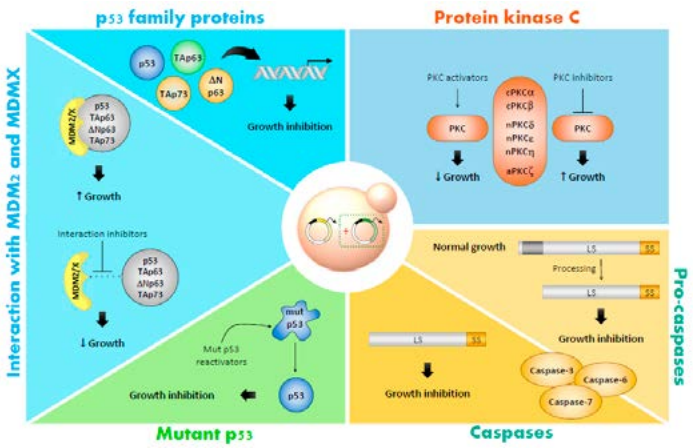
RESEARCH THEMES/
ANTICANCER DRUG DISCOVERY

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 most prevalent types of cancer, namely stomach, lung and colon. The assessment of the anticancer effects of small molecules focuses the impact upon mitochondrial function/status, caspase activity and expression, calcium dynamics and chromatin status. Overall, both caspase-dependent and –independent cell death is studied.

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 new therapeutic opportunities for cancer.

The group will continue to conduct anticancer research using a number of disease models, including 2D/3D cell culture, both from cell lines and primary cells from human donors.



SELECTED PUBLICATIONS

16 C. Sousa, et al. J. Agric. Food Chem. 2015, 63, 2083. doi:10.1021/jf505568h

17 M. A. Armentano, et al. Biomed. Res. Int. 2015, 2015, 561589. doi:10.1155/2015/561589

18 D. C. da Silva, et al. J. Steroid Biochem. Mol. Biol. 2017, 171, 178. doi:10.1016/j.jsbmb.2017.03.009

19 M. Figueiredo-González, et al. Food Chem. Toxicol. 2017, 109, 386. doi:10.1016/j.fct.2017.09.018

20 D. M. Pereira, et al. Mar Drugs. 2014, 12, 54. doi:10.3390/md12010054

21 T. C. Silva, et al. Int. J. Mol. Sci. 2017, 18, 653. doi:10.3390/ijms18030653

22 E. J. T. Silva, et al. Bioorg Med Chem. 2016, 24, 3556. doi:10.1016/j.bmc.2016.05.065

23 J. Soares, et al. Mol. Oncol. 2017, 11, 612. doi:10.1002/1878-0261.12051

24 J. Soares, et al. Oncotarget. 2016, 7, 4326. doi:10.18632/oncotarget.6775

25 J. Soares, et al. Pharmacol. Res. 2015, 95-96, 42. doi:10.1016/j.phrs.2015.03.006

26 M. Leão, et al. Exp. Cell Res. 2015, 330, 164. doi:10.1016/j.yexcr.2014.09.028

27 M. Leão, et al. Life Sci, 2015, 142, 60. doi:10.1016/j.lfs.2015.10.015

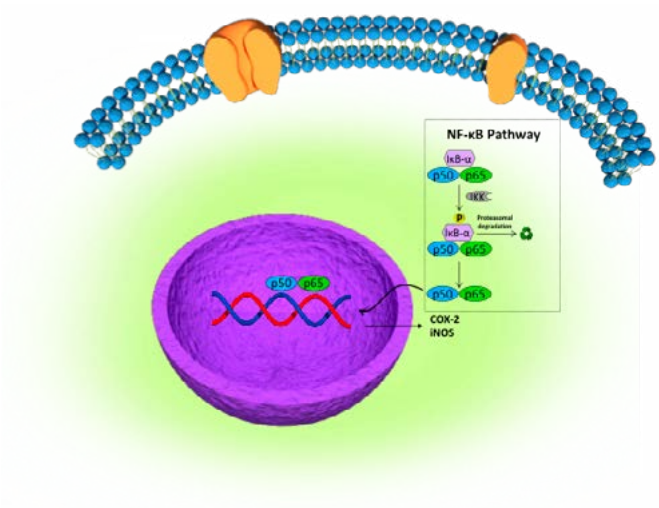
28 J. Soares, et al. Eur. J. Pharm. Sci. 2014, 66, 138. doi:10.1016/j.ejps.2014.10.006

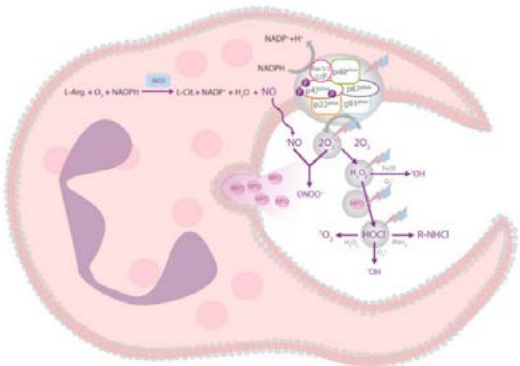
29 C. Quintas, et al. J Neuroinflamm, 2014, 11, 141. doi:10.1186/s12974-014-0141-3

30 M. Leão, et al. Biochem. Pharmacol. 2013, 85, 1234. doi:10.1016/j.bcp.2013.01.032

RESEARCH THEMES/
ANTI-INFLAMMATORY DRUG DISCOVERY

Natural and synthetic molecules have been evaluated for their ability to modulate key targets in the inflammatory cascade, such as enzymes (NADPH oxidase, inducible nitric oxide synthase, phospholipase A2, elastase and hyaluronidase) and pro-inflammatory mediators such (reactive oxygen and nitrogen species, interleukines, leukotrienes and cytokines). The crosstalk between oxidative stress and inflammation will continue to be pursued, with several cellular (human, murine) and non-cellular systems being used as research tools to this end.





SELECTED PUBLICATIONS

31 D. M. Pereira, et al. PLoS One, 2014, 9, e88341. **doi:10.1371/journal.pone.0088341**

32 E. Moita, et al. PLoS One, 2013, 8, e59131. **doi:10.1371/journal.pone.0059131**

33 G. Lopes, et al. Mar Drugs, 2014, 12, 1406. **doi:10.3390/md12031406**

34 M. J. Rebelo, et al. Food Chem. 2014, 163, 16. **doi:10.1016/j.foodchem.2014.04.070**

35 A. P. Oliveira, et al. Molecules. 2015, 20, 15766. **doi:10.3390/molecules200915766**

36 F. Ferreres, et al. Food Chem. Toxicol. 2017, 106, 8. **doi:10.1016/j.fct.2017.05.020**

37 M. Barbosa, et al. Algal Res. 2017, 28, 1. **doi:10.1016/j.algal.2017.09.009**

38 A. P. Oliveira, et al. Arab. J. Chem. 2016. **doi:10.1016/j.arabjc.2016.03.007**

39 A. P. Oliveira, et al. Chem. Biodivers. 2017, 14, e1700002. **doi:10.1002/cbdv.201700002**

40 D. Ribeiro, et al. Eur. J. Med. Chem. 2014, 72, 137. **doi:10.1016/j.ejmech.2013.11.030**

41 M. Freitas, et al. Eur. J. Med. Chem. 2014, 86, 153. **doi:10.1016/j.ejmech.2014.08.035**

42 M. E. Figueira, et al. Food Funct. 2014, 5, 3241. **doi:10.1039/c4fo00376d**

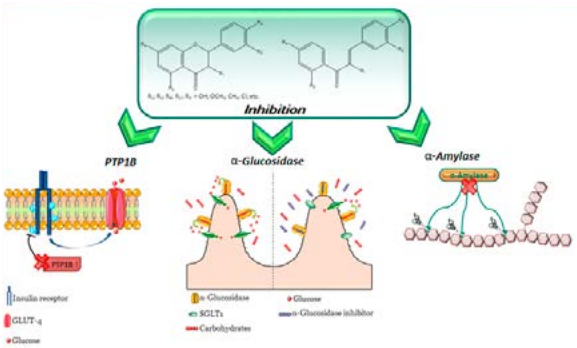
43 B. R. Pinho, et al. PLoS One, 2014, 9, e90122. **doi:10.1371/journal.pone.0090122**

44 D. Ribeiro, et al. Inflammation, 2015, 38, 858. **doi:10.1007/s10753-014-9995-x**

45 J. Rocha, et al. Basic. Clin. Pharmacol. Toxicol. 2015, 116, 398. **doi:10.1111/bcpt.12335**

RESEARCH THEMES/ ANTIDIABETIC DRUG DISCOVERY

Diabetes mellitus is a common chronic disease in our Society. The use of antidiabetic drugs has been increasing in Europe, and Portugal is no exception. Despite the therapeutics evolution, the currently available antidiabetic drugs do not present the desired efficacy and are associated with serious adverse side effects. The group works to develop new antidiabetic drugs that may constitute clinical alternatives in the future. Polyphenols have been considered a potential alternative strategy for the development of effective and safe anti-diabetic drugs. In this sense, this research group wants to uncover the best polyphenol scaffold to modulate enzymatic diabetic targets leading to an innovative treatment of type 2 diabetes.



SELECTED PUBLICATIONS

46 J. Collado-González, et al. Food Chem. 2017, 235, 298. **doi:10.1016/j.foodchem.2017.04.171**

47 M. Figueiredo-González, et al. J. Pharm. Biomed. Anal. 2016, 118, 322. **doi:10.1016/j.jpba.2015.10.042**

48 D. Russo, et al. Int. J. Mol. Sci. 2015, 16, 17696. **doi:10.3390/ijms160817696**

49 F. Ferreres, et al. Food Chem. 2013, 136, 1390. **doi:10.1016/j.foodchem.2012.09.089**

50 A. P. Oliveira, et al. J. Agric. Food Chem. 2013, 61, 8650. **doi:10.1021/jf401884u**

51 C. Proença, et al. J. Enzyme Inhib. Med. Chem. 2017, 32, 1216. **doi:10.1080/14756366.2017.1368503**

52 P. Guedes-Dias, et al. Biochim. Biophys. Acta - Mol. Basis Dis. 2015, 1852, 2484. **doi:10.1016/j.bbadis.2015.08.012**

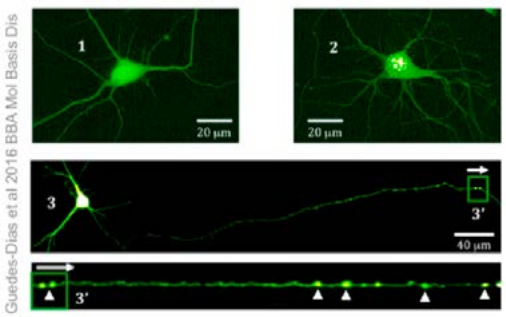
53 B. R. Pinho, et al. Pharmacol. Res. 2016, 103, 328. **doi:10.1016/j.phrs.2015.11.024**

54 D. C. da Silva, et al. J. Steroid Biochem. Mol. Biol. 2017, 171, 178. **doi:10.1016/j.jsbmb.2017.03.009**

RESEARCH THEMES/ PROTEOSTASIS

Proteostasis is a designation that includes a wide range of cellular processes related to the quality control of the proteome. The balance of the proteome is essential to most cellular processes and, in order to this balance to be maintained, it is essential to selectively degrade short-lived, misfolded and/or defective proteins

The group is interested in the discovery of proteostasis modulators, specifically molecules capable of targeting the endoplasmic reticulum and the unfolded protein response, as well as proteasome inhibitors, which can have applications both in cancer, inflammatory diseases and neurodegeneration.

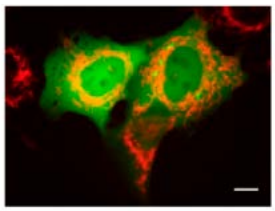


RESEARCH THEMES/ NEURODEGENERATIVE DISEASES

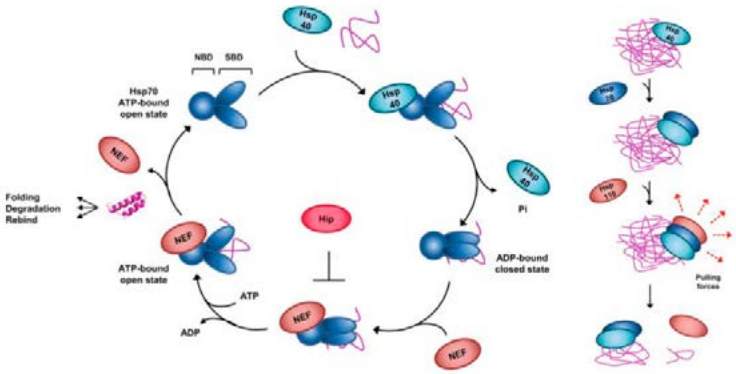
The group is focused on the initial stages of brain degeneration associated with Huntington's, Parkinson's and Alzheimer's diseases (HD, PD and AD), under the working hypothesis that mitochondrial dysfunction is one the key early features transversal to different such diseases. Thus, the problem of age-related neurodegeneration will be addressed considering different therapeutic strategies involving the modulation mitochondrial function (e.g. energy, membrane lipids, homeostasis and signals).

Mitochondrial damage in HD may arise from the production of reactive oxygen species (ROS) induced by huntingtin (mHtt), suggesting that defending mitochondria from ROS should afford neuroprotection. In this context, we will test the hypotheses that promoting mHtt clearance and preventing mitochondrial oxidative damage, hold disease-modifying potential in HD.

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. Pre-clinical models of AD and PD will be used to prove this new concept therapy and to investigate the molecular mechanisms underlying the homeostatic interconnectivity among mitochondrial lipidome, bioenergetic metabolism and the cellular redox state will in brain cells.



HUNTINGTIN PROTEOSTASIS AND MITOCHONDRIA



SELECTED PUBLICATIONS

55 F. Ferreres, et al. Phytochem. Anal. 2013, 24, 534. doi:10.1002/pca.2429

56 F. Ferreres, et al. Food Chem. Toxicol. 2013, 57, 91. doi:10.1016/j.fct.2013.03.012

57 P. Costa, et al. Food Chem. Toxicol. 2013, 57, 69. doi:10.1016/j.fct.2013.03.006

58 F. Ferreres, et al. Phytochem. Anal. 2014, 25, 453-460. doi:10.1002/pca.2515

59 F. Ferreres, et al. J. Pharm. Biomed. Anal. 2014, 88, 157. doi:10.1016/j.jpba.2013.08.040

60 V. F. Monteiro-Cardoso, et al. J. Alzheimers Dis. 2015, 43, 1375. doi:10.3233/JAD-141002

61 V. F. Monteiro-Cardoso, et al. Curr Alzheimer Res, 2015, 12, 100. doi:10.2174/1567205012666150204124852

62 C. Pereira, et al. Exp. Cell Res. 2015, 333, 73. doi:10.1016/j.yexcr.2015.02.018

63 P. Guedes-Dias, et al. Biochim. Biophys. Acta – Mol. Basis Dis. 2013, 1832, 1345. doi:10.1016/j.bbadis.2013.04.005

64 F. Bruni, et al. PLoS One, 2013, 8, e64670. doi:10.1371/journal.pone.0064670

65 B. R. Pinho, et al. Br. J. Pharmacol. 2013, 169, 1072. doi:10.1111/bph.12186

66 A. Almalki, et al. Biochim. Biophys. Acta – Mol. Basis Dis. 2014, 1842, 56. doi:10.1016/j.bbadis.2013.10.008

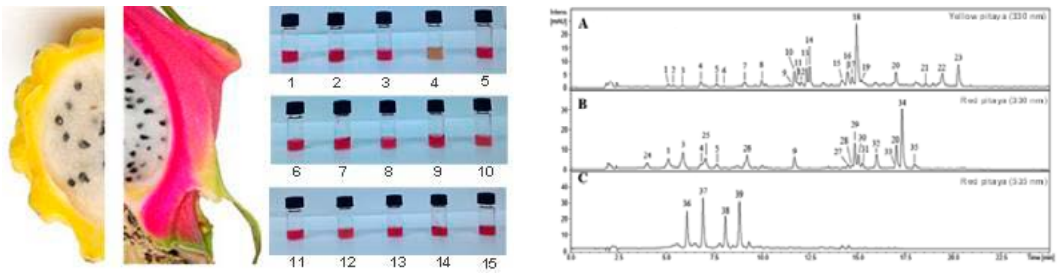
67 P. Guedes-Dias, et al. Biochim. Biophys. Acta – Mol. Basis Dis. 2015, 1852, 2484. doi:10.1016/j.bbadis.2015.08.012

68 B. R. Pinho, et al. Pharmacol. Res. 2016, 103, 328. doi:10.1016/j.bbadis.2015.08.012

HIGHLIGHTS

ECO-FRIENDLY METHODS TO EXTRACT BIOACTIVE COMPOUNDS FROM AGRO-INDUSTRIAL WASTE

A green microwave-assisted extraction of high value-added functional compounds from exotic fruits' peels was optimized by Box-Behnken design. Cinnamoyl derivatives, flavonoid derivatives and betacyanins were identified by HPLC–DAD–ESI/MSn in yellow and white-fleshed red pitayas peel. It was demonstrated that it is possible to reuse these by-products to recover compounds for pharmaceutical, cosmetics and food industries, thus contributing to a sustainable bio-based economy.

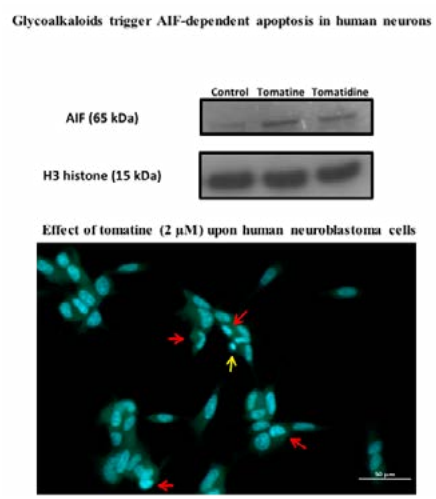


Optimization of the recovery of high-value compounds from pitaya fruit by-products using microwave-assisted extraction

Food Chemistry, 2017, 230, 463-474.

ANTICANCER AND ANTI-INFLAMMATORY MOLECULES FROM TOMATO PLANT AND SPINY SEA STAR

Sterols and alkaloids found in sea stars and anemones were shown to modulate key enzymes and inflammatory signaling cascades at non-cytotoxic concentrations, being potential new anti-inflammatory agents to develop multi-target approaches for several human diseases connected with chronic inflammation. In the case of tomato glycoalkaloids, we have shown they are neurotoxic in human cells. Also, the anticancer activity of a lipophilic sea star extract was demonstrated, with identification of the main compounds responsible for the cell cycle arrest and apoptosis with involvement of the endoplasmic reticulum.



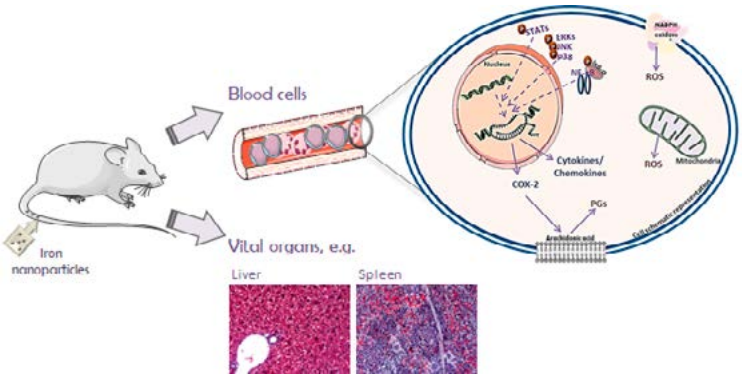
Palmitic acid and ergosta-7,22-dien-3-ol contribute to the ER-stress-mediated apoptotic effect and cell cycle arrest of an extract from *Marthasterias glacialis* L. in neuroblastoma cells.

Marine Drugs, 2014, 12, 54-68.

HIGHLIGHTS

IRON OXIDE NANOPARTICLES TRIGGER INFLAMMATION *IN VIVO*

The *in vitro* study of coated and non-coated iron oxide nanoparticles (IONs) provided evidence of cytokine activation in human blood cells through TAK1, p38 MAPK and JNK pro-inflammatory pathways. IONs did not cause severe organ damage in CD-1 mice following acute administration. However, they accumulate mainly in liver and spleen, being able to trigger an inflammatory process *in vivo*.

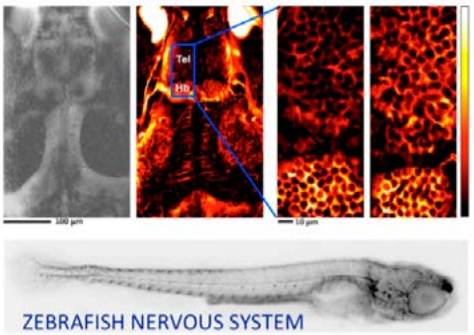


Quantitative histochemistry for macrophage biodistribution on mice liver and spleen after the administration of a pharmacological relevant dose of polyacrylic acid-coated iron oxide nanoparticles.

Nanotoxicology, 2017,11, 256-266.

ZEBRAFISH – AN ADEQUATE MODEL FOR STUDYING HISTONE DEACETYLASES

Zebrafish as animal model for Parkinson Disease (PD) was established considering the main behavioral and metabolic features that characterize the PD phenotypes. The functional homology of its histone deacetylases HDAC1 and HDAC6 isoforms was revealed. This study highlighted parameters dependent on the integrity of zebrafish neuronal circuits as a valuable complement to cell-based studies. Also, the demonstration of the feasibility of targeting HDAC1 and 6 in zebrafish paves the way for future studies investigating KDAC modulators in other disease contexts in this high-throughput model organism.



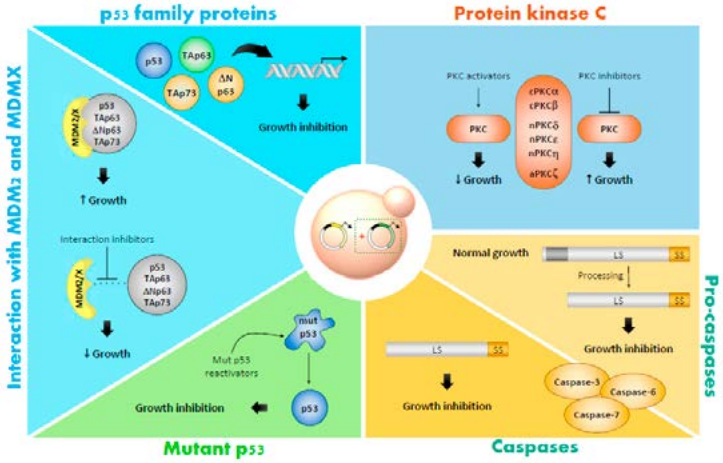
Pharmacological modulation of HDAC1 and HDAC6 in vivo in a zebrafish model: Therapeutic implications for Parkinson's disease.

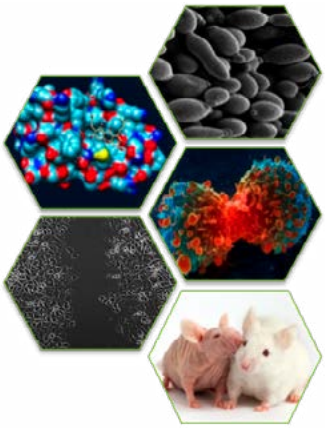
Pharmacological Research, 2016, 103, 328-39.

HIGHLIGHTS

YEAST MODELS AS SCREENING TOOLS FOR HUMAN DISEASES

Innovative yeast targeted screening approaches were developed and used to identify the tryptophanol-derived oxazoloisoindolinones SLMP53-1, as a novel reactivator of wild-type (wt) and mutant p53, as well as DIMP53-1 as a novel dual inhibitor of the p53-MDM2/MDMX interactions. Using human tumor cell lines and xenograft mouse models, it was shown that both SLMP53-1 and DIMP53-1 have multifunctional activity targeting the major hallmarks of cancer through its antiproliferative, proapoptotic, antiangiogenic, anti-invasive and antimigratory properties. Additionally, they did not reveal toxic side effects in animal models. These preclinical results indicate that SLMP53-1 and DIMP53-1 are promising drug candidates in anticancer therapy.



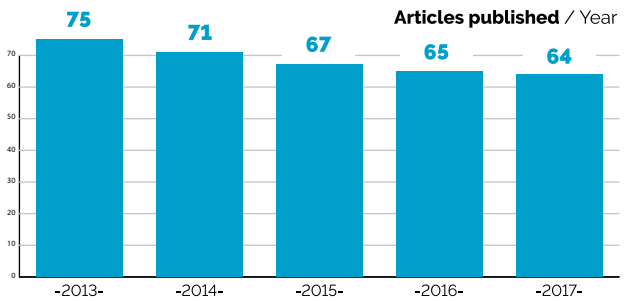


A yeast model of the Parkinson's disease-associated protein Parkin.

Experimental Cell Research, 2015, 333: 73-79.

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION 2013-2017*



342 articles
8185 citations**
H-index: **64**

**From WOS core collection*
***of the published articles in 2013-2017*

FUNDED PROJECTS *(Representative projects)*

- BIO.REM: Integrating multiple toxicological BIOmarkers in a phytoREMemediation assay of Pb and Cd contaminated sites
  FCT, PTDC/AAC-AMB/112804/2009, Maria Santos (PI).
  Total Funding: € 170,336.00.
- KDAC inhibition and intracellular dynamics: impact on NEUROnal development, survival and transmission
  FCT, PTDC/NEU-NMC/0237/2012, Jorge Oliveira (PI).
  Total Funding: € 143,983.00.
- PRE-NEURO-HD: Targeting huntingtin proteostasis and mitochondria to prevent neuronal dysfunction in Huntington's disease
  FCT, PTDC/NEU-NMC/0412/2014, Jorge Oliveira (PI).
  Total funding: € 198,514.00.
- 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.
- Functional, molecular and pharmacological studies of p53 family proteins: from yeast to human cells
  FCT, PTDC/SAU-FAR/110848/2009, Lucília Saraiva (PI),
  Total Funding: € 168,200.00.
- Carotenoid oxidation by reactive oxygen and nitrogen species: Chemical analysis and biological activity
  FCT, PTDC/QEQ-QAN/1742/2014, Eduarda Fernandes (PI),
  Total Funding: € 148,800.00.

9 EU projects
1.2 M€

19 national projects
2.07 M€

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 Científicas, Murcia, Spain
- Università degli Studi della Basilicata, Italy
- Instituto Nacional de Estudos e Pesquisas (INEP), Guinea-Bissau

OUTREACH

- Ciência Viva - Semana da Ciência e da Tecnologia 2015. "Compostos bioactivos: da natureza ao medicamento". Pharmacognosy Laboratory, Open day. FFUP, Porto, November 28, 2015.
- Fascination of plants day. Pharmacognosy Laboratory, Open day. "Plants and Pharmacy: Experiments in the Laboratory". FFUP, Porto, May 20, 2017.
- Science Awareness Initiative. "Projeto SEI: Sociedade, Escola e Investigação". Partnership between FFUP (Laboratory of Pharmacognosy) and Câmara Municipal do Porto. 2014-2015 and 2015-2016.


LABORATÓRIO ASSOCIADO
PARA A QUÍMICA VERDE


requimte
rede de química e tecnologia


U.PORTO


UNIVERSIDADE
NOVA
DE LISBOA


universidade
de aveiro

AnalytDev

ANALYTICAL DEVELOPMENT

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

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 [2018-2022]

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


Clara Sousa


Célia Amorim


Eduarda Silva


Helena Soares


João Paulo Noronha


João Prior


José A. Rodrigues


José Luís Costa Lima


Júlia Magalhães


Mafalda Sarraguça


★ Marcela Segundo


Marco G. Silva


M. Beatriz Quinaz


M. Conceição Branco


Ricardo Páscoa

★ Group coordinator

RESEARCH TEAM

OTHER DOCTORATE RESEARCHERS

Aquiles Barros
Cristina Couto
Jorge Sarraguça
M. Gabriela Ribeiro
Patrícia Peixoto
Paulo Almeida
Rita Duarte
Rui Lapa

POST-DOCTORAL FELLOWS

Inês Valente
J. Rodrigo Santos
Luís Gonçalves
Luísa Barreiros
Raquel Garcia

PhD STUDENTS

Álvaro Torrinha
Bruno Soares
Bruno Leite
Diana Gonçalves
Inês Ferreira
Inês Ramos
Luís M. Fernandes
Manuel Alves
M. José Pereira
Michaela Kohlová
Patrícia Matos
Renato Gil
Rosa Couto
Sandia Machado
Sara Marques
Sara Fernandes

MSc STUDENTS

Ana Rita Pereira
Flávia Freitas
Flávia Mendes
Manuela Sousa
Mariana Carvalho
Marisa Rodrigues
Pedro Cruz
Raquel Garcia
Rute Martins
Sílvia Rocha
Sónia Pedreiro

RESEARCH GRANTEES

Adriana Costa
Ana Cunha
Ana Margarida Teixeira
Ana Telma Leal
Carina Vieira
Catarina Augusto
Catarina Martins
Eduardo Moreira
Gabriela Guerra
Liliana Cordeiro
Maria João Gomes
Pedro Brandão
Rui Ramos

OTHER RESEARCHERS

Maria Isabel Rocha

RESEARCH THEMES/
INNOVATIVE SAMPLE TREATMENT

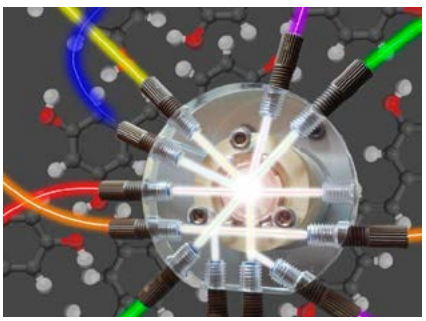
Sample treatment is the bottleneck of analytical procedures as it takes about 70% of total analysis time and is labor intensive. Almost all advanced instrumental methods of analysis require samples to be as much as possible free from interfering molecules, namely biomolecules and dissolved salts. Further, 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.



SELECTED PUBLICATIONS

1 A. C. Alves, et al. Talanta. 2016, 146, 369. doi:10.1016/j.talanta.2015.08.070

2 P. F. Brandão, et al. Anal. Bioanal. Chem. 2017, 409, 2885. doi:10.1007/s00216-017-0233-x

3 R. C. Ferreira, et al. Analyst. 2015, 140, 3648. doi:10.1039/c5an00196j

4 R. Garcia, et al. Electrophoresis. 2016, 37, 1916. doi:10.1002/elps.201600073

5 M. A. Maia, et al. Talanta. 2017, 166, 162. doi:10.1016/j.talanta.2017.01.040

6 M. V. Osório, et al. J. Food Compos. Anal. 2016, 45, 141. doi:10.1016/j.jfca.2015.10.007

7 I. I. Ramos, et al. Anal. Methods. 2014, 6, 3622. doi:10.1039/c3ay42185f

8 R. M. Ramos, et al. Talanta. 2014, 124, 146. doi:10.1016/j.talanta.2014.02.026

9 D. M. C. Rodrigues, et al. Talanta. 2015, 141, 220. doi:10.1016/j.talanta.2015.04.013

10 M. Rosende, et al. Environ. Sci. Technol. 2013, 47, 11668. doi:10.1021/es401872j

11 M. Rosende, et al. Anal. Chim. Acta. 2014, 842, 1. doi:10.1016/j.aca.2014.06.033

12 C. M. Santos, et al. Analyst. 2013, 138, 7233. doi:10.1039/c3an00766a

13 T. F. A. Sousa, et al. Biomed. Chromatogr. 2014, 28, 680. doi:10.1002/bmc.3089

14 I. M. Valente, et al. J. Chromatogr. A. 2013, 1308, 58. doi:10.1016/j.chroma.2013.08.014

15 I. M. Valente, et al. J. Chromatogr. A. 2013, 1271, 27. doi:10.1016/j.chroma.2012.11.026

16 I. M. Valente, et al. Bioanalysis. 2015, 7, 2187. doi:10.4155/bio.15.142

17 I. M. Valente, et al. Talanta. 2017, 167, 747. doi:10.1016/j.talanta.2017.01.091

18 L. Zelená, et al. Anal. Bioanal. Chem. 2016, 408, 971. doi:10.1007/s00216-015-9194-0

RESEARCH THEMES/
MULTIDIMENSIONAL METHODS FOR TOTAL ANALYSIS

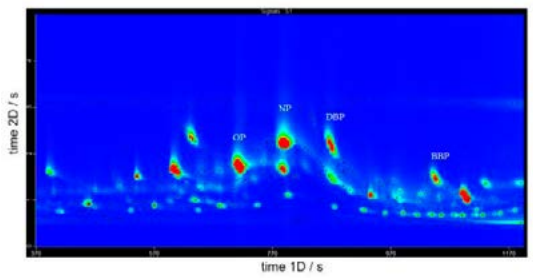
One of the trends in analytical sciences is the implementation of comprehensive methods, able to extract the maximum amount of information from a given sample within a single analytical run. This is possible using multidimensional setups, consisting of several detectors in series, orthogonal separative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

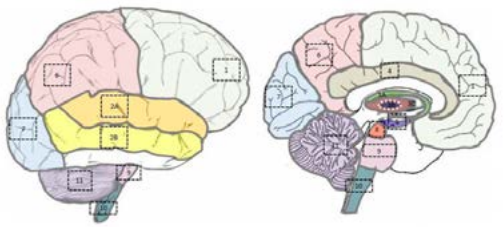
Research efforts in this area will address bidimensional gas chromatography coupled to mass spectrometry for evaluation of traditional products and food commodities, aiming to collect science-based evidence for promotion of economic value added.

Orthogonal separative methods (eg. 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

1 L. Barreiros, et al. J. Pharm. Biomed. Anal. 2017, 136, 120. doi:10.1016/j.jpba.2016.12.028

2 P. F. Brandão, et al. J. Agric. Food Chem. 2017, 65, 1037. doi:10.1021/acs.jafc.6b05370

3 A. R. Carvalho, et al. Food Res. Int. 2017, 99, 485. doi:10.1016/j.foodres.2017.06.008

4 N. Costa, et al. ChemPlusChem. 2013, 78, 1466. doi:10.1002/cplu.201300229

5 A. R. Freitas, et al. Diagn. Microbiol. Infect. Dis. 2017, 87, 299. doi:10.1016/j.diagmicrobio.2016.12.007

6 T. Melo, et al. J. Mass Spectrom. 2013, 48, 1357. doi:10.1002/jms.3301

7 T. Melo, et al. Anal. Chem. 2016, 88, 2622. doi:10.1021/acs.analchem.5b03407

8 T. Melo, et al. Free Radic. Biol. Med. 2017, 106, 219. doi:10.1016/j.freeradbiomed.2017.02.033

9 M. A. Moreira, et al. J. Braz. Chem. Soc. 2015, 26, 531. doi:10.5935/0103-5053.20150006

10 N. F. F. Moreira, et al. Water Res. 2016, 94, 10. doi:10.1016/j.watres.2016.02.003

11 A. R. Neves, et al. J. Agric. Food Chem. 2015, 63, 3114. doi:10.1021/acs.jafc.5b00390

12 E. Pinto, et al. J. Toxicol. Environ. Health Part A Curr. Iss. 2015, 78, 848. doi:10.1080/15287394.2015.1051177

13 C. Quintelas, et al. Int. J. Pharm. 2015, 492, 199. doi:10.1016/j.ijpharm.2015.07.005

14 A. N. Ramdzan, et al. J. Chromatogr. A. 2016, 1429, 284. doi:10.1016/j.chroma.2015.12.051

15 A. Santos, et al. Forensic Sci. Int. 2015, 247, 62. doi:10.1016/j.forsciint.2014.12.006

16 M. A. Segundo, et al. J. Pharm. Biomed. Anal. 2016, 120, 290. doi:10.1016/j.jpba.2015.12.033

17 A. S. Silva, et al. RSC Adv. 2017, 7, 8581. doi:10.1039/c6ra27531a

18 S. Silva, et al. RSC Adv. 2016, 6, 92065. doi:10.1039/c6ra16769a

19 C. A. Teixeira dos Santos, et al. Food Res. Int. 2017, 102, 504. doi:10.1016/j.foodres.2017.09.018

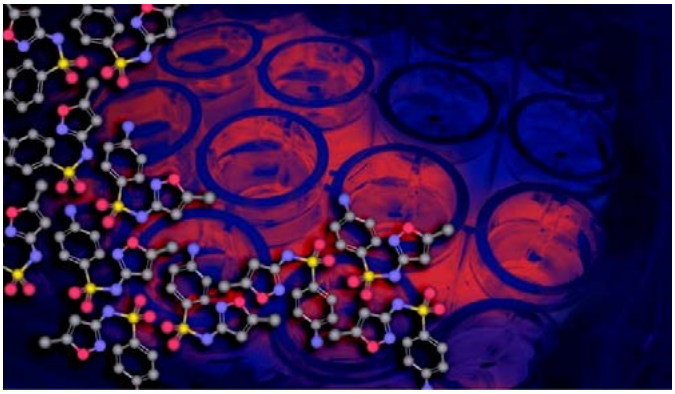
RESEARCH THEMES/
GREENER ANALYTICAL METHODS

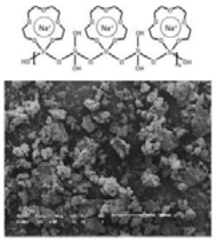
Sustainability is the key word in modern Chemistry. Analytical developments must embrace this paradigm and research within this topic will focus on providing analytical solutions with low environmental impact.

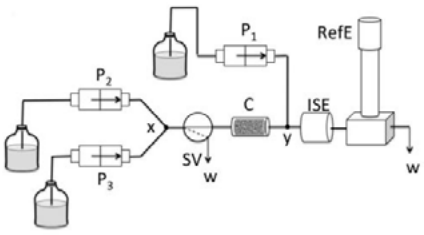
For this, methods based on physical-chemical properties of target analytes will be sought, namely using electrochemical-based detectors and infrared/Raman spectroscopy associated to data fusion chemometrics.

Innovative sensor construction, using 3-D printing for 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 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.







SELECTED PUBLICATIONS

1 T. A. Catelani, et al. Food. Bioprocess Technol. 2017, 10, 630. doi:10.1007/s11947-016-1843-6

2 R. A. S. Couto, et al. J Electrochem Soc. 2017, 164, B103. doi:10.1149/2.0561704jes

3 R. A. S. Couto, et al. Sensors. 2016, 16. doi:10.3390/s16071015

4 T. Cordeiro, et al. Mol. Pharm. 2017, 14, 3164. doi:10.1021/acs.molpharmaceut.7b00386

5 M. Cuartero, et al. Anal. Chim. Acta. 2013, 787, 57. doi:10.1016/j.aca.2013.05.038

6 R. Gil, et al. Electroanalysis. 2015, 27, 2809. doi:10.1002/elan.201500275

7 L. M. Magalhães, et al. Talanta. 2016, 147, 460. doi:10.1016/j.talanta.2015.10.022

8 J. G. Martins, et al. J. Environ. Sci. Health Part A Toxic Hazard. Subst. Environ. Eng. 2014, 49, 344. doi:10.1080/10934529.2014.846706

9 F. T. C. Moreira, et al. Sens Actuators, B Chem. 2013, 182, 733. doi:10.1016/j.snb.2013.03.099

10 F. T. C. Moreira, et al. Biosens. Bioelectron. 2014, 56, 217. doi:10.1016/j.bios.2013.12.052

11 F. T. C. Moreira, et al. Microchim. Acta. 2015, 182, 975. doi:10.1007/s00604-014-1409-0

12 R. N. M. J. Páscoa, et al. Food. Bioprocess Technol. 2015, 8, 865. doi:10.1007/s11947-014-1454-z

13 R. B. Queirós, et al. Sens Actuators, B Chem. 2013, 181, 766. doi:10.1016/j.snb.2013.01.062

14 T. S. C. R. Rebelo, et al. Anal. Chim. Acta. 2014, 850, 26. doi:10.1016/j.aca.2014.08.005

15 M. C. Sarraguça, et al. Int. J. Pharm. 2014, 471, 478. doi:10.1016/j.ijpharm.2014.06.003

16 J. M. G. Sarraguça, et al. Analyst. 2016, 141, 4410. doi:10.1039/c6an00247a

17 M. C. Sarraguça, et al. Int. J. Pharm. 2016, 513, 1. doi:10.1016/j.ijpharm.2016.09.010

18 A. F. T. Silva, et al. Int. J. Pharm. 2017, 520, 29. doi:10.1016/j.ijpharm.2017.01.052

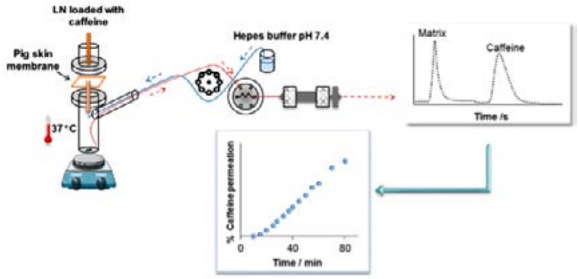
19 T. F. A. Sousa, et al. Sens Actuators, B Chem. 2013, 176, 660. doi:10.1016/j.snb.2012.09.016

20 Á. Torrinha, et al. Electroanalysis. 2017, 29, 1566. doi:10.1002/elan.201600738

HIGHLIGHTS

AUTOMATION FOR MONITORING DYNAMIC SYSTEMS

Assessment of dynamic properties requires suitable, real-time methods because the target concentration will change along time. Automatic strategies were developed to evaluate the permeation of compounds through synthetic membranes or cell layers. In this scope, a low-pressure liquid chromatography system for the on-line quantification of caffeine loaded into lipid nanoparticles that permeates pig skin was proposed. The apparatus includes a Franz diffusion cell with computer-controlled sampling that allows collection of acceptor solution with automatic compensation for sample withdrawing, and a C-18 reversed-phase monolithic column where separation of caffeine from other matrix elements is performed before spectrophotometric quantification. Due to the real time automated sampling and high throughput, transdermal permeation profiles of nanoformulations can be established within a time frame seldom observed by conventional techniques.

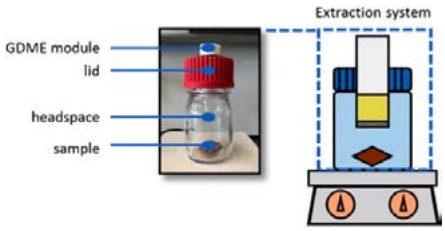


On-line automated evaluation of lipid nanoparticles transdermal permeation using Franz diffusion cell and low-pressure chromatography

Talanta, 2016, 146, 369-374.

TARGETING VOLATILES BY GAS-DIFFUSION MICROEXTRACTION

Gas-diffusion microextraction (GDME) targets volatile and semi-volatile analytes present in liquid and solid samples. Its implementation is based on a dedicated device developed by LAQV researchers, where sample and acceptor fluids are separated by gas-permeable membranes. In fact, GDME is one of the few membrane-based techniques where solids are directly analyzed, without previous treatment or manipulation. The main advantage of this analytical proposal is the built-in capabilities for determination of labile fractions, surpassing reference methods. GDME is also amenable to direct coupling to different detectors (spectrophotometric, fluorimetric or electrochemical) as removal of most matrix interferences is performed in the extraction step and derivatization reagents can be added to the acceptor fluid.



Gas-diffusion microextraction coupled with spectrophotometry for the determination of formaldehyde in cork agglomerates

Analytical and Bioanalytical Chemistry, 2017, 409, 2885-2892.

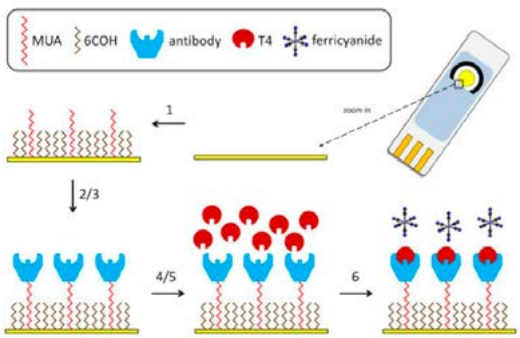
HIGHLIGHTS

SENSORS FOR REAL-LIFE APPLICATIONS

Sensors based on electrochemical features are particularly tailored for real-life applications. They are adaptable to both field and lab conditions, providing almost immediate results and making them suitable for both point-of-care and screening analysis. T4, a thyroid hormone with many relevant roles in human metabolism, was determined with an antibody-based biosensor, consisting on a multi thiol self-assembled monolayer whereas anti-serpina7 polyclonal antibody was attached. Electroanalytical measurements were performed by impedance on a ferricyanide redox probe, achieving detection of target hormone above 4 ppb.

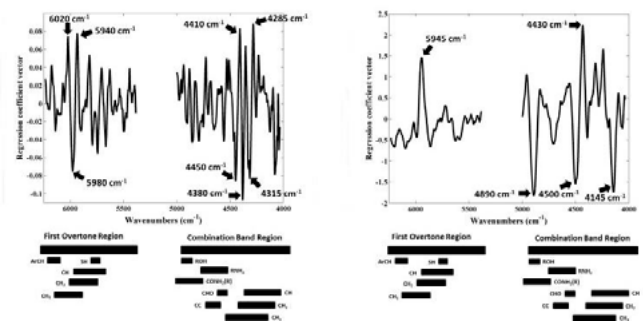
FAST, NON-INVASIVE SCREENING METHODS FOR INDUSTRIAL APPLICATIONS

Industry requires suitable tools for monitoring and quality control. Ideally, these tools should be non-invasive (to prevent contamination of production line, for instance) and non-destructive (to avoid economic losses from sampling for control purposes). Real-time capabilities and multi-parametric features are also sought. Infra-red spectroscopy methods offer suitable solutions for this field, as shown by several successful applications developed for pharmaceutical and food industries. A rapid and non-destructive methodology for assessing the potential of spent coffee grounds as a source of bioactive compounds was developed using near-infrared spectroscopy. High-throughput evaluation of three main phenolics (caffeic acid, (+)-catechin and chlorogenic acid) and three methylxanthines (caffeine, theobromine and theophylline) was implemented in spent coffee grounds samples obtained from different coffee brands and diverse coffee machines.



SAM-based immunosensor for the analysis of thyroxine (T4)

Journal of the Electrochemical Society, 2017, 164, B103-B106.



Rapid assessment of bioactive phenolics and methylxanthines in spent coffee grounds by FT-NIR spectroscopy

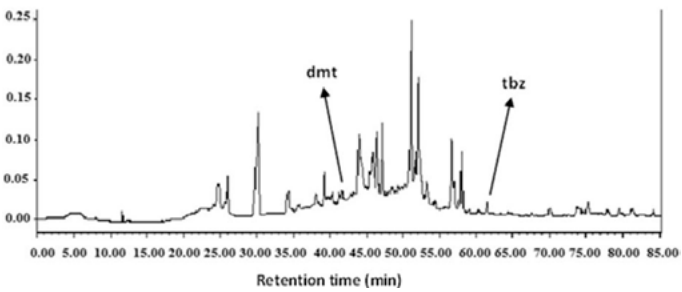
Talanta, 2016, 147, 460-467.

HIGHLIGHTS

MOLECULAR IMPRINTING FOR SELECTIVE ANALYSIS

Molecular imprinting consists of preparing solid material where cavities are created by template molecules. After removal of the template, these cavities will have affinity to the template molecules or their analogues, rendering highly selective material. Their application to analytical development can follow two paths: (i) selective adsorbents for sample treatment prior to chromatographic analysis or (ii) selective recognition elements in sensors. The first approach was implemented for trace analysis of pesticide residues in olive oil, using a dual-layer cartridge packed with molecularly imprinted polymers targeting dimethoate and terbuthylazine.

*From WOS core collection
**of the published articles in 2013-2017

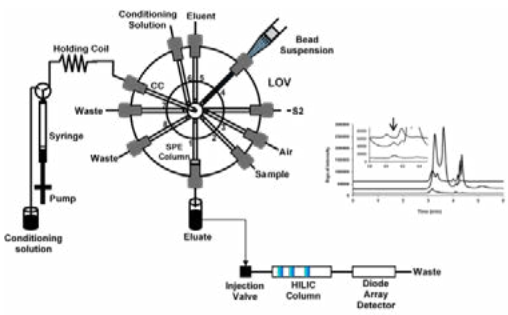


Dual-layer solid-phase extraction based on molecular imprinting technology: Seeking a route to enhance selectivity for trace analysis of pesticide residues in olive oil

Electrophoresis, 2016, 37, 1916-1922.

INNOVATIVE SAMPLE TREATMENT COUPLED TO CHROMATOGRAPHY FOR SOCIETAL CHALLENGES

Current societal challenges demand access to more information regarding environmental conditions, health status, and commodities' quality. This means a growing pressure on analysts, who have to deal with multicomponent analysis in complex samples, targeting low concentrations. In this context, sample is undeniably the bottleneck concerning analytical throughput and automation circumvents this problem. At-line automatic micro-solid phase extraction method for the determination of salivary cotinine followed by its analysis via hydrophilic interaction liquid chromatography was developed. Based on the bead injection concept incorporated in the mesofluidic lab-on-valve platform, all steps of solid-phase extraction procedure were performed without human intervention, providing a high-throughput method for evaluation of environmental tobacco exposure.

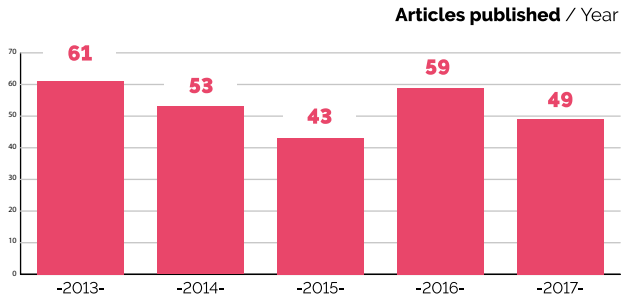


Determination of salivary cotinine through solid phase extraction using a bead-injection lab-on-valve approach hyphenated to hydrophilic interaction liquid chromatography

Journal of Chromatography A, 1429, 2016, 284-291

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION 2013-2017*



265 articles
2079 citations
H-index: **51**

*From WOS core collection
**of the published articles in 2013-2017

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.
- **"Grapevine cultivars metabolic modelling combining weather, soil and non-invasive in-situ vibrational spectroscopy data"**
  FCT, P2020-PTDC/AGRPRO/6817/2014, José Luís Costa Lima (PI).
  Total Funding: € 143,071.00.
- **"On-Line Ammonium Analyzer for water recycling systems, European Space Agency"**
  4000113078/14/NL/SFe, Alberto Araújo (local PI).
  Total Funding: € 76,800.00.
- **"Development and application of fast methodology for evaluation of UV filters levels in coastal bathing waters"**
  FCT, PTDC/AAC-AMB/104882/2008, Marcela Segundo (PI).
  Total Funding: € 180,609.00.
- **"Environmental risk factors for cardiovascular disease in Porto Metropolitan Area",**
  FCT, PTDC/SAU-ESA/108871/2008, Agostinho Almeida (PI).
  Total Funding: € 35,000.00.

2 EU projects
80 k€

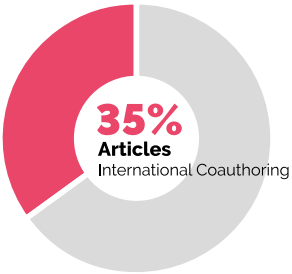
9 national projects
1.64 M€

4 industry-financed projects
1.15 M€

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.
- SENER- Ingenieria y Construccion, Barcelona, Spain
- International Union of Pure and Applied Chemistry (IUPAC) project (#2013-015-1-500), 2013-2015

- Main strategic partner of STARSS - Specialized Team for Advanced Research on Separation Science (CZ.02.1.01/0.0/0 .0/15_003/0000465), Charles University, Czech Republic
- Team members of projects CTM2014-56628-C3-3-R and CTM2014-61553-EXPN, Manuel Miró (PI), Universitat de les Illes Baleares, Spain
- Team members of project NEACCGAP (AGL2014-53647), Universidad de Santiago de Compostela, Spain
- German-Portuguese Bilateral Cooperation nº E-20/16, Federal Institute of Materials Research and Testing, Berlin, Germany
- Brazilian-Portuguese Bilateral Cooperation under a CAPES-FCT financed project (FCT/13277/4/8/2015), Universidade Estadual Paulista, Brazil



OUTREACH

- Project SEI (Projeto Sociedade, Escola e Investigação) for high school students, Faculdade de Farmácia da Universidade do Porto, Agrupamento de Escolas Rodrigues de Freitas, and Câmara Municipal do Porto, 2017.
- Laboratory internship from students enrolled at Colégio Vasco da Gama, Sintra, 2017.
- Presidium and organizing committee of the 18th International Conference on Flow Injection Analysis (Marcela Segundo, co-Chair), Porto, 15-20 September 2013.
- Organizing committee of the 18th Meeting of the Portuguese Electrochemical Society, Porto, 25-27 March 2013.
- Organizing committee of the EUPAT 6 – 6th pan-European Science Conference on Quality by Design and Process Analytical Technology Sciences, Porto, 23-24 September 2013.
- Presidium and organizing committee of the XX Encontro Luso-galego de Química ((José Luís Costa Lima, Chair), Porto, 26-28 November 2014.
- Organizing committee of the XXV Encontro Nacional da Sociedade Portuguesa de Química, Lisbon, 16-19 July 2017.
- Portuguese representation at General Assembly of EuCheMS – Division of Analytical Chemistry, Marcela Segundo, from 2012.


LABORATÓRIO ASSOCIADO
PARA A QUÍMICA VERDE


requimte
rede de química e tecnologia


U.PORTO


UNIVERSIDADE
NOVA
DE LISBOA


universidade
de aveiro

BCO

(BIO)CHEMISTRY & OMICS

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

The (Bio)Chemistry & OMICS group is a multidisciplinary international research group integrated by analytical and inorganic chemists, biochemists, biologist, biochemist, veterinaries, materials science and biotechnological researchers, whose common goal is to gain insight in complex biological systems using multidisciplinary approaches. C_4O comprises 10 senior researchers and 7 research labs in an integrative and cooperative approach, with a strong relationship with several universities, hospitals and industries.

There is an extensive experience in synthesis of organic, inorganic and multifunctional dyes and nanoparticles and nanomaterials, in innovative approaches for large-scale identification of biomolecules, characterization and quantification of small molecules, characterization of metalloenzymes and proteins (structural and function), and in the analysis of bacteriology, mycology and viruses samples.

RESEARCH OBJECTIVES [2018-2022]

The (Bio)Chemistry & OMICS group will continue to pursue work aiming the identification, characterization and quantitation of a wide array of biomolecules to in order to gain insights into underling molecular mechanisms in complex biological systems by integrating nanotechnology and multiplex-probing systems, biophysical techniques, a wide range of spectroscopies, and mass spectrometry. In particular, we intend to strengthen:

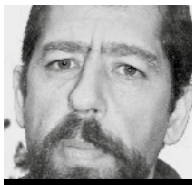
- The design of new nanotechnology-based multiplex-probing systems with application in the fields of environment, sustainable health and point-of-care. Innovating in new synthetic protocols using environmental friendly reagents applied for nanomaterials and new smart functionalized nanoparticles.
- The development of innovative methods to unravel the biochemical mechanisms of antibiotics resistance .
- 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.
- 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.

From 2018 the group will benefit from the incorporation of new members upcoming from the University of Aveiro. This circumstance will reinforce the expertise in mass spectrometry both in terms of new equipment and targeted analytes.

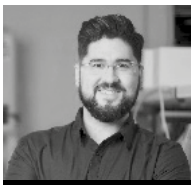
RESEARCH TEAM

SENIOR RESEARCHERS

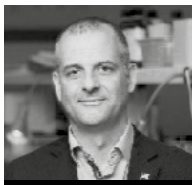

★ Carlos Lodeiro


Francisco Amado


Gilberto Igrejas


Hugo M. Santos


Isabel Moura


José L. Capelo


José Moura


Patrícia Poeta


Pedro Domingues


Rita Ferreira

★ Group coordinator

RESEARCH TEAM

OTHER DOCTORATE RESEARCHERS

Bruno Neves
Cristina Costa
Jorge Lampreia
Luisa Helguero
M. Rosário Domingues
Rui Vitorino
Stéphane Besson

POST-DOCTORAL FELLOWS

Alejandro Samhan-Arias
Catarina Ramos
Cristina Cordas
Cíntia Carreira
Elisabete Oliveira
Javier Férnandez-Lodeiro
Luísa Maia
Maia Maciel
Marta Carepo
Nuno Moura
Tânia Melo

PhD STUDENTS

Adrian Fernandez-Lodeiro
Ana Figueredo
António Paulino
Augusto Gonçalves
Catarina Nunes
Cláudia Covas
Daniela Pinheiro
Filipa Gomes
Gonçalo Marcelo
Gonçalo Martins
Isabel Carvalho
Jamila Djafari
Javier Bullón
Jemmysson de Jesus
José Araújo
Júlio Miranda
Luís Pinto
Margarida Sousa
Ricardo Teixo
Susana Jorge
Vanessa Silva

MSc STUDENTS

Alexandra Pais
Ana Ferreira
Ana Sabença
Anicia Gomes
Bárbara Matos
Carina Baía
Catarina Luz
Cátia Leitão
Fernando Peixoto
Filipe Cristóvão
Inês Marques
Joana Flores
João Antunes
João Braga
João Prates
José Figueiredo
Laura de Sousa
Luís Carvalho
Marco Araújo
Mariana Campaniço
Michael Freitas
Nuno Cunha
Patrick Ferreira
Soraia Oliveira
Stephanie Reis
Telma Sousa
Vânia Santos

RESEARCH GRANTEES

Bruna Santos
Flávia Santos
Francisco Almeida
Gabriel Valério
Heitor Coelho
Inês Paiva
Joana Santos
João Magalhães
José Almeida
Rafaela Sabino
Rita Baptista
Sebastião Villax
Vasco Silva

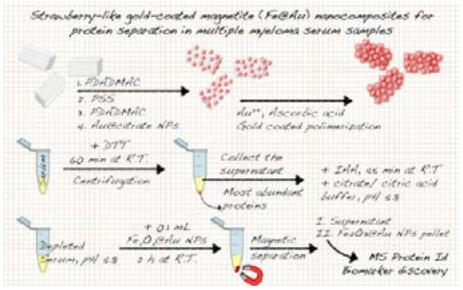
OTHER RESEARCHERS

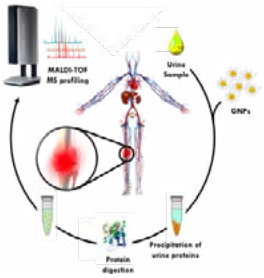
Carla Carneiro

RESEARCH THEMES/
SYNTHESIS OF PROBES AND NANOMATERIALS

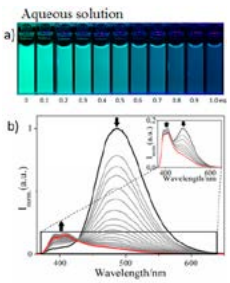
Synthesis of new Fluorescent and Colorimetric dyes, functionalized nanoparticles and composites (Au, Ag, Pt, Pd, SiO_2, Fe_2O_3, Polymers and mesoporous materials, and Nano Probes, for environmental detection of Pollutants, Drug delivery, Biomedical and Proteomics Applications have been developed in the last years. Strong efforts have been focused on the development of new green synthetic methodologies for Nanoparticles and Composites.

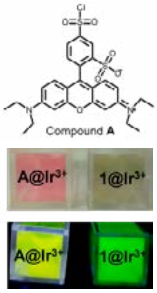
BIOMEDICAL AND PROTEOMICS APPLICATIONS[1-3]

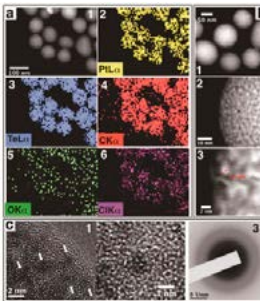




NEW EMISSIVE@NANO MATERIALS[4-7] AND NANOMATERIALS FOR TARGETING DETECTION[8-10]







SELECTED PUBLICATIONS

1 J. E. Araujo, et al. NanoResearch. 2015, 8(4), 1189. doi 10.1007/s12274-014-0599-4

2 R. López-Cortes, et al. Talanta. 2016, 150, 638. doi:10.1016/j.talanta.2015.06.043

3 C. Nuñez, et al. Biomaterials. 2016, 97, 34. doi:10.1016/j.biomaterials.2016.04.027

4 C. Cuerva, et al. Chemistry Eur J. 2016, 22, 10168. doi:10.1002/chem.201601115

5 J. Djafari, et al. ChemistryOpen. 2016, 5, 206. doi:10.1002/open.201600016

6 A. C. Gonçalves, et al. Sensor Act. B Chem. 2017, 239, 311. doi:10.1016/j.snb.2016.08.014

7 E. Oliveira, et al. Dalton Trans. 2016, 3, 45, 1254. doi:10.1039/c5dt03666f

8 J. Fernández-Lodeiro, et al. ACS Omega. 2016, 1, 1314. doi:10.1021/acsomega.6b00309

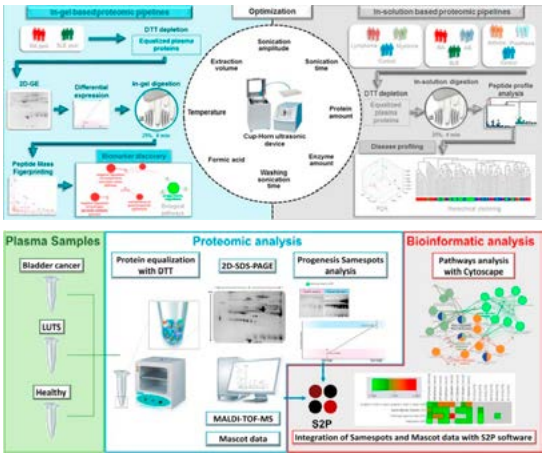
9 J. Fernández Lodeiro, et al. Scientific Reports. 2017, 7, 9889. doi:10.1038/s41598-017-10239-8

10 E. Oliveira, et al. ChemistryOpen. 2018, 7-1, 9. doi:10.1002/open.201700135

RESEARCH THEMES/
BIOANALYTICS & PERSONALIZED NANO@PROTEOMICS

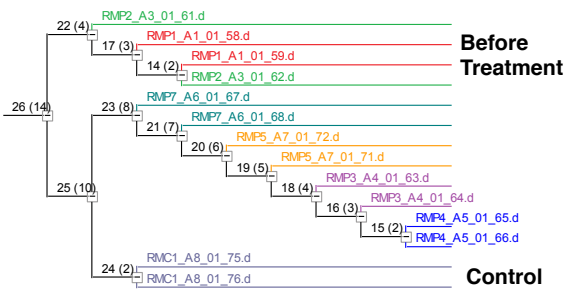
BIOANALYTICS & PERSONALIZED NANO@PROTEOMICS

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, in order to gain insight into the underlying molecular mechanisms.[11-15]



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 investigating the role of several post-translational modifications, such as phosphorylation, ubiquitination and sumoylation in health and disease. We are using the multiplexing capabilities of mass spectrometry to build permanent digital quantitative maps of proteins to follow disease progression and response to therapy[16-20]



SELECTED PUBLICATIONS

11 J. E. Araújo, et al. Talanta. 2018, 180, 36. doi:10.1016/j.talanta.2017.11.063

12 H. López-Fernández, et al. Comput. Methods Programs Biomed. 2018, 155, 1. doi:10.1016/j.cmpb.2017.11.024

13 S. Jorge, et al. Talanta. 2018, 178, 1067. doi:10.1016/j.talanta.2017.07.079

14 S. Correia, et al. Expert Rev Proteomics. 2017, 14, 941. doi:10.1080/14789450.2017.1375856

15 J. L. Capelo, et al. Int. J. Biochem. Cell Biol. 2017, 91, 82. doi:10.1016/j.biocel.2017.08.008

16 J. E. Araújo, et al. J. Proteomics. 2016, 145, 207. doi:10.1016/j.jprot.2016.05.010

17 J. E. Araújo, et al. Talanta. 2016, 152, 364. doi:10.1016/j.talanta.2016.02.026

18 H. López-Fernández, et al. BMC Bioinformatics, 2015, 16, 318. doi:10.1186/s12859-015-0752-4

19 E. Oliveira, et al. Clin. Proteom. 2014, 11, 17. doi:10.1186/1559-0275-11-17

20 R. López-Cortés, et al. Talanta. 2012, 100, 239. doi:10.1016/j.talanta.2012.08.020

RESEARCH THEMES/ BIOLOGICAL CHEMISTRY

Aims 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[21-23]
- biophysical and structural characterization of electron transfer complexes, and molecular recognition processes[23]
- development of effective disposable biosensors for nitrite, using nitrite reductases, and nitric oxide, using nitric oxide reductase[24]

CARBON DIOXIDE REDUCTION

- establishment of an innovative reaction mechanism for the formate dehydrogenase catalysis[25]
- identification and characterization of a new, very efficient carbon dioxide reductase[25]

NOVEL HETEROMETALLIC CLUSTERS

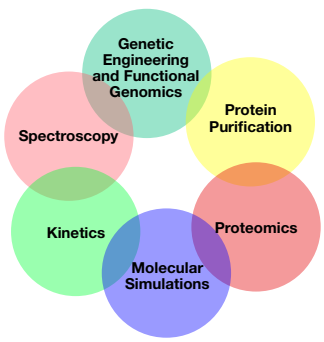
- characterization of the novel and unique molybdenum/copper heterometallic cluster of the bacterial "Orange Protein"[26]

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[27-28]

BACTERIAL ROS METABOLISM AND DETOXIFICATION MECHANISMS

- mechanistic characterization of hydrogen peroxide and superoxide detoxification in bacteria[29]
- 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[30]

SELECTED PUBLICATIONS

21 E. M. Johnston, et al. Chem. Sci. 2015, 6, 5670. **doi:10.1039/c5sc02102b**

22 E. M. Johnston, et al. J. Am. Chem. Soc. 2017, 139, 4462. **doi:10.1021/jacs.6b13225**

23 RSC Metallobiology Series No. 9. Editors I. Moura, et al. The Royal Society of Chemistry, Cambridge, 2017. **doi:10.1039/9781782623762**

24 T. Monteiro, et al. Talanta. 2015, 142, 246. **doi:10.1016/j.talanta.2015.04.057**

25 L. Maia, et al. J. Am. Chem. Soc. 2016, 138, 8834. **doi:10.1021/jacs.6b03941**

26 B.K. Maiti, et al. Inorg. Chem. 2017, 56, 8900. **doi:10.1021/acs.inorgchem.7b00840**

27 L. Maia, et al. Chem. Rev. 2014, 114, 5273. **doi: 10.1021/cr400518y**

28 L. Maia, et al. Biochemistry. 2015, 54, 685. **doi:10.1021/bi500987w**

29 R.M. Almeida, et al. ChemBioChem. 2013, 14, 1858. **doi:10.1002/cbic.201300196**

30 B.K. Maiti, et al. Coord. Chem. Rev. 2017, 352, 379. **doi:10.1016/j.ccr.2017.10.001**

RESEARCH THEMES/ COMPREHENSION OF DISEASE-RELATED BIOLOGICAL MECHANISMS

NEW BIOMARKERS OF OXIDATIVE STRESS: A MOLECULAR APPROACH

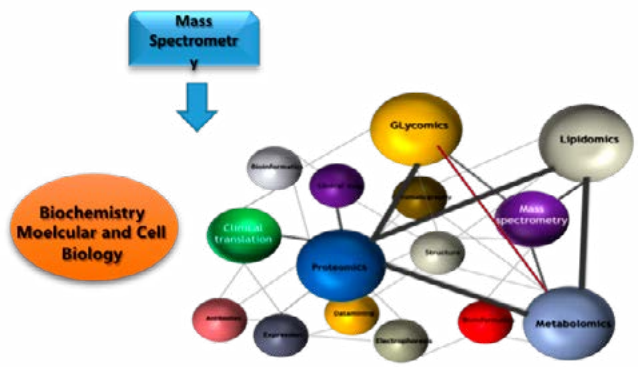
This line of research is concerned with applications of mass spectrometry for the study of oxidative stress. Main work has been developed in the detection and characterization of free radicals by mass spectrometry, the study of oxidative stress in lipids and phospholipids and amino acids. Present and future special interests are the study and characterization of oxidized lipids, peptides and proteins using mass spectrometric approaches.

DISEASE PROTEOMICS

This line of research is concerned with the study of noncommunicable diseases using as core methodologies immunohistochemistry and proteomics, cell cultures, human body fluids and archival human patient biopsies our research aims are: a) access the subcellular post-translational modifications (e.g. phosphorylation; b) evaluate adaptive reprogramming mechanisms; c) develop proteomics quantitative strategies for potential disease and therapeutic biomarkers; d) develop new practical tools of low technology used for diagnostic, prognostic, and predictive biomarkers evaluation, easily applied in daily clinical practice.

LIFESTYLE IMPACT ON CANCER-INDUCED MUSCLE REMODELING

This line of research is concerned with the study of muscle remodeling with the topics: a) striated muscle remodeling in cancer cachexia; b) the role of exercise training on the molecular mechanisms underlying muscle wasting conditions; c) mitochondrial plasticity in pathophysiological conditions; d) proteomics applied to the identification of biological processes modulated by wasting conditions.



SELECTED PUBLICATIONS

31 Amado, et al. Expert Rev. Proteomics. 2014, 11, 383. doi:10.1586/14789450.2014.899470

32 Ferreira, et al., J. Proteome Res. 2014, 13, 2045. doi:10.1021/pr4011926

33 Monteiro, et al. Cancer Lett. 2017, 28, 396, 42. doi:10.1016/j.canlet.2017.03.007

34 Silva, et al. Biochem. J. 2014, 461, 33. doi:10.1042/BJ20140133.

35 Couto, et al. J. Am. Soc. Mass Spectrom. 2016, 27(12), 1965. doi:10.1007/s13361-016-1474-1

36 Melo, et al. Free Radic Biol Med. 2017, 106, 219. doi:10.1016/j.freeradbiomed.2017.02.033

37 Antunes, et al. Biochim. Biophys. Acta Mol. Cell Biol. Lipids. 2014, 1841, 896. doi:10.1016/j.bbalip.2014.03.004

38 Ferreira, et al. Basic Res. Cardiol. 2015, 110(1), 454. doi:10.1007/s00395-014-0454-5

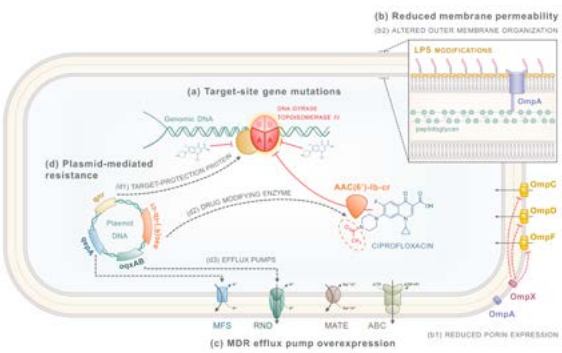
39 Nogueira-Ferreira, et al. J Cell Physiol. 2017, 232(11), 3128. doi:10.1002/jcp.25763.

40 Padrão, et al. Acta Physiologica. 2017, 219, 4, 803-813. doi:10.1111/alpha.12721

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 molecular and storage proteins characterization of populations/ landraces of vegetables, cereals, grain legumes, fruit trees, medicinal and aromatic species and industrial crops; recovery and breeding of Portuguese landraces of vegetables and cereals; identification of genes responsible for important economic fruit traits and antibiotic resistance in bacterial strains evaluation through genomic-transcriptomic-proteomic platform linked to agriculture and natural ecosystems.

- Genomic, transcriptomic and proteomic characterization of genetic resources of graminae;
- Proteomic of new genes controlling grain functionality and allergenicity applied to wheat, rye and triticale;
- Nutrigenomics and nutriproteomics applied to proteaginous species;
- Probiotics in biotechnology and health;
- BACT_ONE_OMICS: Genomic and proteomic evaluation of antibiotic resistance in bacterial strains of wild and domestic animals and humans.



SELECTED PUBLICATIONS

41 T. Santos, et al. Crop Pasture Sci. 2017, 68, 1041. doi:10.1071/CP17307

42 J. Nunes-Miranda, et al. J. Proteomics, 2017, 169, 136. doi:10.1016/j.jprot.2017.05.019

43 S. Correia, et al. Proteomics Clin. Appl. 2017, 11, 1600107. doi:10.1002/prca.201600107

44 F. Cristóvão, et al. FEMS Microbiol. Lett. 2017, 364, 1. doi:10.1093/femsle/fnx039

45 A. Inácio, et al. Int. J. Legal Med. 2017, 131, 657. doi:10.1007/s00414-016-1484-3

46 P. Magalhães, et al. J. Proteomics, 2016, 145, 103. doi:10.1016/j.jprot.2016.03.042

47 C. Marinho, et al. Front. Microbiol. 2016, 7, 1650. doi:10.3389/fmicb.2016.01650

48 S. Ramos, et al. OMICS. 2016, 20, 362. 362. doi:10.1089/omi.2016.0044

49 M. Ribeiro, et al. Sci. Rep. 2015, 5, 18041. doi:10.1038/srep18041

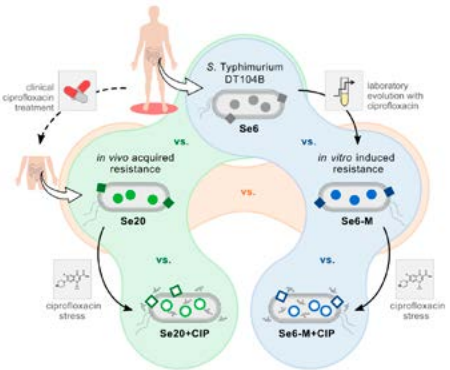
50 C. Portugal, et al. Int. J. Food Microbiol. 2015, 210, 113. doi:10.1016/j.ijfoodmicro.2015.06.005

RESEARCH THEMES/ ANTIBIOTIC RESISTANCE

The Medical Microbiology Laboratory (MML) offers quality veterinary microbiology diagnostic testing and research services to University Veterinary Hospital, government organizations, private sector, and individuals. The MML covers both bacteriology and mycology investigates, as well virus analysis. The lab service processes a wide variety of clinical samples from companion, farm and wild animals, as well as tissues from animals submitted for post-mortem investigations.

MECHANISMS OF MULTIDRUG RESISTANCE

The group drives part of its research activities on detection of foodborne pathogens and specific spoilage organisms from food of animal origin along different food production chains. Under these research subjects, important microbiological hazards (*Salmonella sp., E. coli,* MRSA) involved in foodborne outbreaks, are analyzed. The group will still develop new approaches to analyze and interpret more complex and emerging microbial pathogen using molecular, serotyping and phylogenetic analysis. Also, research will be developed to improve knowledge on prevalence, definition of contamination sources, risk to public health and strategies to improve food safety and quality.



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. We produce higher quality research results and knowing which antimicrobial resistant bacteria variants are associated with each focus of infection, each animal species and in a particular habitat may be important to carry a greater control over the dissemination of zoonotic bacteria and better understand their transmissibility.

SELECTED PUBLICATIONS

51 A. Garcês, et al. J Hazard. Mater. 2018, in press. doi:10.1016/j.jhazmat.2017.12.053

52 V. Silva, et al. Microb Drug Resist. 2018, 24, 89. doi:10.1089/mdr.2017.0040J

53 S. Correia, et al. Proteomics Clin. Appl. 2017, 11, 7–8, 1600107. doi:10.1002/prca.201600107

54 F. Cristóvão, et al. FEMS Microbiol. Lett. 2017, 364, 1. doi:10.1093/femsle/fnx039

55 M. Sousa, et al. Sci. Total Environ. 2017, 596-597, 26. doi:10.1016/j.scitotenv.2017.04.054

56 R. Monteiro, et al. J. Proteomics, 2016, 145, 167. doi:10.1016/j.jprot.2016.04.032

57 C. Marinho, et al. Front. Microbiol. 2016, 7, 1650. doi:10.3389/fmicb.2016.01650

58 S. Ramos, et al. OMICS. 2016, 20, 362. doi:10.1089/omi.2016.0044

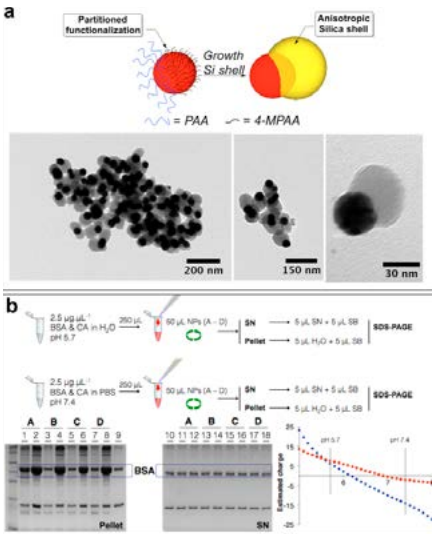
59 E. Guerrero-Ramos, et al. Food Microbiol. 2016, 53, 156. doi:10.1016/j.fm.2015.09.007

60 J. Djafari, et al. ChemistryOpen. 2016, 5, 206. doi:10.1002/open.201600016

HIGHLIGHTS

ORGANOTELLURIUM CHEMISTRY: APPLICATION IN GOLD NANOMATERIALS

Long-term preservation of Gold nanoparticles properties either in solution or as a dry powder can be difficult. We have overcome this challenge by using organotellurium derivatives as both reducing agents and stabilizers in the synthesis of gold nanoparticles. The new synthetic protocol takes advantage of the photochemical and oxidative properties of diphenyl ditelluride (Ph_2Te_2), which so far has never been exploited in the synthesis of gold nanoparticles. The Au/Te core/shell (inorganic/organic) hybrid nanomaterial can be obtained in a one-step reaction, using only Ph_2Te_2 and $HAuCl_4$. By modifying the reaction conditions, different resonance conditions of the gold core are archived as a consequence of different external shell thickness formed. The organotellurium shell can be easily removed by re-suspension of the nanoparticles in environmentally friendly solvents, such as water or ethanol, making the Au core available for subsequent applications. A mechanism for the formation core/shell nanoparticles was also discussed.

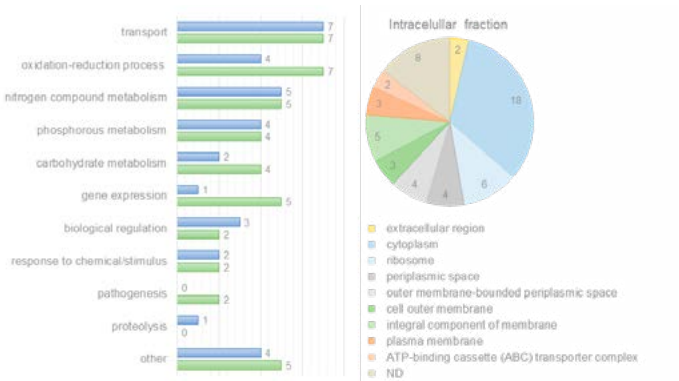


Unravelling the organotellurium chemistry applied to the synthesis of gold nanomaterials

ACS Omega, 2016, 1, 1314.

BIOCHEMICAL MECHANISMS DRIVING ANTIBIOTICS RESISTANCE

Salmonela tryphimutium DT104 multiresistant strains with additional quinolone resistance are highly adaptive and have been responsible for global outbreaks and high mortality. In order to give new insights about the resistance mechanisms involved, the developed work pointed out subproteome changes between a DT104B clinical strain that acquired quinolone resistance after patient treatment and an in vivo induced clonally related highly-resistant mutant.



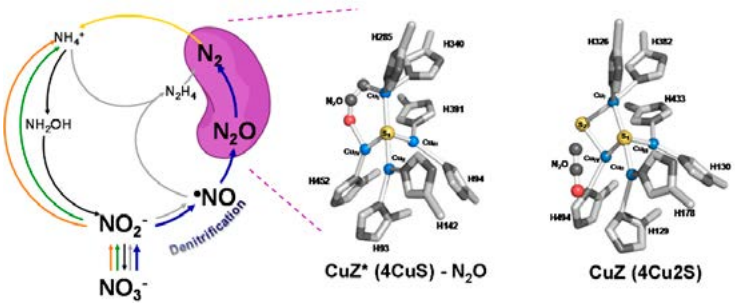
Impacts of experimentally induced and clinically acquired quinolone resistance on the membrane and intracellular subproteomes of Salmonella Typhimurium DT104B.

Journal of Proteomics, 2016, 145, 46–59.

HIGHLIGHTS

UNVEILING THE DENITRIFICATION SECRETS: UNDERSTANDING THE REDUCTION OF N_2O

In denitrification, bacteria reduce NO_3- to N_2 gas in 4 metalloenzymes-catalyzed steps to derive energy. In the last step, the N_2O reduction to N_2 is catalyzed by 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, in two redox states, $2Cu^{+}/2Cu^{2+}$ and $3Cu^{+}/1Cu^{2+}$, and identified the protonation states. We have established that the CuZ form has very low catalytic activity and cannot participate in the catalytic cycle, which should be carried out by CuZ*.



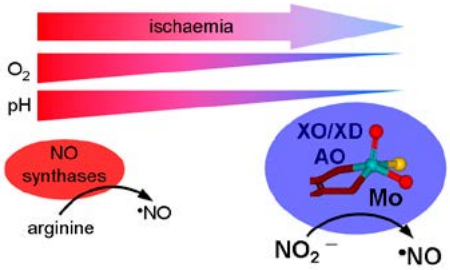
Spectroscopic definition of the CuZ* intermediate in turnover of nitrous oxide reductase and molecular insight into the catalytic mechanism

Journal of the American Chemical Society, 2017, 139, 4462-4476.

HOW HUMANS ARE USING NO_3^- AND NO_2^- TO GENERATE •NO FOR SIGNALING PURPOSES?

Remarkably, part of the bacterial denitrification is replicated in human signaling pathways to generate •NO from NO_2- and NO_3-, for signaling purposes under challenging conditions. We have characterized kinetically and mechanistically the NO-forming nitrite reductase activity of the human xanthine dehydrogenase (XD), xanthine oxidase (XO) and aldehyde oxidase (AO).

We have established that the NO_2- reduction to •NO (an oxygen atom abstraction) by those molybdoenzymes is carried out by the reduced Mo^{4+} and Mo^{5+} cores and is dependent on a protonation step assisted by a key glutamate residue. The same reaction mechanism should be followed by the bacterial molybdoenzymes.



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.

Biochemistry, 2015, 54, 685-710.

HIGHLIGHTS

LIFELONG EXERCISE TRAINING MODULATES CARDIAC MITOCHONDRIAL PHOSPHOPROTEOME

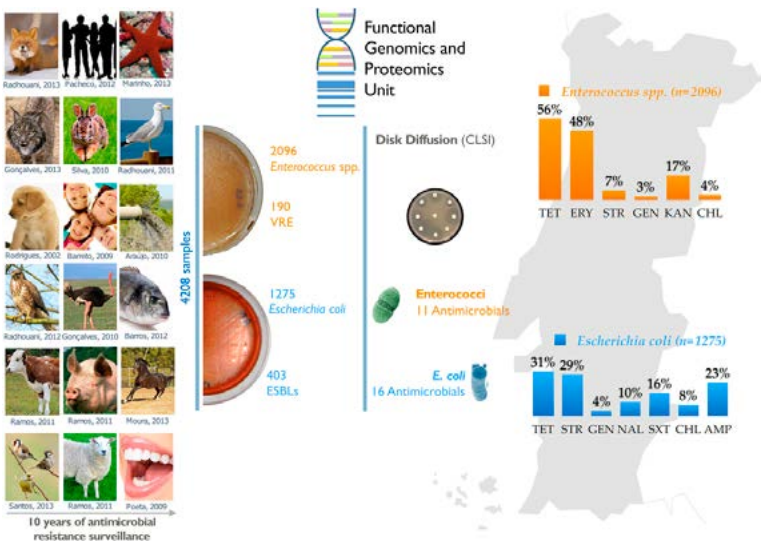
Moderate physical activity has been associated to the improvement of the cardiac function and, consequently, to the extension of the life span. In order to disclose the molecular mechanisms underlying the beneficial effect of lifelong physical activity in the cardiac function, we performed label-free quantitative mass spectrometry-based proteomics of heart mitochondrial proteome and phosphoproteome. Data shown that 54-weeks of moderate treadmill exercise modulates the abundance of proteins involved in the generation of precursor metabolites and cellular respiration, suggesting an increase in carbohydrate oxidation-based metabolism.

Lifelong Exercise Training Modulates Cardiac Mitochondrial Phosphoproteome in Rats

Journal of Proteome Research, 2014, 13 (4), 2045–2055.

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.



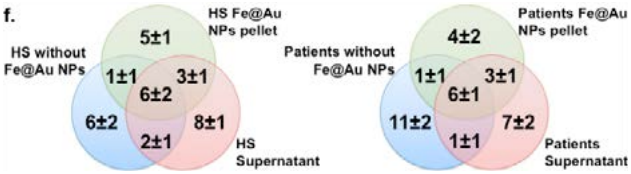
A decade-long commitment to antimicrobial resistance surveillance in Portugal.

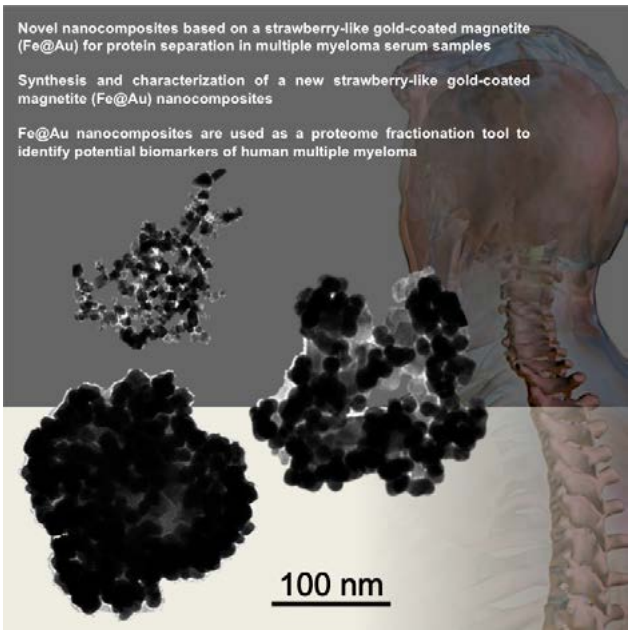
Frontiers in Microbiology, 2016, 7, 1650.

HIGHLIGHTS

NOVEL NANOCOMPOSITES BASED ON A STRAWBERRY-LIKE GOLD-COATED MAGNETITE FOR PROTEIN SEPARATION IN MULTIPLE MYELOMA SERUM SAMPLES

New synthetic gold-coated magnetite (Fe@Au) magnetic strawberry-like nanoparticles have been assessed in biomarker discovery as a tool for pre-concentration and separation of proteins from complex proteomes. Combined with MS spectrometry has allowed for the identification of 53 proteins in sera from healthy people compared with patients diagnosed with multiple myeloma, revealing the heat shock protein HSP75 and the plasma protease C1 inhibitor as potential biomarkers for diagnostics and control of multiple myeloma progression.



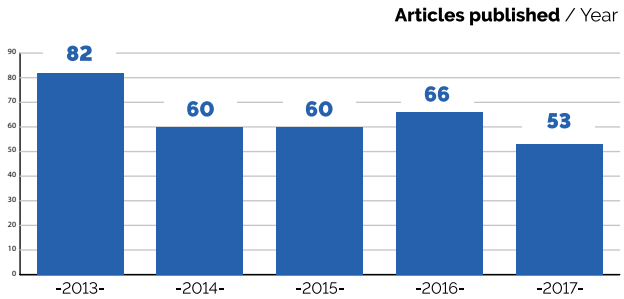


Novel nanocomposites based on a strawberry-like gold-coated magnetite (Fe@Au) for protein separation in multiple myeloma serum samples

Nano Research 2015, 8(4) 1189.

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION 2013-2017*



321 articles
2424 citations**
H-index: **65**

*From WOS core collection
**of the published articles in 2013-2017

FUNDED PROJECTS *(Representative projects)*

1 EU projects
476 k€

17 National projects
760 k€

- **"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 N2O"**
  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.
- **"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.
- **"Biomaterials for Regenerative Medicine Total"**
  CENTRO-07-ST24-FEDER-002030, Francisco Amado (PI),
  Total funding: €150.000,00.

INTERNATIONAL COOPERATION AND NETWORKING

- COST Action CM1001, "Chemistry of non-enzymatic protein modification - modulation of protein structure and function", 2010-2014.
- COST Action FA1306, "The quest for tolerant varieties: phenotyping at plant and cellular level", 2014-2018.

- Portuguese member of the Expert Working Group (EWG): Improving wheat quality for processing and health of the Wheat Initiative.
- 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), 2014-2018, Universidade de Campinas, Brazil.
- International Cooperation's with several research centers, hospitals and universities from: Argentina, Australia, Belgium, Brazil, Canada, Cyprus, Denmark, France, Finland, Germany, The Netherlands, Italy, Poland, Romania, Spain, Sweden, United Kingdom, United States of America.

OUTREACH

- The national newspaper "Público", and the national TV channel RTP1 highlighted the C. Lodeiro and J.L. Capelo Team research in Nanotechnology with "A Bandeira Portuguesa tem Quimica? Tem é muita", November 2017.
- Research in Celiac Illness and Wheat (G. Igrejas) in the TV SIC Noticias.
- Organizing committee of a winter and a summer Hands-on school for young researchers and academics related to the research lines of the team since 2013.
- Organizing committee of the National Biological Olympics (G. Igrejas and P. Poeta) in UTAD, Vila Real.
- Organizing and scientific committee of the Proteomass Scientific Society International Conferences (C. Lodeiro, J. Capelo, G. Igrejas, H. M. Santos) since 2013.
- Chairs (C. Lodeiro and J.L. Capelo) of the Proteomass Scientific Society International Conferences Series 32 since 2013.
- Chair (J. Moura) and of "International Molybdenum and Tungsten Enzymes Conference, MoTEC 2013", 16-19 July 2013, Sintra, Portugal
- Scientific committee (J. Moura) of MoTEC 2015, 06-10 September 2015, Balatonfured, Hungary, and MoTEC 2017, 18-23 June, 2017, Santa Fe, USA

- Member of the Scientific Commission I Simpósio em Microbiologia: a tríade alimentos, saúde e ambiente, P. Poeta, UTAD, Vila Real, November 2017.
- Recognized Fellows of the RSC (C. Lodeiro and J.L. Capelo) in 2014.
- USP Brazil highlight in chemistry for health and energy, C Lodeiro, 2014.
- H. M. Santos Awarded with Young Research Award 2015 Proteomass by ICAP 2015 Conference.
- E. Oiveira Awarded with Young Research Award 2015 Proteomass by PTIM 2015 Conference.
- Participation in several public diffusion initiatives, including: BIOIN PT (2013); Ano Europeu do Cérebro (2014); NOITE da LUZ (2015); Light Design "Emotions and Light" (2016); NoSIC-7: Not Strictly Inorganic Chemistry (2016); Seminar "Cartoons, Chemistry, Art and Society"; FUTURALIA, FIL (2016), FCT FABLAB (2016); Summer Festival (2016); "How to Cock a dog", Vegetarianism and Vegan Conferences; EXPO FCT (2013-2017).
- Demonstrations of the "Biochemistry Lab" and "BIOSCOPE Lab" by several group members.
- Creation of the Chemical Startup Nan@rts by C. Lodeiro, J. F. Lodeiro, J.L. Capelo, H. Santos, and the "Proteomass Laboratory for Biological Mass Spectrometry "Isabel Moura" Facility" by C. Lodeiro, J.L. Capelo, H. Santos.
- Collaboration with industries: Denator (Sweden), Paralab (Portugal) and Bruker (Germany).
- Collaboration with Hospitals: Cedars Sinai Hospital LA USA, Pittsburgh University Hospital USA, IPO Portugal, Egas Moniz Hospital and Garcia de Horta Hospital in Lisbon, Portugal.

LABORATÓRIO ASSOCIADO
PARA A **QUÍMICA VERDE**

requimte
rede de química e tecnologia

U.PORTO

UNIVERSIDADE NOVA DE LISBOA

universidade de aveiro

EnvChem

ENVIRONMENTAL CHEMISTRY

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

Nowadays, the quality of the environment and its effects on citizens' welfare is one of the world's major issues of the uttermost 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 [2018-2022]

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); the environmental evaluation (in surface and drinking waters, wastewaters, soils, sediments, sludge, air, and biological samples, such as tissues, urine, 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 for application 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


Ana Paula Carvalho


César Oliveira


★Cristina Delerue Matos


Hendrikus Nouws


Henrique Vicente


José T. Albergaria


M. Eduarda Pereira


M. João Ramalhosa


M. Manuela Correia


M. Teresa Oliva Teles


Mónica Dias Teixeira


Nuno Nunes


Simone Morais


Sónia Figueiredo


Valentina Domingues

★ Group coordinator

RESEARCH TEAM

OTHER DOCTORATE RESEARCHERS

Abel Duarte
Florinda Martins
Iqbal Ahmad
M. Carmo Vaz
M. Manuela Carvalho
Olga Freitas
Salomé Teixeira

POST-DOCTORAL FELLOWS

Aleksandar Lolic´
Ana Teresa Reis
António Soares
Bruno Henriques
Carolina Portella
Cláudia Mieiro
Cláudia Lopes
Cristina Soares
Elsa Vieira
Estefanía Rama
João Paulo Pacheco
João Pedro Coelho
Joilson Jesus
Klára Slezáková
Koigoora Srikanth
Lúcia Santos
Luciana Rocha
Manuela Moreira
María Begoña García
M. Fátima Barroso
M. Luisa Sá
Marta Oliveira
Naser Aziz Anjum
Paula Campos
Rita Alves
Sónia Rodrigues
Virgínia Fernandes
Wojciech Stawin´ski

PhD STUDENTS

Alexandre Nascimento
Ana Bessa
Carla Palma
Daniela Tavares
Diogo Dias
Elaine Fabre
Elena Surra
Filipa Gomes
Idalina Bragança
Iram Mohmood
Joana Sousa
José Vera
José Seco
Liliana Freitas
M. Cristina Freitas
Maria da Luz Maia
M. João Fernandes
Marta Neves
Nádia Silva
Patrícia Rebelo
Patrícia Leitão
Pedro Carneiro
Pedro Silva
Regiane Bonilha
Rui Monteiro
Sérgio Morais
Sérgio Sousa
Thiago Oliveira

MSc STUDENTS

Adriana Ribeiro
Andreia Melo
Alexandra Dias
Alexandre Deodato
Alexys Boim
Ana Monteiro
Ana Filipa Costa
Ana Isabel Silva
Ana João Vinhas
Ana Sofia Cerqueira
Ana Teresa Matos
Ana Rute Santos
Ana Rute Teixeira
Andreia Coelho
Andreia Rocha
Andreia Silva
Arany Rocha
Bárbaro Matos
Carla Macedo
Cátia Peixoto
Carolina Silva
Cindy Carvalho
Claudia Pellegrini
Catarina Pinheiro
César Tavares
Diana Cruz
Diana Castro
Diana Ribeiro
Fabiana Teixeira
Fabiana Silva
Filipa C. Silva
Filipa R. Silva
Francesco Valentini
Frederico Lopes
Hélder Silva
Igor Azevedo
Ilária Mercuri
Inês Maia
Isa Nogueira
Isolete Gonçalves
Iris Oliveira
Iuri Martinho
Jéssica Correia
Joana Silva
Joana Lopes
Joana Abreu
Jorge Teixeira
Jorge Azevedo
Juan Romacho
Karina Ferreira
Karolina Filipkowska
Leonor Costa
Liliana Alves
Liliana Duarte
Liliana Soares
Maria Cavaliere
Maria C. Ferreira
Maria João Gomes
Mariana Magalhães
Marisa Ribeiro
Marlene Pimentel
Marta Machado
Maria Isabel Silva
Marta Sofia Silva
Mattia Orazi
Miguel Nogueira
Nathalie Ferreira
Nuno Morgado
Pawel Zajac
Pedro Vicente
Pedro Pinto
Piotr Zajac
Raquel Marques
Raquel Maia
Rui Monteiro
Rui Taborda
Sandra Neto
Sandra Rodrigues
Sara Sousa
Sara Ramos
Sílvia Capelas
Sílvia Martinho
Sílvia Bastos
Sofia Costa
Susana Faria
Thomas Have
Tatiana Valente
Tiago Veloso
Tiago Machado
Tiago Ferreira
Tiago Teixeira
Vera Barbosa
Vitor Pereira

RESEARCH GRANTEES

Ana Teresa Reis
Andreia Coelho
Bruno Moreira
Carmen Palenzuela
Cláudia Coelho
Daniela Tavares
Diana Cruz
Diana Lopes
Diana Rede
Fabíola Fogaça
Filipa Oliveira
Francisco Ribeiro
Helena Becker
Juliana Sousa
Leiz Véras
Manuela Rodrigues
M. João Ribeiro
Mário Silva
Mário Paz
Nathalie Ferreira
Nuno Cruz
Paula Figueira
Ricardo Santos
Rui Magalhães
Rui Monteiro
Sara Barreiro
Sílvia Martinho
Susana Machado
Wagner Correr

OTHER RESEARCHERS

Maria Aurora Silva
Paula Paíga

RESEARCH THEMES/
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 flame retardants, polychlorinated biphenyls, metals) in environmental samples (surface 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 water 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 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 P. Paíga, et al. J. Pharm. Biomed. Anal. 2017, 135, 75. doi:10.1016/j.jpba.2016.12.013

2 M. Oliveira, et al. Sci. Total Environ. 2017, 575, 1156. doi:10.1016/j.scitotenv.2016.09.195

3 K. Slezakova, et al. J. Toxicol. Env. Health Part A 2017, 80, 630. doi:10.1080/15287394.2017.1286931

4 P. Paíga, et al. J. Sep. Sci. 2016, 39, 3436. doi:10.1002/jssc.201600412

5 M. Oliveira, et al. Environ. Pollut. 2016, 214, 430. doi:10.1016/j.envpol.2016.04.046

6 P. Paíga, et al. Sci. Total Environ. 2016, 573, 164. doi:10.1016/j.scitotenv.2016.08.089

7 M. Oliveira, et al. Environ. Pollut. 2016, 208, 382. doi:10.1016/j.envpol.2015.10.004

8 J. Coelho et al. Mar. Pollut. Bull. 2016, 111, 488. doi:10.1016/j.marpolbul.2016.06.053

9 A. Reis, et al. TrAC - Trends Anal. Chem. 2015, 64, 136. doi:10.1016/j.trac.2014.08.015

10 M. Barroso, et al. Environ. Earth Sci. 2015, 73, 2881. doi:10.1007/s12665-014-3297-3

11 M. Oliveira, et al. Indoor Air 2015, 25, 557. doi:10.1111/ina.12164

12 A. Lolić, et al. Sci. Total Environ. 2015, 508, 240. doi:10.1016/j.scitotenv.2014.11.097

13 A. Ribeiro, et al. J. Chromatogr. A 2014, 1363, 226. doi:10.1016/j.chroma.2014.06.099

14 K. Slezakova, et al. Environ. Sci. Pollut. Res. 2014, 21, 4492. doi:10.1007/s11356-013-2391-5

15 K. Slezakova, et al. Environ. Sci. Poll. Res. 2014, 21, 3604. doi:10.1007/s11356-013-2316-3

16 A. Gomes, et al. Water Resour. Manage. 2014, 28, 1345. doi:10.1007/s11269-014-0547-9

17 V. Fernandes, et al. J. Sep. Sci. 2013, 36, 376. doi:10.1002/jssc.201200673

18 S. Rocha, et al. Bull. Environ. Contam. Toxicol. 2013, 90, 73. doi:10.1007/s00128-012-0887-1

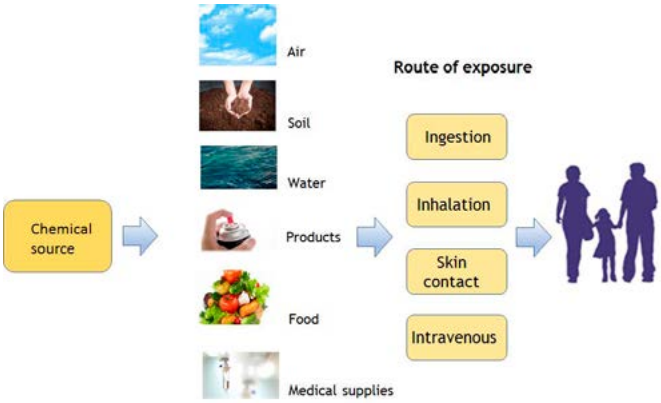
19 L. Santos, et al. Sci. Total Environ. 2013, 461-462, 302. doi:10.1016/j.scitotenv.2013.04.077

20 P. Paíga, et al. Environ. Sci. Pollut. Res. 2013, 20, 2410. doi:10.1007/s11356-012-1128-1

RESEARCH THEMES/
BIOMONITORING: SOURCES AND EXPOSURE ASSESSMENT

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

21 L. Correia-Sá, et al. Environ. Sci. Pollut. Res. 2017, 24, 27502. doi:10.1007/s11356-017-0358-7

22 A. Abreu, et al. J. Toxicol. Env. Health Part A 2017, 80, 596. doi:10.1080/15287394.2017.1286896

23 F. Lessmann, et al. Environ. Int. 2017, 104, 25. doi:10.1016/j.envint.2017.03.028

24 D. Pestana, et al. Sci. Rep. 2017, 7, 2738. doi:10.1038/s41598-017-02885-9

25 M. Oliveira, et al. J. Hazard. Mater. 2017, 323, 184. doi:10.1016/j.jhazmat.2016.03.012

26 L. Correia-Sá, et al. Environ. Int. 2017, 102, 79. doi:10.1016/j.envint.2017.02.001

27 M. Oliveira, et al. . J. Hazard. Mater. 2017, 322, 357. doi:10.1016/j.jhazmat.2016.10.004

28 M. Oliveira, et al. J. Hazard. Mater. 2017, 334, 10. doi:10.1016/j.jhazmat.2017.03.057

29 M. Oliveira, et al. Int. J. Hyg. Environ. Health 2016, 219, 857. doi:10.1016/j.ijheh.2016.07.011

30 D. Teixeira, et al. J. Clin. Endocrinol. Metab. 2015, 100, 1792. doi:10.1210/jc.2014-4136

31 D. Pestana, et al. Environ. Res. 2014, 133, 170. doi:10.1016/j.envres.2014.05.026

32 S. Santos, et al. J. Environ. Sci. Health Part B 2013, 48, 364. doi:10.1080/03601234.2013.742374

RESEARCH THEMES/
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. Also 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, agriculture wastes, and clays) or after modification (physical, physico-chemical and chemical) to produce environmental and economical sustainable materials with high performance in micropollutant removal.

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, and their economic and environmental evaluation with SWOT and Life Cycle Assessment tools. This systematic approach will minimize potential negative impacts of wastewater reuse in the environment, decreasing the undesirable introduction of micropollutants and their spread within the food chain.

SELECTED PUBLICATIONS

33 W. Stawiński, et al. Microporous Mesoporous Mat. 2017, 250, 72. **doi:10.1016/j.micromeso.2017.05.017**

34 W. Stawiński, et al. Sci. Total Environ. 2017, 576, 398. **doi:10.1016/j.scitotenv.2016.10.120**

35 W. Stawiński, , et al. Chemosphere. 2017, 173, 107. **doi:10.1016/j.chemosphere.2017.01.039**

36 W. Stawiński, et al. Chemosphere. 2016, 153, 115. **doi:10.1016/j.chemosphere.2016.03.004**

37 M. Bernardo, et al. Int. J. Environ. Sci. Technol. 2016, 13, 1989. **doi:10.1007/s13762-016-1030-3**

38 P. Figueira et al. Environ. Sci. Pollut. Res. 2016, 23, 11985. **doi:10.1007/s11356-016-6398-6**

39 B. Henriques et al. Chem. Eng. J. 2015, 281, 759. **doi:10.1016/j.cej.2015.07.013**

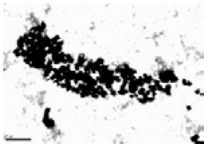
40 A. Silva, et al. Environ. Technol. 2014, 35, 3124. **doi:10.1080/09593330.2014.932438**

41 M. Bernardo, et al. J. Colloid Interface Sci. 2013, 409, 158. **doi:10.1016/j.jcis.2013.07.050**

RESEARCH THEMES/
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 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.

SELECTED PUBLICATIONS

42 S. Machado, et al. Int. J. Environ. Sci. Technol. 2017, 14, 1109. **doi:10.1007/s13762-016-1197-7**

43 D. Rede, et al. Chemosphere, 2016, 159, 193. **doi:10.1016/j.chemosphere.2016.06.002**

44 S. Rodrigues et al. TrAC - Trend in Anal. Chem. 2016, 75, 129. **doi:10.1016/j.trac.2015.07.003**

45 S. Rodrigues et al. Environ. Pollut. 2013, 183, 234. **doi:10.1016/j.envpol.2012.10.006**

46 S. Machado, et al. Sci. Total Environ. 2013, 461-462, 323. **doi:10.1016/j.scitotenv.2013.05.016**

RESEARCH THEMES/
VALORIZATION OF AGRO-FOOD AND INDUSTRIAL WASTES

In Europe, about 90 million tones of food are wasted annually and according to a recent FAO report, the food wastage will grow by an additional rate of 40% by 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, including livestock and crop production, food processing and retail sector is crucial in terms of economic and environmental sustainability standpoints. Our research group has been working on the valorization of several residues from the agro-food industry (wine, spent grain, yeast, hop, beer, fish, dairy products, rice and maize crop production), as well as marine (microalgae and seaweeds) and vegetable (chayote, apple) residues and resources. These matrices are recognized to possess a high nutrient content, added-value substances, or calorific value, thus making them optimal for valorization into bioenergy, bioactive compounds, biomaterials, bio-fertilizers, animal feedstock or nutraceuticals and 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, thereby 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 *in vitro* (and *in vivo*) of extracts with biological activity;
- Demonstration of technical feasibility of different valorisation technologies using laboratorial and pilot assays;
- Intensive collaboration with agriculture and food/pharmaceutical industries to promote a sustainable value-added chain.

SELECTED PUBLICATIONS

47 S. Sousa, et al. Molecules 2017, 22, 1545. **doi:10.3390/molecules22091545**

48 M. Moreira, et al. Ind. Crops Prod. 2017, 104, 210. **doi:10.1016/j.indcrop.2017.04.038**

49 A. Cvetanović, et al. J. Supercrit. Fluids 2017, 128, 173. **doi:10.1016/j.supflu.2017.05.023**

50 D. Dias, et al. Waste Manage. 2017, 65, 186. **doi:10.1016/j.wasman.2017.04.011**

51 O. Freitas, et al. Color. Technol. 2016, 132, 421. **doi:10.1111/cote.12234**

52 M. Bernardo, et al. Int. J. Environ. Sci. Technol. 2016, 13, 1989. **doi:10.1007/s13762-016-1030-3**

53 S. Machado, et al. Sci. Total Environ. 2015, 533, 76. **doi:10.1016/j.scitotenv.2015.06.091**

54 M. Araújo, et al. Trends Food Sci. Technol. 2015, 45, 200. **doi:10.1016/j.tifs.2015.06.010**

55 C. Lopes et al. Environ. Sci. Pollut. Res. 2014, 21, 2108. **doi:10.1007/s11356-013-2104-0**

56 S. Machado, et al. Sci. Total Environ. 2014, 496, 233. **doi:10.1016/j.scitotenv.2014.07.058**

57 L. Rocha et al. Water, Air, Soil Pollut. 2013, 224, 1599. **doi:10.1007/s11270-013-1599-9**

58 S. Figueiredo, et al. Environ. Eng. Manag. J. 2013, 12, 2061.

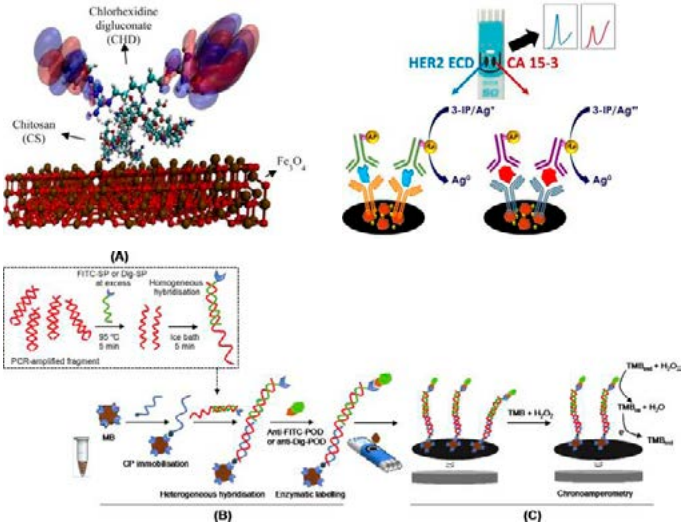
59 M. Moreira, et al. Food Res. Int. 2013, 54, 382. **doi:10.1016/j.foodres.2013.07.023**

60 S. Machado, et al. Sci. Total Environ. 2013, 445-446, 1. **doi:10.1016/j.scitotenv.2012.12.033**

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 will be focused on various domains for which novel sensors, using chemical, biological or bio-inspired molecular recognition elements, will be developed: application to environmental control (e.g. micropollutants and their corresponding metabolites and/or degradation products, namely antibiotics and pesticides in natural and wastewaters), assessment of food quality and safety (e.g. pathogenic microorganisms such as Salmonella) and disease diagnostics and follow-up (e.g. chronic kidney disease and cancer). Some of these challenges are the aim of several ongoing national and international financed projects.



SELECTED PUBLICATIONS

61 M. Firmino, et al. Chem. Eng. J. 2017, 323, 47. doi:10.1016/j.cej.2017.04.077

62 F. Lopes, et al. Sens. Actuators B 2017, 243, 745. doi:10.1016/j.snb.2016.12.031

63 D. Fernandes, et al. J. Solid State Electrochem. 2017, 21 1059. doi:10.1007/s10008-016-3463-5

64 P. Carneiro, et al. Sens. Actuators B 2017, 239, 157. doi:10.1016/j.snb.2016.07.181

65 M. Freitas, et al. Sens. Actuators B 2016, 237, 702. doi:10.1016/j.snb.2016.06.149

66 M. Freitas, et al. ACS Sensors 2016, 1, 1044. doi:10.1021/acssensors.6b00182

67 F. Ribeiro, et al. Electrochim. Acta 2016, 194, 187. doi:10.1016/j.electacta.2016.02.086

68 C. Manzanares-Palenzuela, et al. Sens. Actuators B 2016, 222, 1050. doi:10.1016/j.snb.2015.09.013

69 H. Silva, et al. Sens. Actuators B 2015, 219, 301. doi:10.1016/j.snb.2015.04.125

70 R. Alves, et al. Biosens. Bioelectron. 2015, 64, 19. doi:10.1016/j.bios.2014.08.026.

71 N. Silva, et al. Anal. Methods 2015, 7, 4008. doi:10.1039/C5AY00053J

72 M. Barroso, et al. Talanta 2015, 134, 158. doi:10.1016/j.talanta.2014.10.017

73 R. Marques, et al. Talanta 2014, 129, 594. doi:10.1016/j.talanta.2014.06.035

74 H. Silva, et al. Biosens. Bioelectron. 2014, 52, 56. doi:10.1016/j.bios.2013.08.035

75 T. Oliveira, et al. Bioelectrochem. 2014, 98, 20. doi:10.1016/j.bioelechem.2014.02.003

76 M. Freitas, et al. Biosens. Bioelectron. 2014, 51, 195. doi:10.1016/j.bios.2013.07.048

77 M. Neves, et al. Sens. Actuators B 2013, 187, 33. doi:10.1016/j.snb.2012.09.019

78 M. Neves, et al. Analyst 2013, 138, 1956. doi:10.1039/C3AN36728B

79 T. Oliveira, et al. Talanta 2013, 106, 249. doi:10.1016/j.talanta.2012.10.074

80 T. Oliveira, et al. Biosens. Bioelectron. 2013, 47, 292. doi:10.1016/j.bios.2013.03.026

RESEARCH THEMES/
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, specially with a life cycle perspective can help the different stakeholders to adopt and implement sustainable practices and behaviors.
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 by pointing-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.

SELECTED PUBLICATIONS

81 F. Martins, et al. Int. J. Life Cycle Assess. 2017, 22, 707. **doi:10.1007/s11367-016-1258-7**

82 M. Brito, et al. Fuel 2017, 208, 476. **doi:10.1016/j.fuel.2017.07.050**

83 F. Martins, Renew. Sust. Energ. Rev. 2017, 74, 173. **doi:10.1016/j.rser.2017.02.026**

84 S. Morais, et al. Sci. Total Environ. 2014, 490, 342. **doi:10.1016/j.scitotenv.2014.04.082**

85 S. Morais, et al. Chemosphere 2013, 93, 252. **doi:10.1016/j.chemosphere.2013.04.074**

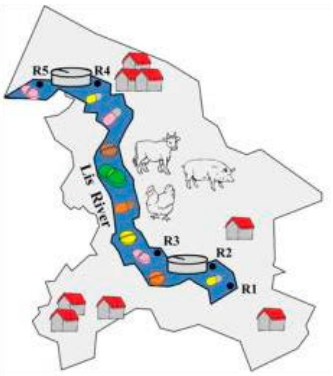
86 S. Morais, et al. J. Hazard. Mater. 2013, 248-249, 461. **doi:10.1016/j.jhazmat.2013.01.002**

87 J. Morais, et al. Resour. Conserv. Recycl. 2011, 55, 1109. **doi:10.1016/j.resconrec.2011.06.011**

HIGHLIGHTS

PRESENCE OF PHARMACEUTICALS IN THE LIS RIVER (PT)

The occurrence of 33 pharmaceuticals and metabolites was evaluated along the Lis river and in the influents and effluents of two wastewater treatment plants (WWTPs) located along the river. Ibuprofen, ketoprofen, carbamazepine and fluoxetine, and the metabolite salicylic acid are widespread along the Lis river, showing 100% of detection frequency, at levels up to 1.3 μg L^{-1}. The highest concentrations were often found downstream near the river mouth.

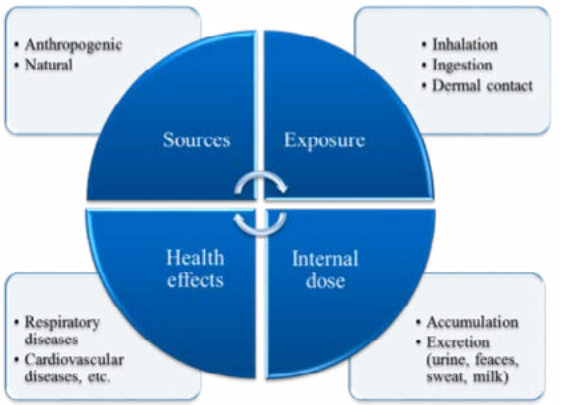


Presence of pharmaceuticals in the Lis river (Portugal): Sources, fate and seasonal variation

Science of the Total Environment, 2016, 573, 164–177.

ASSESSMENT OF EXPOSURE TO POLYCYCLIC AROMATIC HYDROCARBONS IN PRESCHOOL CHILDREN

The exposure of Portuguese preschool children to polycyclic aromatic hydrocarbons (PAHs) was assessed by environmental monitoring of eighteen compounds in air and biomonitoring of six urinary biomarkers of exposure (OH-PAHs). Total (including probable/possible) carcinogenic PAHs represented 26-45% of PAHs. Significant correlations were found between airborne PAHs and urinary OH-PAHs.



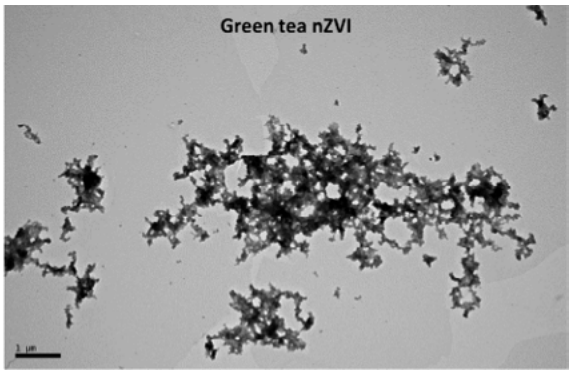
Assessment of exposure to polycyclic aromatic hydrocarbons in preschool children: Levels and impact of preschool indoor air on excretion of main urinary monohydroxyl metabolites

Journal of Hazardous Materials, 2017, 322, 357–369.

HIGHLIGHTS

NANOCLEAN - REMEDIATION OF SOILS CONTAMINATED WITH PHARMACEUTICAL PRODUCTS USING "GREEN" ZERO VALENT IRON NANOPARTICLES

Green zero valent iron nanoparticles (gn-ZVI) were synthesized using extracts from tree leaves with high antioxidant capacity as a substitute of the "toxic" sodium borohydrate. These gn-ZVI were applied to the degradation of pharmaceuticals (such as ibuprofen and amoxicillin), acting as a reductant (as zero valent iron), or as a catalyst (in the Fenton reaction), and presented several advantages: lower synthesis cost, lower toxicity and capping effect that the extract matrix provides to the nanoparticles.

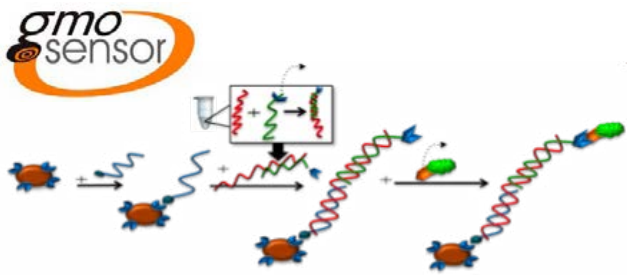


Application of green zero-valent iron nanoparticles to the remediation of soils contaminated with ibuprofen

Science of the Total Environment, 2013, 461-462, 323-329.

GMOSENSOR: MONITORING GENETICALLY MODIFIED ORGANISMS IN FOOD AND FEED BY INNOVATIVE BIOSENSOR APPROACHES

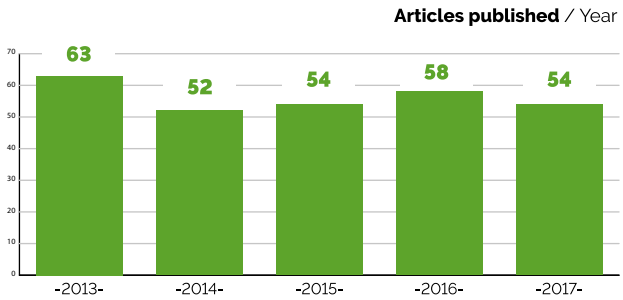
The GMOsensor project established an international network (EU and South America) focusing on the development of novel, innovative, cheap and integrated bioanalytical devices (mainly DNA- and protein-based) for the detection of GMO in food and feed. Three types of GMO sensing platforms were designed to be used in a stepwise approach: i) element specific (such as the promoter and terminator elements and the encoded protein); ii) gene-specific; and iii) event-specific.



FP7-PEOPLE-2013-IRSES | 612545

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION 2013-2017*



281 articles
2502 citations**
H-index: **46**

'From WOS core collection
''of the published articles in 2013-2017

FUNDED PROJECTS *(Representative projects)*

- "REWATER - Sustainable and safe water management in agriculture: Increasing the efficiency of water reuse for crop growth while protecting ecosystems, services and citizens' welfare"
  WaterJPI/0007/2016, Cristina Delerue-Matos (PI),
  Total Funding: € 555,960.00, Team Funding: 119,449.00 €
- "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),
  Total Funding: € 536,227.00, Team Funding: 395,000.00 €
- "Energetic valorization of wastes obtained during rice production in Portugal - RICEVALOR"
  PTDC/AAG-REC/3477/2012, Filomena Pinto (PI),
  Total Funding: € 197,944.00, Team Funding: 62,869.00 €
- "GMOsensor - Monitoring Genetically Modified Organisms in Food and Feed by Innovative Biosensor Approaches"
  FP7-PEOPLE-2013-IRSES | 612545, Cristina Delerue-Matos (PI),
  Total Funding: € 340,200.00, Team Funding: 79,800.00 €
- "TrophicENPs - Bioavailability and trophic transfer of metal-based engineered nanoparticles in terrestrial foodchains"
  PTDC/AGR-PRO/4091/2012, Eduarda Pereira (PI),
  Total Funding: € 185,000.00, Team Funding: 98,504.00 €
- "Monitorização ambiental dos efeitos da implementação da Unidade Aquícola de engorda de pregado em Mira na Qualidade da Água do Meio Recetor"
  AQUINOVA, Eduarda Pereira (PI),
  Total Funding: € 276,452.00

9 EU projects
658 k€

42 national projects
1.9 M€

8 industry-financed projects
170 k€

INTERNATIONAL COOPERATION AND NETWORKING

- 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)
- International Cooperation with several research centres and universities from: Argentina, Belgium, Brazil, Czech Republic, Denmark, France, Germany, India, Italy, Paraguay, Poland, Romania, Serbia, Spain, Sweden, Netherlands, United States of America

OUTREACH

- Ciência Viva Short Placements in Laboratories is a programme that offers young people the opportunity to get involved in research teams in science and technology institutions, during their Summer holidays. This research group hosted a range of hands-on activities for the secondary education students, 2013-2017.
- Organization of a contest "Recycling is an art", 2015.
- Organization of a workshop "Contaminated Soils: Remediation Technologies and Solutions", 2015.
- Organization of a workshop "Waste management", 2017.
- TECHDAYS 2017, "Tecnologias para a proteção, gestão e reutilização da água", Mar e Ria, Centro de Exposições de Aveiro, 2017.
- Open days of the university and polytechnic institutes.
- BUSINESS2SEA, "Alternative tecnologies for water treatment", Centro de Congressos da Alfândega do Porto, 2016.
- Escola de Verão "Ria de Aveiro", Fábrica de Ciência Viva de Aveiro, 2014.
- Introductory course on scientific research, 2013-2017.


LABORATÓRIO ASSOCIADO
PARA A QUÍMICA VERDE


requimte
rede de química e tecnologia


U.PORTO


UNIVERSIDADE
NOVA
DE LISBOA


universidade
de aveiro

BCPE

(BIO)CHEMICAL PROCESS ENGINEERING

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

Our group has 34 integrated (senior) members, distributed among 8 research laboratories, whose main scientific background is in Chemical and Biochemical Engineering. From 2018 onwards the group will benefit from the integration of new members from the University of Évora with a strong track record in thermophysics and molecular modelling.

Our research covers a wide spectrum of disciplines, such as biocatalysis, separation/purification, solvents and reaction media, synthesis/processing, systems biology and metabolic modelling, and thermophysics. The development of environmentally friendly processes to produce highly added-value products in a sustainable and economical way is a unifying research theme.

A sizable volume of intellectual property involving different labs has been produced, as reflected by 4 recent patent submissions, 8 industrial contracts, including 4 in EU projects, 32 externally funded projects, with 11 directly from EU, and 4 new start-ups. A process engineering pilot plant, with 120 sq.m, includes (bio)reactors, membrane units, extraction and separation equipment and a supercritical
fluid unit.

RESEARCH OBJECTIVES [2018-2022]

The (Bio)chemical Process Engineering group will continue using its diversified experience in state-of-the-art environmentally friendly technologies to develop innovative processes that combine expertise from its different labs in key areas such as:

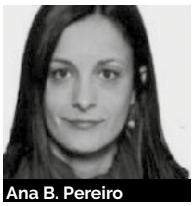
- Purification, extraction, and in situ transformation of solutes;
- Downstream processing of industrial effluents containing complex (bio) molecules;
- Carbon dioxide utilization, comprising capture with ionic liquids, eutectic solvents, membrane, and novel adsorption processes, carbon dioxide (electro-/bio-)chemical reduction to fuels or use as green solvent in extraction or (bio) reactions;
- Extraction of added-value compounds, using ionic liquids, eutectic solvents, enzymatic pre-treatments, near-critical water or supercritical carbon dioxide;
- Functionalized ionic liquids and eutectic solvents for delivery of biomolecules, protein crystallization, microfluidics, electrochemical devices, and gas separation;
- Implementation of new microbial processes and optimization using functional enviromics methods for cell culture medium engineering, and microbial ecology.

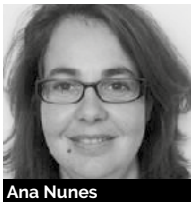
RESEARCH TEAM

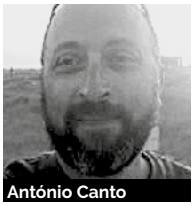
SENIOR RESEARCHERS


Alexandre Paiva


Alfredo Carvalho


Ana B. Pereiro


Ana Nunes


António Canto


Carla Portugal


Ewa Bogel-Lukasik


Isabel Esteves


Isabel Coelhoso


João M. M. Araújo


João Ramalho


João G. Crespo


José M. Esperança


José P. Mota


Luís Martins


Luís P. Rebelo


Luísa Neves


Manuel da Ponte


Madalena Dionísio


Patrícia M. Reis


Paulo C. Lemos


Pedro Simões


Rui Oliveira


★ Susana Barreiros


Svetlozar Velizarov

★ Group coordinator

RESEARCH TEAM

OTHER DOCTORATE RESEARCHERS

Ana Maria Machado
Mário Eusébio
Maria Margarida Cardoso

POST-DOCTORAL FELLOWS

Ana Dias
Ana Isabel Ferreira
Ana Rita Gameiro
Carla B. Ferreira
Carolina H. Merino
Cláudia G. Loureiro
Fátima M. Diaz
Fernando J. L. Cruz
Gonçalo Carrera
Helena I. M. Veiga
James Yates
Magdalena Kowacz
Marija Petkovic
Mohammad Tariq
Rita Craveiro
Rosa Huertas
Rui P. P. L. Ribeiro
Sylwin Pawlowski

PhD STUDENTS

Abimaelle Chibério
Ameessa Tulcidas
Ana Carina Manjua
Ana I. Paninho
Ana Mimoso
Ana Rita Ferreira
Ana Rita Fidalgo
Ana Rute Ferreira
Anabela Costa
André Martins
André Silva
Andriy Lyubchyk
Bárbara Camacho
Bruno Pedras
Bruno Santos
Carla Daniel
Carla Martins
Carmo Fraga
Catarina M. Barbosa
Daniela Souza
Diana Oliveira
Duarte L. Martins
Elena Surra
Filipa Franco
Filipe S. Oliveira
Francisca Mano
Helga Garcia
Idalina Bragança
Inês Meireles
Inês Valente
Isabel Martins
Joana C. Bastos
Joana Monte
Joana S. Pereira
Lakshmeesha Upadhyaya
M. João Pereira
Mafalda Lopes
Márcia Alves
Margarida Ferreira
Magdalena Malankowska
Mariella Polino
Mário Soromenho
Marta da Silva
Marta Sá
Mohammad Almanasrah
Mohammed Yahia
Nayan Nayak
Nicole Vieira
Pedro Bastos
Pedro Lisboa
Piergiuseppe Nestola
Ricardo Silva
Rita Leones
Rita Valério
Rui Ferreira
Sara F. Carvalho
Sérgio da Costa
Sergio Santoro
Shabnam Majudi
Sofia Fraga
Sofia Messias
Sowmiah Subbiah
Susana Santos
Teresa Brás
Teresa Cordeiro
Usman Taqui Syed
Zenamarkos Sendekie

MSc STUDENTS

Alison Setim
Ana Calheiros
Ana Martins
Ana Patrícia Martins
Ana Rita Nabais
Ana T. Rebocho
Ana Vera Torres
André Oliveira
André Portela
Andreia Carvalho
Bárbara Camacho
Beatriz Moura
Bruno Marta
Carla Casas Garcia
Carlos Gomes
Carmen Villarta
Catarina Rodrigues
Cátia Marques
Daniela Carvalho
Frederico Martins
Helga Correia
Henrique Marçal
Hugo Andrade
Inês Bernardo
Inês Ferreira
Inês Hilário
Inês Valente
Jéssica Viegas
Joana Silva
João Gomes
João P. Azevedo
Júlio Parra
Mafalda Isidro
Miguel Palhas
Misgina Tilahun
Ng Kok Seng
Olga Sulim
Oriol Ribera Serra
Paulina Sosa
Pedro Camilo
Pedro Bastos
Pedro Melo
Rizza Ardiyanti
Romana Martins
Sara Cândido
Sofia Pereira
Susana Ferreira
Tanmoy Kanti Deb
Tiago Diniz
Tiago Ferreira
Tiago Santos
Vânia Silva
Vera Nunes
Ye Wee

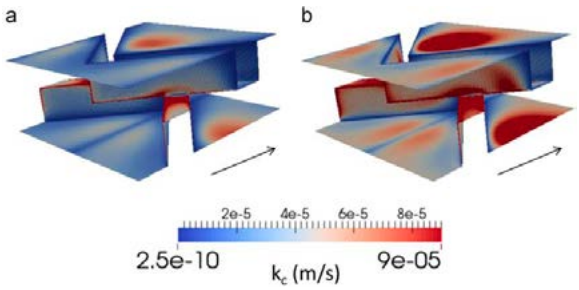
RESEARCH GRANTEES

Adrianna Nogalska
Amina Noubli
Ana Luísa Neves
Ana Raquel Batuca
André M. Ferro
Andreia Sousa
Andryi Lyubchyk
Ângela Machado
Asmaâ Zakmout
Bárbara Camacho
Eleonora Lalli
Eliana Orfão
Elisa Esposito
Elsa Mora
Fabiana Teixeira
Filipa Teixeira
Gaëlle Capitaine
Halima Gallouze
Jaouen Florian
Joana Marques
Juliette Boudaud
Karen Ranochia
Katarzyna Knozowska
Maëlle Morellec
Mateuz Marchel
Nawel Rahmoune
Sofiane Bensaadi
Susana Martinho
Tiago Santos

RESEARCH THEMES

MEMBRANE PROCESSES: DEVELOPMENT AND MONITORING[1-8]

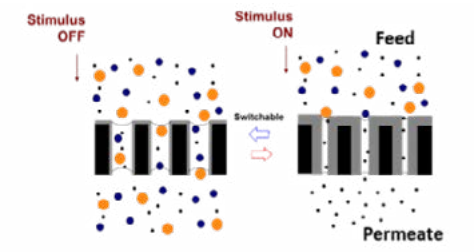
- Recovery of high-value compounds from complex (bio)medium (agro-industrial effluents and microalgae biomass)
- Treatment of (agro)industrial and domestic effluents for water reuse (implementation of this work allowed GALP to save 500 k€/year in wastewater costs and target additional savings of 1.5 M€/year)
- Integration of membranes and advanced oxidation processes
- Removal of hazardous ionic pollutants from drinking water supplies
- Membrane contactors for crystallization and nano-emulsification
- "Blue" energy for a sustainable world
- Modelling of membrane processes using computational fluid dynamics



- Real-time process monitoring using 2D fluorescence spectroscopy
- Molecular probes for in-situ and on-line membrane monitoring
- On-line, real-time monitoring of gas and vapour permeation by mass-spectrometry

DEVELOPMENT OF NEW MEMBRANE MATERIALS[9-12]

- Membranes integrating ionic liquids and MOFs for gas separation
- Membranes based in biopolymers for biomedical applications, food packaging and dehydration processes
- Stimuli-responsive membranes for biotechnological, biomedical and environmental applications
- Photocatalytic membranes



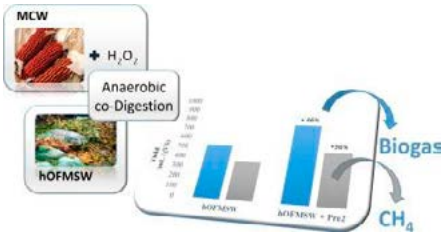
SELECTED PUBLICATIONS

1 U. T. Syed, et al. Sep. Purif. Technol. 2017, 172, 404. doi:10.1016/j.seppur.2016.07.039
2 B. Santos, et al. Sep. Purif. Technol. 2013, 119, 51. doi:10.1016/j.seppur.2013.09.009
3 S. Sanches, et al. J. Chem. Technol. Biotechnol. 2017, 92, 1727. doi:10.1002/jctb.5172
4 M. Pessoa-Lopes, et al. Sep. Purif. Technol. 2016, 166, 125. doi:10.1016/j.seppur.2016.04.032
5 S. Pawlowski, et al. J. Membr. Sci. 2016, 502, 179. doi:10.1016/j.memsci.2015.11.031
6 M. Sá, et al. Algal Res. 2017, 24, 325. doi:10.1016/j.algal.2017.04.013
7 S. Santoro, et al. J. Membr. Sci. 2017, 536, 156. doi:10.1016/j.memsci.2017.05.001
8 S. C. Fraga, et al. Sep. Purif. Technol. 2018, 197, 18. doi:10.1016/j.seppur.2017.12.026
9 B. Monteiro, et al. Energy Technol. 2017, 5, 1. doi:10.1002/ente.201700228
10 A. R. V. Ferreira, et al. Carbohydr. Polym. 2016, 147, 8. doi:10.1016/j.carbpol.2016.03.089
11 C. I. Daniel, et al. J. Membr. Sci. 2016, 505, 36. doi:10.1016/j.memsci.2015.11.025
12 R. M. Huertas, et al. Sep. Purif. Technol. 2017, 180, 69-81. doi:10.1016/j.seppur.2017.02.047

RESEARCH THEMES

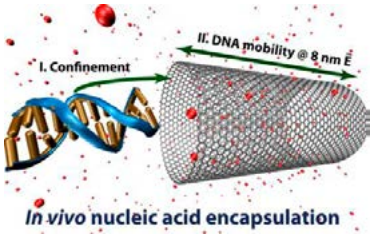
SUSTAINABLE BIOREFINERY FOR BIOGAS UPGRADING[13-19]

- Novel Adsorption-based Technological Pathways Towards a Low-Carbon Economy, GHG Mitigation and Renewable Energy Resources
- Biorefinery for the Production of Activated Carbon from maize wastes and Biogas Upgrading
- Screening of New Adsorbent Media for Biogas Upgrading as a Source of Renewable Energy

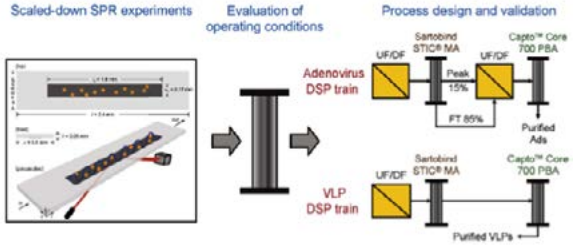


ADSORPTION SCIENCE AND TECHNOLOGY[20-24]

- Experimental and computational studies of gas adsorption in metal-organic frameworks
- Optimization of the industrial-scale simulated moving-bed Parex unit for p–xylene separation.
- Rational development of flow-through purification strategies for viruses and virus-like particles



- Nanoscopic characterization of DNA confined within hydrophobic and hydrophilic carbon nanotubes
- Improved virus purification processes for vaccines and gene therapy



SELECTED PUBLICATIONS

13 C. R. Correa, et al. J. Anal. Appl. Pyrolysis. 2017, 124, 461. doi:10.1016/j.jaap.2017.02.014

14 E. Surra, et al. Waste Manag. 2018, 72, 193. doi:10.1016/j.wasman.2017.11.004

15 B. C. R. Camacho, et al. Sep. Purif. Technol. 2015, 141, 150. doi:10.1016/j.seppur.2014.11.040

16 R. P. P. L. Ribeiro, et al. Sep. Purif. Technol. 2017, 182, 19. doi:10.1016/j.seppur.2017.03.037

17 J. P. B. Mota, et al. J. Phys. Chem. C. 2017, 121, 24252. doi:10.1021/acs.jpcc.7b06861

18 R. P. P. L. Ribeiro, et al. Microporous Mesoporous Mater. 2016, 230, 154. doi:10.1016/j.micromeso.2016.05.006

19 M. S. P. Silva, et al. AIChE J. 2016, 62, 241. doi:10.1002/aic.15022

20 F. J. A. L. Cruz, et al. J. Phys. Chem. C. 2017, 121, 16568. doi:10.1021/acs.jpcc.7b03167

21 F. J. A. L. Cruz, et al. Biochem. Eng. J. 2015, 104, 41. doi:10.1016/j.bej.2015.04.027

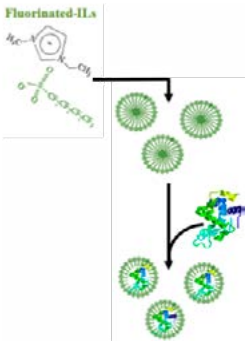
22 F. J. A. L. Cruz, et al. J. Chem. Phys. 2014, 140, 225103. doi:10.1063/1.4881422

23 C. Peixoto, et al. Human Gene Ther. 2015, 26, A71. doi:10.1089/hum.2015.29008.abstracts

24 P. Nestola, et al. J. Chromatogr. A. 2015, 1426, 91. doi:10.1016/j.chroma.2015.11.037

RESEARCH THEMES

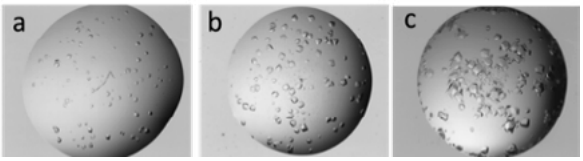
FLUORINATED IONIC LIQUIDS[25-28]



- Influence of nanosegregation on the behavior of ionic liquids
- Drug delivery systems of biomolecules using ionic liquids
- Enhanced tunability afforded by aqueous biphasic systems and ionic liquids
- Increasing the surfactant behavior and solubilization capacity of ionic liquids

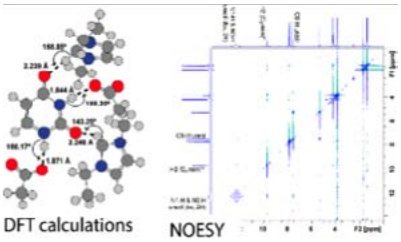
FUNCTIONALIZED IONIC LIQUIDS[29-32]

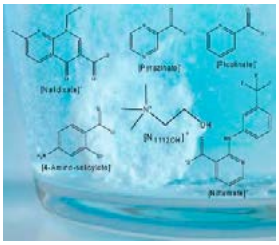
- Protonic ammonium nitrate ionic liquids
- Charge-inverted ionic liquid pairs
- Ionic liquids for the crystallization of proteins
- Magnetic ionic liquids and their applications on the development of high performance materials
- Playing with ionic liquids structure to discover unusual properties and applications



NATURE-INSPIRED IONIC LIQUIDS[33-36]

- 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
- 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





SELECTED PUBLICATIONS

25 A. Luís, et al. Langmuir. 2016, 32, 6130. doi:10.1021/acs.langmuir.6b00209
26 M. Alves, et al. Int. J. Pharm. 2017, 526, 309. doi:10.1016/j.ijpharm.2017.05.002
27 A. M. Ferreira, et al. Green Chem. 2016, 18, 1070. doi:10.1039/C5GC01610J
28 A. B. Pereiro, et al. Langmuir. 2015, 31, 1283. doi:10.1021/la503961h
29 J. N. C. Lopes, et al. J. Phys. Chem. B. 2016, 120, 2397. doi:10.1021/acs.jpcb.5b11900
30 M. Kowacz, et al. Cryst. Growth Des. 2015, 15, 2994. doi:10.1021/acs.cgd.5b00403
31 R. Leones, et al. Electrochim. Acta. 2017, 240, 474. doi:10.1016/j.electacta.2017.04.042
32 J. C. Dias, et al. Polym. Test. 2015, 48, 199. doi:10.1016/j.polymertesting.2015.10.012
33 J. M. M. Araújo, et al. J. Phys. Chem. B. 2013, 117, 4109. doi:10.1021/jp400749j
34 S. Shahriari, et al. RSC Adv. 2013, 3, 1835. doi:10.1039/C2RA22972B
35 F. J. Deive, et al. RSC Adv. 2015, 5, 3386. doi:10.1039/C4RA15021J
36 J. M. M. Araújo, et al. RSC Adv. 2014, 4, 28126. doi:10.1039/C3RA47615D

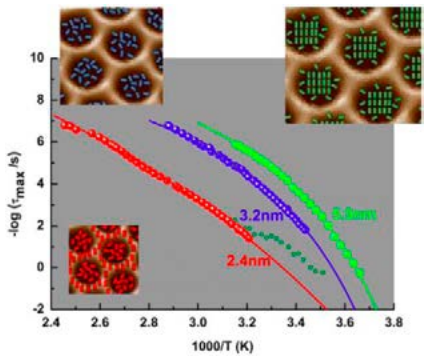
RESEARCH THEMES

CO_2 UTILIZATION[37-41]

- Valuable new platform chemicals obtained by valorization of succinic and bio-succinic acid with an ionic liquid and high-pressure CO_2
- New organic carbonates from CO_2 and bio-based epoxides
- High pressure electrochemical reduction of carbon dioxide and water, in an ionic liquid electrolyte, to produce syngas with controlled proportions of CO and Hydrogen
- Hydrogenation of CO_2 into methane, catalyzed by ruthenium nanoparticles, stabilized by ionic liquid solvents
- Novel systems, based on highly abundant saccharides, in combination with an organic superbase, were studied for carbon dioxide capture

THERMOPHYSICS[42-47]

- Probing phase transformations and molecular mobility of materials in bulk and upon nanoconfinement: pharmaceutical drugs, polymers
- Improvement of drug delivery performance by stabilization of high energetic drug states
- Characterization of conductive properties of ionic liquid based materials



SELECTED PUBLICATIONS

37 D. Silva, et al. Green Chem. 2017, 19, 4048. doi:10.1039/C7GC00952F

38 C. A. Montoya, et al. J. Catal. 2016, 335, 135. doi:10.1016/j.jcat.2015.12.027

39 T. Pardal, et al. J. CO2 Util. 2017, 18, 62. doi:10.1016/j.jcou.2017.01.007

40 C. Melo, et al. ChemSusChem. 2016, 9, 1081. doi:10.1002/cssc.201600203

41 G. V. S. M. Carrera, et al. Faraday Discuss. 2015, 183, 429. doi:10.1039/C5FD00044K

42 T. Cordeiro, et al. J. Phys. Chem. C. 2016, 120, 14390. doi:10.1021/acs.jpcc.6b04078

43 A. R. Brás, et al. J. Phys. Chem. C. 2014, 118, 13857. doi:10.1021/jp500630m

44 M. T. Viciosa, et al. J. Phys. Chem. B. 2014, 118, 6972. doi:10.1021/jp5045783

45 T. Cordeiro, et al. Mol. Pharm. 2017, 14, 3164. doi:10.1021/acs.molpharmaceut.7b00386

46 T. Carvalho, et al. J. Phys. Chem. B. 2014, 118, 9445. doi:10.1021/jp502870q

47 M. T. Viciosa, et al. Phys. Chem. Chem. Phys. 2015, 17, 24108. doi:10.1039/C5CP03715H

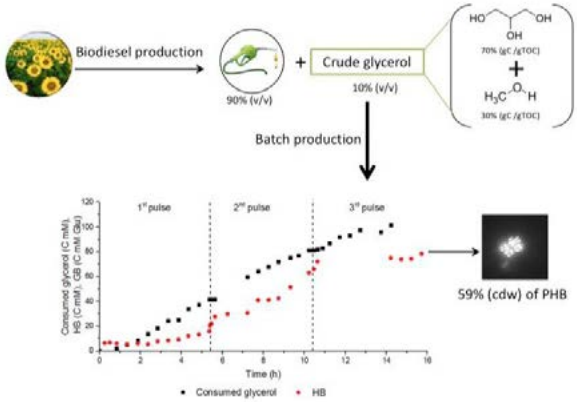
RESEARCH THEMES

SYSTEMS BIOLOGY AND ENGINEERING[48-52]

- Novel hybrid modelling methods combining traditional mathematical modelling with machine learning and Artificial Intelligence (AI) to support efficient industry 4.0 digitalization
- Modelling, Measurement, Monitoring & Control (M3C) of bioprocesses: supporting Process Analytical Technology (PAT) using hybrid systems theory
- Cell functional enviromics: reconstruction of cellular function from the side of the environment whereby time series of cellular footprints are used to identify and reconstruct active biologic functions
- Novel systems biology methods for designing synthetic biologic parts, such as core promoter DNA sequences, for fine-tuning heterologous protein expression
- Value creation and entrepreneurship in the field of systems biology through education, industrial collaboration and science based start-ups

MICROBIAL ECOLOGY AND TECHNOLOGY[53-58]

- Combining thermochemical and biological processes for agro-industrial/forestry residues valorization
- Conversion of biodiesel by-product (crude glycerol) to biodegradable polymers
- Microbial Ecology of mixed microbial cultures processes
- Two/three-step process for polyhydroxyalkanoates production using hardwood spent sulfite liquor from pulp and paper industry
- Molecular biology methods in Microbial Ecology of mixed microbial cultures processes



SELECTED PUBLICATIONS

48 R. Marques, et al. J. Biotechnol. 2017, 246, 61. doi:10.1016/j.jbiotec.2017.01.017

49 I. A. Isidro, et al. Bioprocess Biosyst. Eng. 2016, 39, 1351. doi:10.1007/s00449-016-1611-z

50 M. Stosch, et al. Bioprocess Biosyst. Eng. 2016, 39, 773. doi:10.1007/s00449-016-1557-1

51 M. Stosch, et al. BMC Bioinf. 2016, 17, 200. doi:10.1186/s12859-016-1063-0

52 R. M. Portela, et al. ACS Synth. Biol. 2017, 6, 471. doi:10.1021/acssynbio.6b00178

53 R. Moita, et al. N. Biotechnol. 2014, 31, 297. doi:10.1016/j.nbt.2013.10.009

54 R. Moita, et al. Water Res. 2014, 58-9, 9. doi:10.1016/j.watres.2014.03.066

55 D. Queirós, et al. Appl. Microbiol. Biotechnol. 2014, 9, 10433. doi:10.1007/s00253-015-7010-6

56 D. Queirós, et al. J. Chem. Technol. Biotechnol. 2016, 91, 2480. doi:10.1002/jctb.4841

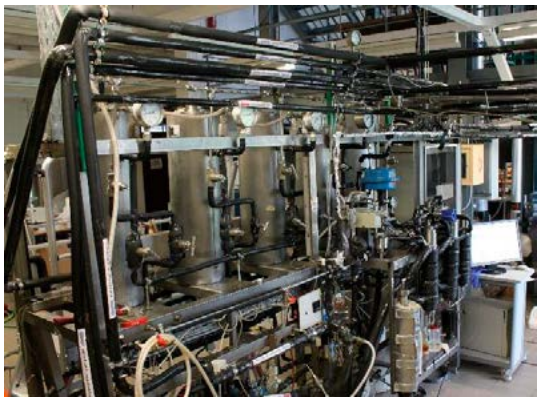
57 A. Freches, et al. N. Biotechnol. 2017, 39, 22. doi:10.1016/j.nbt.2017.05.011

58 D. Queirós, et al. J. Ind. Microbiol. Biotechnol. 2017, 44, 1215. doi:10.1007/s10295-017-1951-y

RESEARCH THEMES

VALORIZATION OF AGRO-INDUSTRIAL AND FISH BY-PRODUCT[59-64]

- Subcritical water (SBW) and supercritical CO_2 (sc-CO_2) have been used in the recovery of added-value compounds from agro-industrial matrices and fish waste
- Deep eutectic solvents (DES) have been used to decrease cellulose crystallinity
- Recovered lipids and carbohydrates have been used as alternative sources to grow yeast and bacteria
- Integrated extraction/(bio)transformation/separation processes have been implemented for lipids from agro-industrial by-products. Phase equilibrium data have been generated and modelled
- Some processes have been carried out at pilot scale under contract with National or European industrial companies, and their economic viability assessed



NEW FORMULATIONS FOR COSMETICS, PHARMACEUTICALS, CO_2 CAPTURE AND CONVERSION[65-70]

- Sc-CO_2 has been used to prepare/alter functional materials, often materials that incorporate a task specific ionic liquid or DES, through swelling, impregnation/extraction, and foaming
- Data on the properties of DES and DES/sc-CO_2 systems have been generated
- Added-value compounds from agro-industrial by-products, as well as therapeutic DES and enzymes, have been encapsulated in films, particles, sol-gel matrices, electrospun fibres, or incorporated in formulations for cosmetics, controlled release, and CO_2 capture and conversion

SELECTED PUBLICATIONS

59 A. R. R. Pinto, et al. J. Anal. Appl. Pyrolysis. 2017, 127, 68. **doi:10.1016/j.jaap.2017.08.021**

60 B. Pedras, et al. J. Supercrit. Fluid. 2017, 128, 138. **doi:10.1016/j.supflu.2017.05.020**

61 J. Del Valle, et al. J. Supercrit. Fluid. 2016, 107, 321. **doi:10.1016/j.supflu.2015.09.021**

62 M. Gameiro, et al. Fuel. 2015, 153, 135. **doi:10.1016/j.fuel.2015.02.100**

63 P. Lisboa, et al. J. Supercrit. Fluid. 2014, 85, 31. **doi:10.1016/j.supflu.2013.10.018**

64 M. V. Cruz, et al. Biores. Technol. 2014, 157, 360. **doi:10.1016/j.biortech.2014.02.013**

65 A. Gertrudes, et al. ACS Sustain. Chem. Eng. 2017, 5, 9542. **doi:10.1021/acssuschemeng.7b01707**

66 A. S. D. Ferreira, et al. Magn. Reson. Chem. 2017, 55, 452. **doi:10.1002/mrc.4427**

67 R. Craveiro, et al. J. Mol. Liq. 2016, 215, 534. **doi:10.1016/j.molliq.2016.01.038**

68 G. Barreira, et al. RSC Adv. 2014, 4, 25099. **doi:10.1039/C4RA01620C**

69 A. Paiva, et al. ACS Sustain. Chem. Eng. 2014, 2, 1063. **doi:10.1021/sc500096j**

70 H. Ribeiro, et al. Eur. J. Lipid. Sci. Technol. 2013, 115, 330. **doi:10.1002/ejlt.201200239**

HIGHLIGHTS

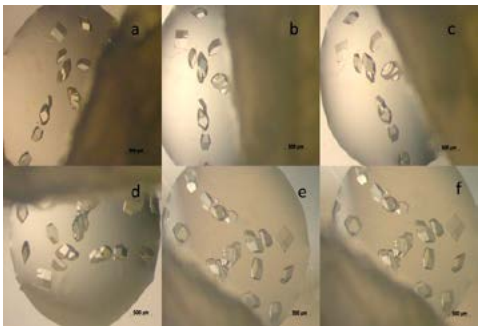
DESIGN OF FUNCTIONAL MEMBRANES

Functional membranes are task specific molecular barriers designed to fulfil specific process requisites or promote well-defined processing operations allowing for a non-invasive control, monitoring and improvement of the performance of processes from different application fields – biotechnology, health, food, environment and energy.

Functional porous materials and biodegradable dense thin films, with tailor made chemistries, hierarchical 3D porous structures and topographies were designed and used in the development of (bio)sensors, edible food packaging and cutting edge (bio)separation processes.

Stimuli-responsive membrane based devices for tissue engineering applications, membranes with magnetically modulated permeability and microfluidic systems for high throughput protein crystallization and derivatization processes were developed.

For the first time, it was possible to produce isomorphous protein crystals without laborious handling, using membranes to control diffusion for *in-situ* crystal's derivatization.



Ion-exchange membranes for stable derivatization of protein crystals

Crystal Growth & Design, 2017, 17, 4563-4572.

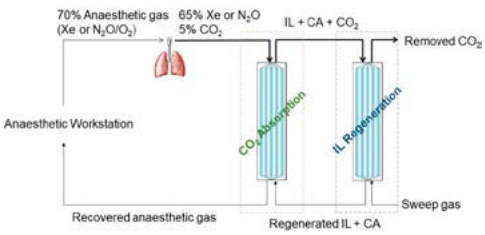
TECHNOLOGY FOR THE REMOVAL OF CARBON DIOXIDE (CO2) PRESENT IN ANAESTHETIC GAS CIRCUITS

Anaesthetic closed circuits are used to promote the reuse of the exhaled anaesthetic gas that circulates through a canister containing soda lime which reacts with CO2. Despite of being used in hospital operating rooms, soda lime is a caustic compound which produces toxic products when in contact with the anaesthetic gas mixture. This work proposes a clean, efficient and self-renewable technology to remove CO2 from anaesthesia circuits. It consists of using hollow fibre membrane contactors with a biocompatible ionic liquid and an enzyme (carbonic anhydrase) as the liquid absorber. This procedure allows for capturing CO2 and regenerating the ionic liquid in a continuous operation mode.

Due to the novelty of this work, a National Patent (N°106902), a PCT PCT/IB2014/060797 and a World Patent (WO2014/170858A1) were submitted.

The L'Oréal Portugal Medal of Honour for Women in Science 2013 was awarded with visibility in press and national TV.

It also gave rise to the creation of the spin-off company InovBreath, Lda (February 2016), and the first prize award in the entrepreneurship business idea contest of CINC Cascais (June 2016).



Process for the purification of anesthesia gases using membrane contactors and its applications

PCT/IB2014/060797

HIGHLIGHTS

STATISTICAL MECHANICS & MOLECULAR SIMULATION

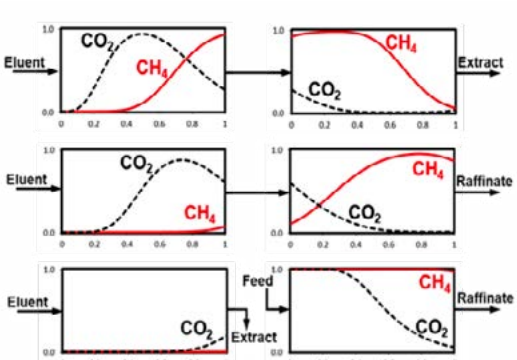
We have employed theoretical tools developed within the framework of statistical mechanics (Molecular Dynamics, Monte Carlo, Hamiltonian-biasing algorithms) to solve contemporary issues in biophysics and materials science. In particular, we have theoretically studied DNA nanotechnology using carbon nanotubes for it is currently leading the way in personalized (less risk intense) therapeutics for specific drug delivery to living human cells.
Enhanced sampling techniques spanning a sub-microsecond time scale revealed that a double-stranded DNA dodecamer can be spontaneously encapsulated into (51,0) and (40,0) single-walled carbon nanotubes under the influence of an electric field, leading to hybrids with a 40 kJ/mol enhanced free energy. Moreover, our molecular study has been shown the nanotube-encapsulated nucleic acid maintains translational mobility within the endohedral nanotube volume, but the diffusional mechanism is markedly dependent on pore diameter.

Dynamics of B-DNA in electrically charged solid nanopores

Journal of Physical Chemistry C, 2017, 121, 16568.

ADSORPTION SCIENCE AND PROCESS SYSTEMS ENGINEERING

We have evaluated state-of-the-art adsorbents, namely metal-organic frameworks (MOFs), carbon nanotubes, zeolites and activated carbons for application in adsorption-based separations and gas storage (e.g. methane, CO_2, and hydrogen). Experimental adsorption equilibria and kinetics studies have been combined with molecular modelling and classical simulation for a general interpretation of the thermodynamic phenomena.
We have designed novel adsorption-based processes, for gas and liquid separations, through model-based process simulation & optimization and experimental validation. The main separation/process targets have been Pressure Swing Adsorption (PSA) for biogas upgrading and carbon dioxide (CO_2) capture, novel Simulated Moving Bed (SMB) schemes for ethane/ethylene and CO_2/CH_4 separation, and the purification of fine chemicals and biopharmaceuticals by compact SMB chromatography.



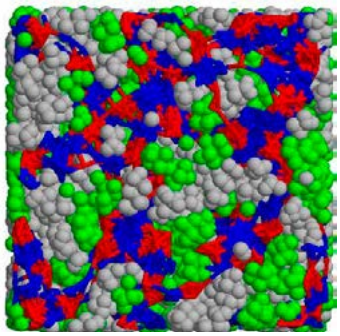
Two-column relay simulated moving-bed process for gas-phase separations

Separation and Purification Technology, 2017, 182, 19.

HIGHLIGHTS

FLUORINATED IONIC LIQUIDS AS NOVEL TASK-SPECIFIC MATERIALS

Fluorinated ionic liquids (FILs) are growing into greener materials for engineering applications. For the first time, the presence of a unique nanostructuring effect was proven – the appearance of a third nanosegregated domain (fluorous), which permits converting FILs into 3-in-1 solvents with enhanced solubilization power. The different types of interactions and the size and nature of the domains promote an enriched surfactant behavior and solubility in water. This fact permit us to use FILs in different bio-applications where conventional fluorocarbon compounds display some handicaps.

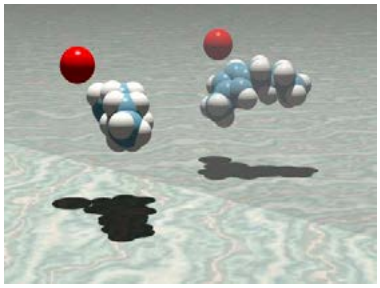


On the formation of a third, nanostructured domain in ionic liquids

Journal of Physical Chemistry B, 2013, 117, 10826-10833.

CHARGE-INVERTED IONIC LIQUID PAIRS

It is well-known that salts based on the halides anions show much lower melting temperatures than those in which their isoelectronic alkali counterparts are present as cations. Salts based on potassium are not members of the ionic liquids family, whereas many containing chloride are. There are more than 400 halide-based ILs (e.g. Cl^-) but none based on its isoelectronic counterpart, K^+. For the first time, ionic liquid pairs in which their constitutive ions can be regarded, in terms of charge, as the mirror images of each other, were synthesized and characterized. The proof-of-concept that inverted-IL salts can also be fluid at relatively low temperatures opens new possibilities for the preparation of novel, paradigm-shifting IL families.



ILs through the looking glass: electrostatics and structure probed using charge-inverted ionic liquid pairs

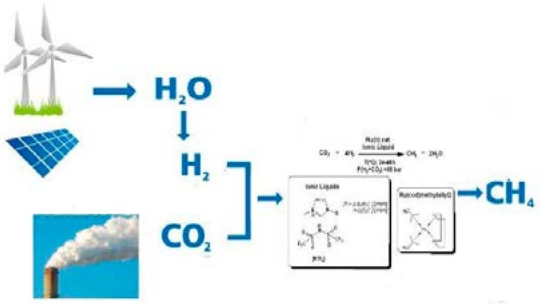
Faraday Discuss., 2018, 206, 203-218.

CO_2 HYDROGENATION TO METHANE USING RUTHENIUM NANOPARTICLES IN IONIC LIQUIDS

Power-to-gas schemes use hydrogen from water electrolysis to reduce captured carbon dioxide into fuels.

An efficient, high yield route to obtain methane directly form CO_2 was discovered, using as catalyst ruthenium nanoparticles prepared in situ in imidazolium-based ionic liquid media, at relatively low temperature (150 °C).

Yields in different ionic liquids were highly dependent on the nanoparticle stabilizing effect of each liquid.



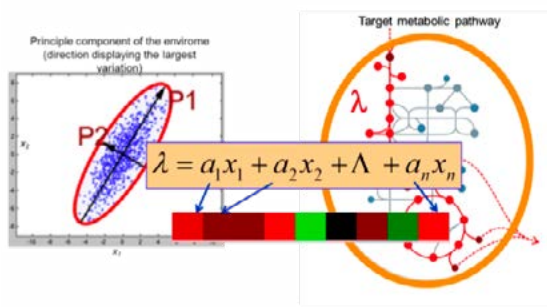
Ruthenium nanoparticles prepared in situ in the presence of an ionic liquid catalyze the hydrogenation of CO_2

ChemSusChem, 2016, 9, 1081–1084.

HIGHLIGHTS

FUNCTIONAL ENVIROMICS MAPPING OF CHO CELLS

We have developed of functional enviromics maps for Pichia pastoris cells expressing heterologous proteins. Such mapping provides unprecedented detail of cellular interaction with their environment. Metabolic pathway tailored culture medium optimization to enhance the expression of heterologous proteins by Pichia pastoris cells and Chinese hamster ovary (CHO) cells.
We have also developed of a software tool for hybrid semiparametric mathematical modelling for systems bio(techno)logy problems. Implementation of Process Analytical technologies (PAT) and Quality by Design (QbD) for mammalian cell cultures and show case with CHO expressing monoclonal antibodies using hybrid systems theory.

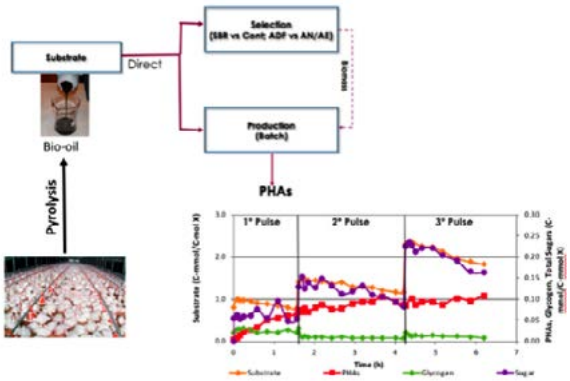


A principal components method constrained by elementary flux modes: Analysis of flux data sets

BMC Bioinformatics, 2016, 17, 200.

UTILIZATION OF PYROLYTIC OIL FROM CHICKEN BEDS FOR PHA AEROBIC PRODUCTION BY MIXED MICROBIAL CULTURES

Polyhydroxyalkanoates (PHA) are biodegradable polymers with similar properties to fuel-derived ones. PHA production from low-value substrates and/or by-products is an economical and environmental promising alternative to established industrial processes. Chicken beds are a hazard waste namely due to its high N content. From the thermochemical conversion of the solid waste the obtained liquid fractions (bio-oil) was used as substrate to select a mixed microbial culture able to produce PHA under feast/famine conditions.
A PHA content of 9.2% was achieved in an SBR operated for culture selection, later maximized in a side-stream step. Other studies that use real complex substrates for culture selection show that bio-oil can be a promising feedstock to produce PHAs. To maximize carbon conversion a three-step process is preferable to the present two-step one. The introduction of an acidogenesis step would convert available carbon sources into short-chain organic acids that would be more easily converted to PHAs.



Bio-oil upgrading strategies to improve PHA production from selected aerobic mixed cultures

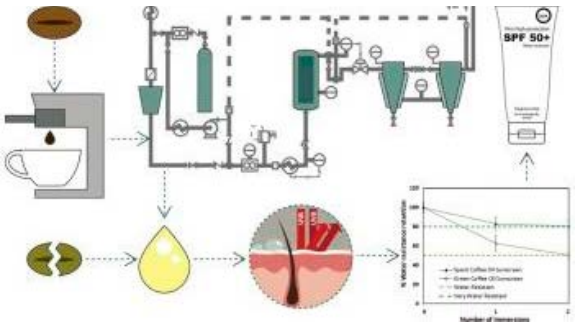
New Biotechnology, 2014, 31, 297-307.

HIGHLIGHTS

GREEN GENERATION SUNSCREENS BASED ON COFFEE INDUSTRIAL BY-PRODUCTS

Spent coffee grounds and green coffee defective beans, which are industrial by-products of coffee processing, have a potential use for cosmetic applications, due to their safety and high content in lipids with interesting physicochemical properties.

The biological effects of using the oil fraction of spent coffee grounds extracted with supercritical CO2, and of green coffee oil in the development of a new generation of sunscreens with improved sun protection performance, were assessed. The two oil fractions were used to prepare w/o sunscreens. The emulsion containing the spent coffee grounds oil fraction presented promising characteristics in the improvement of water performance, with a broad spectrum sun protection when compared to an emulsion containing green coffee oil, which improved the sun protection factor in physical sunscreens.

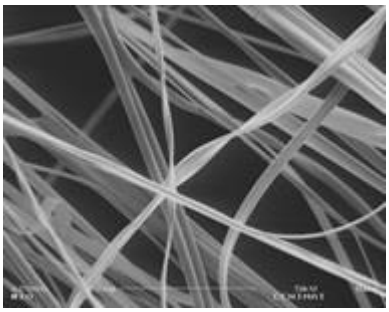


The green generation of sunscreens: Using coffee industrial sub-products

Industrial Crops and Products, 2016, 80, 93-100.

FAST-DISSOLVING DRUG DELIVERY SYSTEMS WITH ENCAPSULATED THERAPEUTIC EUTECTIC SYSTEMS

Oral drug delivery is still the preferred route for the administration of pharmaceutical ingredients, but some patients, e.g. children or elderly people, have difficulties in swallowing solid tablets. Fast-dissolving delivery systems (FDDS) allow quick drug administration, while avoiding physical obstruction as well as the need of access to water. High surface area gelatin membranes containing an encapsulated therapeutic deep eutectic solvent (THEDES) were produced by electrospinning. The fibre membranes had no cytotoxicity effects, exhibited a fast-dissolving release profile in PBS, and the encapsulated THEDES retained its antibacterial activity, thus opening up new opportunities for the design of more affordable and biodegradable drug delivery mechanisms.

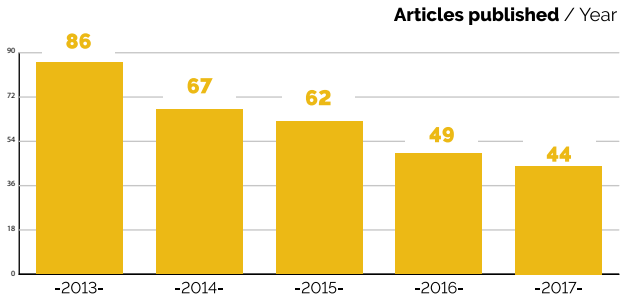


Production of Electrospun Fast-Dissolving Drug Delivery Systems with Therapeutic Eutectic Systems Encapsulated in Gelatin

AAPS Pharm Sci Tech, 2017, 18, 2579-2585.

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION 2013-2017*



308 articles
3286 citations**
H-index: **81**

**From WOS core collection*
***of the published articles in 2013-2017*

FUNDED PROJECTS *(Representative projects)*

- SALTGAE - Demonstration project to prove the techno-economic feasibility of using algae to treat saline wastewater from the food industry
  H2020-WATER-2015, Project ID: 689785, João G. Crespo (Local PI).
  Total Funding: 469,987.00 €.
- D-FACTORY - The micro algae biorefinery
  FP7-KBBE-2013-7, Project ID: 613870, João G. Crespo (Local PI).
  Total Funding: 465,550.00 €.
- Bio-FESS: Biorefinery for the Production of Low- and High-Grade Activated Carbon from forestry wastes, maize residues and biogas digestate.
  ERA NET LAC 2014, Isabel Esteves (Local PI).
  Total funding: 395,000.00 €.
- CEOPS: CO2 - Loop for Energy storage and conversion to Organic chemistry Processes through advanced catalytic Systems
  FP7-NMP-2012-SMALL-6, Project ID: 309984. Manuel Nunes da Ponte (Local PI)
  Total Funding: 225,177.00 €.
- Design of fluorinated ionic liquids as novel task-specific fluids.
  FCT, PTDC/QEQ-EPR/5841/2014. Ana Belén Pereiro (PI).
  Total funding: 199,879.00 €.
- DES-ZYME: Biocatalytic separation of enantiomers using natural deep eutectic solvents
  FCT, PTDC/BBB-EBB/1676/2014. Alexandre Paiva (PI).
  Total funding: 168,535.00 €.

11 EU projects
2.25 M€

17 national projects
2.17 M€

4 industry-financed projects
170 k€

INTERNATIONAL COOPERATION AND NETWORKING

- Joint PhD Programs: MIT Portugal Bioengineering Systems Doctoral program and Erasmus Mundus Doctorate in Membrane Engineering (EUDIME)
- Joint Master's program: Erasmus Mundus Master in Membrane Engineering for a Sustainable World (EM3E-4SW)
- Student exchange at Master's level with the University of São Paulo (Brazil)
- Coordination of H2020-MSCA-RISE 2015 NANOGUARD2AR - Nanomaterials-based innovative engineering solution to ensure sustainable safeguard to indoor air
- Participation in H2020-MSCA-RISE 2015 HUNTER - Advanced Humidity to Electricity Converter
- Participation in EIT RawMaterials activities (as members of Core partner of Co-location Centre CLC West);
- Founding member of the CO_2 Value Europe Association.

OUTREACH

- Participation in EXPO FCT (annual 1-day event for high school students).
- Participation in the Science and Technology Week, organized by FCT.
- Recipient of the Medal of Honour for Women in Science (L. Neves), followed by press and TV coverage.
- Article in Pan European Networks Horizon 2020 Projects: "Novel membranes from biopolymers", I. Coelhoso, Portal – 7th Edition, July 2015.
- Digital media Key Scientific Article at Advances in Engineering, 2015.
- Member, Board of Directors, International Adsorption Society, 2010-16 (J.P. Mota).
- Member, Council of Chairs, International Congress on Ionic Liquids, since 2005 (L. Rebelo).
- Vice-President, European Membrane Society (EMS), since 2017 (C. Portugal).
- Joint organization: 3rd Hybrid Modelling Summer School, University of Life Science and Natural Resources, Vienna, Austria, 2017 (R. Oliveira), 2nd Hybrid Modelling Summer School, Max Planck Institute Magdeburg, Germany, 2015 (R. Oliveira), EMSF2017 – 16th European Meeting on Supercritical Fluids, Lisbon, 2017 (A. Paiva, M. Nunes da Ponte, P. Simões);
- Co-chair: Imagine Membrane, Horta, Azores, 2017 (J. Crespo), ChemPor, Porto, 2014 (J. Crespo), 5th International Congress on Ionic Liquids (COIL-5), Vilamoura 2013 (L. Rebelo), 16th European Meeting on Supercritical Fluids, Lisbon, 2017 (M. Nunes da Ponte);
- Plenary lectures: 2nd EuCheMS Congress on Green and Sustainable Chemistry, Lisbon, 2015 - Carbon Dioxide: from Supercritical to Circular (M. Nunes da Ponte), Russian Congress on Chemical Thermodynamics, Moscow, 2013 - Salty chemistry: interdisciplinary case studies involving ionic liquids (L. Rebelo), ECTP 2014 – 20th European Conference on Thermophysical Properties, Porto, 2014 - Upon what may exist in the "gap" between traditional ionic liquids and molten salts (L. Rebelo).


LABORATÓRIO ASSOCIADO
PARA A QUÍMICA VERDE


requimte
rede de química e tecnologia


U.PORTO


UNIVERSIDADE
NOVA
DE LISBOA


universidade
de aveiro

Charm

CULTURAL HERITAGE AND RESPONSIVE MATERIALS

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

The Cultural Heritage And Responsive Materials (CHARM) group concentrates in the design of responsive molecules and materials where external stimuli allow 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 a number 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 CO2 and Ionic Liquids.

The interdisciplinary environment conveys an integrated approach where state of the art materials and techniques are applied in conservation and the knowledge over how ancient materials have endured inspire the design or development of materials with enhanced properties.

RESEARCH OBJECTIVES [2018-2022]

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 CO2 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 as 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 in the development of Interdisciplinary Approaches, in particular to Medieval Iberian Heritage. The creation of a new research line dedicated to the study and conservation of 19th c. and contemporary heritage is in action, including Ângelo de Sousa collection, contributions for a history of plastics in Portugal, preserving historic photographic collections 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 & PhD students.

We are enthusiastic to celebrate the European Year of Cultural Heritage, sharing our research with the general public and strengthening our position in the community.

RESEARCH TEAM

SENIOR RESEARCHERS


A. Jorge Parola


Ana M. Ramos


César Laia


Fernando Pina


★ J. C. Lima


Joana L. Ferreira


Leslie Carlyle


Luís C. Branco


M. João Melo


M. C. Casanova


Sandra Gago

★ Group coordinator

RESEARCH TEAM

OTHER DOCTORATE RESEARCHERS
Cláudia Pereira
Isabel P. Cardoso
Susana F. Sá

POST-DOCTORAL FELLOWS
Alfonso Alejo-Armigo
Artur Moro
Hugo Cruz
Karolina Zalewska
Noémi Jordão
Nuno Basílio
Vânia Pais
Miguel Santos
Zeljko Petrovski

PhD STUDENTS
Ambrósio Camuenho
Ana Lúcia Pinto
Ana Margarida Rocha
Ana Rita Araújo
Andreia Forte
Andreia Santos
Artur Neves
Catarina Florindo
Daniel Esteban Veja
David Sousa
Élia Roldão
Eva M. Angelin
Filipa Santos
Gonçalo Tiago
Inês Martins
Joana M. Devesa
Joana L. Silva
Johan Chacon
Juliana B. Oliveira
Mani Hosseinzadeh
Marta F. Campos
Paula Nabais
Raquel Marques
Samaneh Shariff
Sara Sá
Sara Sobral Babo
Sofia Friães
Susana B. Caxeiro
Tatiana Vitorino
Vanessa O. Matias

MSc STUDENTS
Ana Galo Luis
Catarina Viola
Débora Magalhães
Inês Soares
Liliane Raposo
Mafalda Rebola
Márcia Vieira
Mariana Antunes
Paulo André
Pedro Reis
Rita Fernandes
Victória Paz

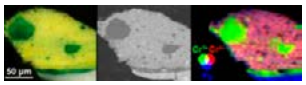
RESEARCH GRANTEES
Carina Figueiredo
Jack Fletcher-Charles
Rafael Mamede
Tiago Moreira

OTHER RESEARCHERS
Antoine Stopin
Massimo Tosolini

RESEARCH THEMES/ CULTURAL HERITAGE

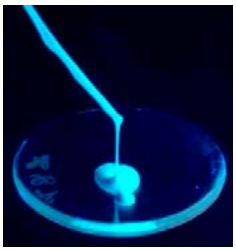
CAUSES AND MECHANISMS OF ALTERATION

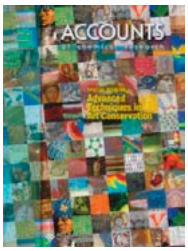
- Medieval illuminated manuscripts and polychrome sculpture[1-5]
- Amadeo de Souza-Cardoso and 19th century artists' paints[6-10]
- 19th century, Modern & Contemporary Cultural Heritage[11-13]

SUSTAINABLE INNOVATIVE METHODS

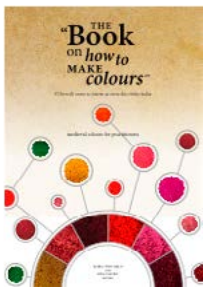
- Applications of super critical and liquid CO_2[14]
- Applications of ionic liquids[15]
- New advanced methods of dyes analysis[8, 16-17]

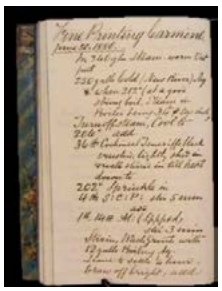
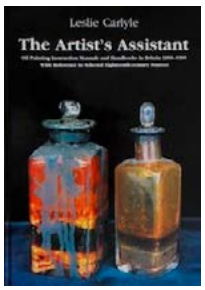




HISTORICAL RECONSTRUCTIONS DATABASE

- The book on how to make colours[8, 18]
- The Winsor & Newton artist materials supplier, 19th century archive[8,16-19]



SELECTED PUBLICATIONS

1 M. J. Melo, et al. Microchem. J. 2016, 124, 837. doi:10.1016/j.microc.2015.10.014

2 P. Nabais, et al. JMIS. 2016, 8, 283. doi:10.1080/17546559.2016.1234061

3 A. M. Cavero, et al. JMIS. 2016, 8, 217-251 doi:10.1080/17546559.2016.1221116

4 I. P. Cardoso, et al. J. Archaeol. Sci. 2017, 79, 86. doi:10.1016/j.jas.2017.01.014

5 I. P. Cardoso, et al. J. Archaeol. Sci. 2017, 79, 96. doi:10.1016/j.jas.2017.01.015

6 V. Otero, et al. Heritage Sci. 2017, 5, 46. doi:10.1186/s40494-017-0160-3

7 V. Otero, et al. Stud. Conserv. 2016, 62, 123. doi:10.1080/00393630.2015.1131478

8 T. Vitorino, et al. Stud. Conserv. 2016, 61, 255. doi:10.1179/2047058415Y.0000000006

9 D. Sanches, et al. Polym. Degrad. Stab. 2017, 138, 201. doi:10.1016/j.polymdegradstab.2017.02.010

10 C. Montagner, et al. Multimed Tools Appl. 2016, 75, 4039. doi:10.1007/s11042-015-3197-x

11 S. F. Sá, et al. J. Raman Spectrosc. 2016, 47, 1494. doi:10.1002/jrs.4984

12 S. F. Sá, et al. Polym. Degrad. Stab. 2017, 144, 354. doi:10.1016/j.polymdegradstab.2017.08.028

13 J. Silva, et al. ICOM-CC 18th Triennial Conference Preprints, 2017, ed. J. Bridgland, art. 1403. Paris: International Council of Museums. icom-cc-publications-online.org/PublicationDetail.aspx?cid=eed87cff-f731-4b7e-9649-fc75c81e8b0d

14 M. Sousa, et al. Green Chem. 2007, 9, 943. doi:10.1039/B617543K

15 J. M. Delgado, et al. Corr. Sci. 2017, 118, 109. doi:j.corsci.2017.01.027

16 R. Castro, et al. J. Raman Spectrosc. 2014, 45, 1172. doi:10.1002/jrs.4608

17 M. J. Melo, et al. Philos Trans A Math Phys Eng Sci. 2016, 374, 20160050 doi:10.1098/rsta.2016.0050

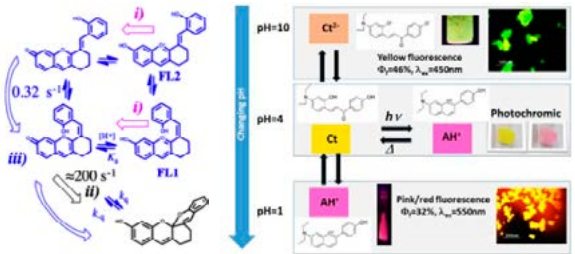
18 M. J. Melo and R. Castro, eds. The "Book on how to make colours". www.dcr.fct.unl.pt/LivComoFazemCores

19 L. Carlyle, 'The Artist's Assistant': Oil Painting Instruction Manuals and Handbooks in Britain 1800-1900 With Reference to Selected Eighteenth-century Sources, Archetype Publications, 2001.

RESEARCH THEMES/ RESPONSIVE MATERIALS

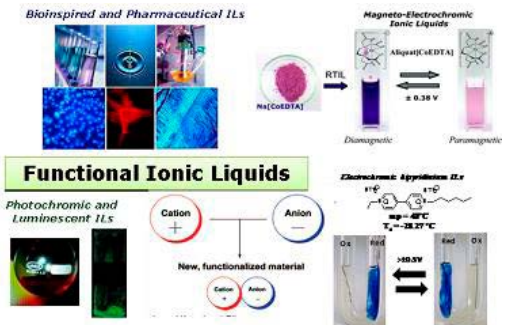
ANTHOCYANINS AND FLAVYLIUM SALTS

- Photochromic systems based on anthocyanin family derivatives[20-22]
- Host-guest systems for improved performance[21-24]
- New anthocyanin familiy derivatives for DSSCs[25,26]



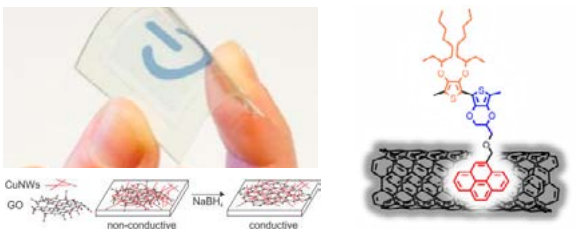
IONIC LIQUIDS AND ALTERNATIVE SOLVENTS

- Innovative active pharmaceutical drugs based ionic liquids[27]
- Photochromic Ionic liquids to control rheology with light[28,29]
- Green electrolytes for electrochromic devices[30]
- Ionic liquids for CO_2 capture and conversion[31]



ELECTROCHROMIC DEVICES

- New organic components for electrochromic devices[32,33]
- New wet methods for material deposition[34]
- New ITO-free conductive coatings for improved transparence[35,36]



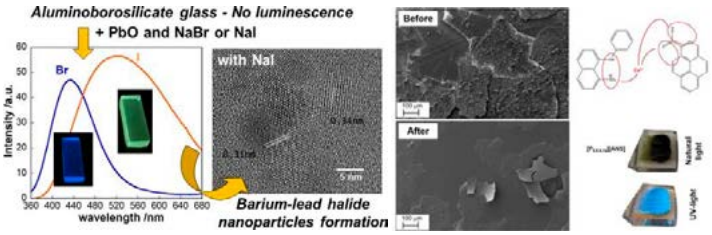
SELECTED PUBLICATIONS

20 S. Gago, et al. Chem. Commun. 2015, 51, 7349. doi:10.1039/C5CC01677K
21 S. Gago, et al. ACS Omega. 2017, 2, 122. doi:10.1021/acsomega.6b00381
22 N. Basílio, et al. Chem. Commun. 2017, 53, 6742. doi:10.1039/C7CC02432K
23 N. Lavande, et al. Phys. Chem. Chem. Phys. 2017, 19, 13640. doi:10.1039/C7CP01889D
24 N. Basílio, et al. J. Phys. Chem. B. 2015, 119, 2749. doi:10.1021/jp511351w
25 A. Alejo-Armijo, et al. Chem. Eur. J. 2016, 22, 12495. doi:10102/chem.201601564
26 G. Calogero, et al. Photochem. Photobiol. Sci. 2017, 16, 1400. doi:10.1039/C7PP00039A
27 I. C. Martins, et al. ChemSusChem. 2017, 10, 1360. doi:10.1002/cssc.201700153
28 J. Avó, et al. J. Phys. Chem. B. 2015, 119, 6680. doi:10.1021/acs.jpcb.5b00254
29 J. Avó, et al. Org. Lett. 2014, 16, 2582. doi:10.1021/ol501111d
30 H. Cruz, et al. Green Chem. 2017, 19, 1653. doi:10.1039/C7GC00347A
31 C. I. Melo, et al. ChemSusChem. 2016, 9, 1081. doi:10.1002/cssc.201600203.
32 N. Jordão, et al. RSC Adv. 2015, 5, 27867. doi:10.1039/C5RA02368H
33 N. Jordão, et al. ChemPlusChem. 2015, 80, 202. doi:10.1002/cplu.201402232
34 S. M. Fonseca, et al. Sol. Energy Mater. Sol. Cells. 2017, 159, 94. doi:10.1016/j.solmat.2016.09.002
35 L. Gomes, et al. Displays. 2013, 34, 326. doi:j.displa.2013.06.004
36 A. Aliprandi, et al. Adv. Mat. 2017, 29, 1703225. doi:10.1002/adma.201703225

RESEARCH THEMES/ RESPONSIVE MATERIALS

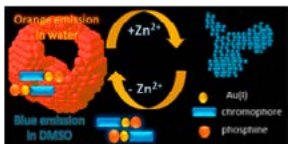
LUMINESCENT GLASS MATERIALS

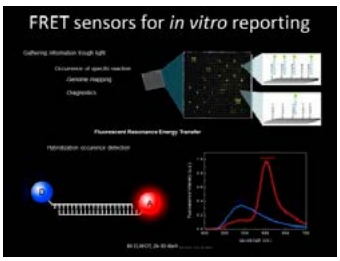
- Rare-earth photoluminescence[37,38]
- Towards fabrication of quantum-dots in aluminoborosilicate glasses[39,40]
- Corrosion mechanisms of glass surfaces and cleaning strategies Application in stained-glass restoration[15]



LIGHT ACTIVATED SENSORS AND ACTUATORS

- Multichanel fluorescent sensors for O2, temperature and biologically relevant targets[41-44]
- Light control over nucleic acid enzimatic polimerization[45]
- Heating through UV/Vis light absorption and non-radiative dumping[46]
- Aggregation induced emission of metalophylic hydrogels[47-49]





SELECTED PUBLICATIONS

37 A. Ruivo, et al. J. Quant. Spectrosc. Radiat. Transfer. 2014, 134, 29. doi:10.1016/j.jqsrt.2013.10.010

38 B. Monteiro, et al. Chem. Comm. 2017, 53, 850. doi:10.1039/C6CC08593H

39 A. Ruivo, et al. J. Phys. Chem. C. 2014, 118, 12436. doi:10.1021/jp5003758.

40 A. Ruivo, et al. J. Phys. Chem. C. 2016, 120, 24925. doi:10.1021/acs.jpcc.6b04552

41 C. C. L. Pereira, et al. Appl. Clay Sci. 2017, 146, 216. doi:10.1016/j.clay.2017.06.002

42 S. Santoro, et al. J. Memb. Sci. 2016, 514, 467. doi:10.1016/j.memsci.2016.05.019

43 M. Cordeiro, et al. J. Nanobiotechnology. 2016, 14, 38. doi:10.1186/s12951-016-0192-y

44 M. Cordeiro, et al. J Biotechnol. 2013, 168, 90. doi:10.1016/j.jbiotec.2013.08.005

45 M. M. Reimão-Pinto, et al. Photochem. Photobiol. Sci. 2014, 13, 751. doi:10.1039/C3PP50438G

46 R. Mendes, et al. Sci. Rep. 2017, 7, 10872. doi:10.1038/s41598-017-11491-8

47 E. Aguiló, et al. Inorg. Chem. 2017, in press. doi:10.1021/acs.inorgchem.7b02343

48 L. Giestas, et al. Supramol. Chem. 2017, in press. doi:10.1080/10610278.2017.1355462

49 A. Pinto, et al. Dalton Trans. 2017, 46, 11125. doi:10.1039/C7DT02349A

HIGHLIGHTS

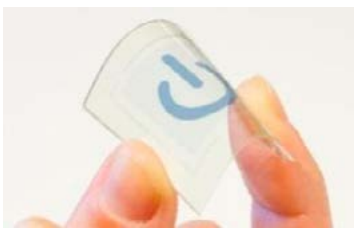
LORVÃO BEATUS (1189) UNESCO´S MEMORY OF THE WORLD REGISTER

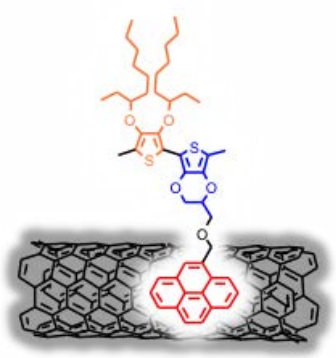
Our team contributed to the interdisciplinary chemical and historical research on the Manuscripts of the Commentary to the Apocalypse (Beatus of Liébana) in the Iberian tradition, which led to the successful entry of 12th century Portuguese Beatus into UNESCO´s Memory of the World Register. Pigment analysis combined with documentary evidence allowed a complete reinterpretation of the color use and depiction of figures in Lorvão Beatus (1189). This research resulted in the codex being recognized as a unique and important contribution to World Heritage.

ELECTROCHROMIC DEVICES

Printed graphics are emerging to the age of interactivity with innovative advanced materials sets allowing the design of smart objects and environments. Electrochromics enables mass producible ultra low-power interactive displays to create the so-called "Internet-of-Things" (IoT). Recently, we have chemically designed semiconductor polymers interactions with carbon nanomaterials and proposed novel electrochromic ionic liquids based on low-cost deep eutectic solvents.

As a result, a strong international collaboration with Academia and Industry (e.g., Ynvisible and Sonae Industria de Revestimentos) gave rise to two recent H2020 Projects, bringing together a strong interdisciplinary consortium in 9 different countries, industry and research, that will provide toolkits to introduce printed electrochromics to designers and the printing industry.



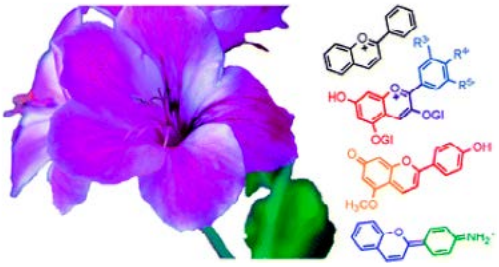


Hybrid copper-nanowire–reduced-graphene-oxide coatings: a "green solution" toward highly transparent, highly conductive, and flexible electrodes for (opto)electronics

Advanced Materials, 2017, 29, 1703225.
INFUSION-H2020-MSCA-RISE-2016 n.734834
DecoChrom-H2020-NMBP-2017 n . 760973

HIGHLIGHTS

ANTHOCYANIN MULTISTATE SYSTEMS



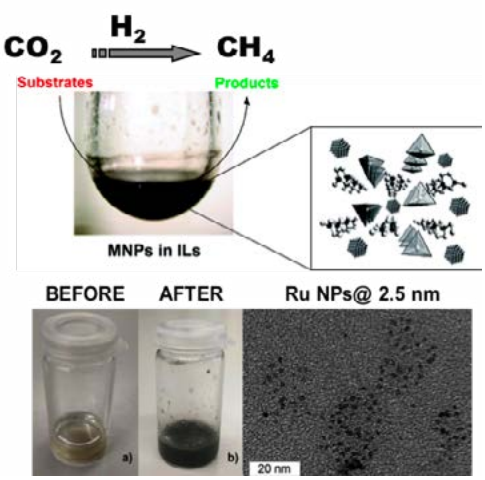
Anthocyanins are an important family of compounds belonging to the flavonoid group, responsible for the different shades of reds and blues of most flowers and fruits. Besides their role as plant colorants there is evidence that regular consumption of anthocyanins and other polyphenols, reduce the risk of some chronic diseases, due to their anti-oxidant properties. During the last two decades we pioneered work on anthocyanins and related flavylium compounds and a rich experimental and theoretical knowledge has been accumulated, recognized. While there are only six common natural anthocyanins, it is possible to design and prepare bioinspired derivatives, more adapted to specific functions. Information systems based on the photochromism within the flavylium network of chemical reactions, able to writereaderase, have been reported, including an illustration of how these system can mimic elementary properties of neurons, and molecular logic gates. The work on anthocyanins provided the seed for contributing to cleaner energy solutions, a societal challenge; anthocyanins were used for building bioinspired Dye Sensitised Solar Cells (DSSC), and a DSSC with 3.1% efficiency has been built and the next generation of flavylium compounds for DSSC is under study.

Electronic and charge transfer properties of bio-inspired flavylium ions for applications to TiO2-based dye-sensitized solar cells

Photochemical & Photobiological Sciences, 2017, 16, 1400-1414

CO2 CAPTURE AND CONVERSION (CCU) IN FUELS

Prominent among the technological challenges to be reached is the development of photochemical mechanisms that lead to the efficient production of H_2 from water and sunlight. Once produced, H_2 may be used directly to power fuel cells or may be further converted into CH_4 or fixed into liquid fuels via hydrogenation of CO_2. Our team have contributed to the integration of TiO_2 and an Au(I) complex containing a thiocoumarin moiety resulting in a very efficient photocatalyst for the generation of H_2. We have also contributed for Carbon Capture and Utilization (CCU) achievements by the discovery of efficient reversible carbon dioxide capture using bioinspired systems (aminoacids, saccharides, cellulose) in combination with suitable organic superbases, as well as the innovative approaches for catalytic conversion of carbon dioxide in methane using metal nanoparticles/ionic liquid systems.



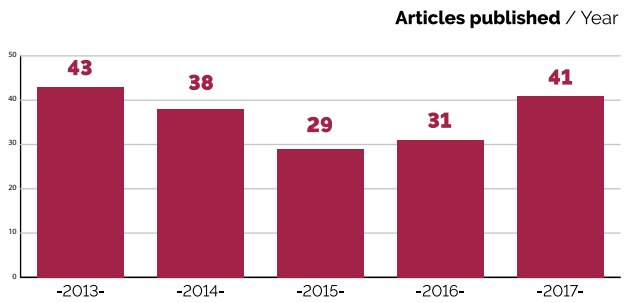
Gold(I)-complex–titania hybrid photocatalyst for hydrogen production

ChemCatChem, 2017, 9, 3289–3292.

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION 2013-2017*

182 articles
1203 citations
H-index: **56**



FUNDED PROJECTS *(Representative projects)*

3 EU projects
1.1 M€

6 national projects
1.2 M€

- **"SACS – Self-Assembly in Confined Space"**
  FP7-NMP4-SL2012 - grant 310651, Fernando Pina (Portuguese coordinator)
  Total funding: € 4,584,067.40
- **"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
- **"SunStorage - Harvesting and Storage of Solar Energy"**
  POCI-01-0145-FEDER-016387, Adélio Mendes (PI, FCUP),
  Total funding: € 2,050,049.77
- **"Crossing Borders. History, Materials and Techniques of Portuguese Painters, 1850-1918: Romantism, Naturalism and Modernism."**
  PTDC/EAT-EAT/113612/2009, Maria João Melo (PI),
  Total funding: € 144,423.60
- **"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

INTERNATIONAL COOPERATION AND NETWORKING

- COST Action CM1005, "Supramolecular Chemistry in water", 2011-2015.
- 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).

OUTREACH

- CHARM members participate actively in the construction of science and technology demonstrators and hands-on activities for high school students at open labs days, (EXPO FCT), visits to schools and other outreach communication events (Futuralia, Researchers Night) occuring yearly.
- CHARM members lecture Lab lessons to high school students and teachers in a unique outreach activity aiming at providing access to laboratory classes to students from underequiped/underprepared institutions (LAQV receives ca. 1000 students/year under this activity).
- J. C. Lima coordinates the yearly training of 17 year old students competing at European Union Science Olympiad since 2006.
- M. J. Melo and other CHARM members participated in several TV documentaries dedicated to Amadeo de Souza-Cardoso, 2016, Public Exhibitions (e.g. BNP, "Livros de Horas: o imaginário da devoção privada", 2014, Workshops on medieval illuminations for the general public, high school students as well as for training and tutoring of partner institutions as the National Library and Archives (BNP, TT).
- J. L. Ferreira participate, together with architect Eduardo Souto de Moura and curator Nuno Faria, in a weekly show organized by Câmara Municipal do Porto, dedicated to the sculpture of Ângelo de Sousa for Torre do Burgo.
- CHARM have a long-term involvement with the archive, creation of a page-image database of over 17,000 records covering recipes for pigments, binders and varnishes in collaboration with Winsor & Newton artist materials supplier, 19th century archive.


LABORATÓRIO ASSOCIADO
PARA A QUÍMICA VERDE


requimte
rede de química e tecnologia


U.PORTO


UNIVERSIDADE
NOVA
DE LISBOA


universidade
de aveiro

MatSusWell

MATERIALS FOR SUSTAINABILITY AND WELLBEING

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

The Materials for Sustainability and Wellbeing (MatSusWell) group aims at contributing towards the 21st Century Grand Global Challenges: i) Bioeconomy; ii) Secure, clean and efficient energy; iii) Climate action, environment, resource efficiency and raw materials; and iv) Health and wellbeing, through a strong emphasis on innovation, by continuing R&TD, investing on knowledge valorization and by bringing together a multidisciplinary team with background in Chemistry, Materials Science & Engineering, Biomedical Sciences, Entrepreneurship & Business Development, encompassing as the ultimate goal the scientific knowledge transfer and technological valorisation.

In this context, the overall purpose of MatSusWell is the development and production of advanced multifunctional (nano)materials using sustainable methodologies for core scientific areas: i) Catalysis for a Sustainable Environment, ii) Renewable Energy and Climate Change Mitigation, iii) Environmental Protection and Remediation, and iv) Drug Delivery and Tissue Regeneration, with complementary research work on iv) Theoretical and Computational Modelling and on v) Wearable Technologies and Devices; the utmost results of scientific areas boost Technology Transfer and Business Development.

RESEARCH OBJECTIVES [2018-2022]

Within 2018-22, MatSusWell group will continue its strong commitment with the Global Challenges that encompasses the rational design and production of advanced materials by green and innovative strategies: (bio)polymers/nanostructured films, (nano) biomaterials, inorganic (nano)materials and natural deep eutectic solvents - with target properties for catalysis, adsorption, drug delivery, tissue regeneration, medical devices, energy and responsive prototypes, devices and smart textiles, going beyond laboratory research to pilot scale in collaboration with industry or through the creation of University spin-offs, with the ultimate goal of contributing to innovative products/technologies for society. Group objectives also comprise the understanding of fundamental physicochemical properties relevant for the core areas of catalysis, adsorption, energy, drug delivery and tissue regeneration processes, biocompatibility assessment, prototypes/devices and textiles, in order to establish composition functionalityperformance relationships, fundamental to the rational design of materials for the chosen target application, always based on a strong support of theoretical studies.

Researchers will be also highly committed with funding procurement, collaboration with other Academic Institutions and Industrial partners at national and international levels, as well as to participate in science dissemination in strict alignment with society demands and needs.

RESEARCH TEAM

SENIOR RESEARCHERS


★ Ana Aguiar-Ricardo


Ana Rita Duarte


André Melo


Clara Pereira


Cristina Freire


Inês Matos


Isabel Fonseca


Joaquim Vital


José Domingos Santos


Liliana Grenho


Manuela R. Carrott


M. Ascenção Lopes


M. Helena Fernandes


M. Natália Cordeiro


Paulo Mourão


Pedro Sousa Gomes


Peter Carrott


Salete S. Balula


Svetlana Lyubchyk


Teresa Casimiro


Zuzana Benkova

★ Group coordinator

RESEARCH TEAM

OTHER DOCTORATE RESEARCHERS
Isabel Cansado
Márcia Ventura
Olena Lygina

POST-DOCTORAL FELLOWS
Amal K. Giri
Amit K. Halder
Andreia F. Peixoto
Carlos Granadeiro
Diana Fernandes
Elisabete Ferreira
Filipe Teixeira
Iuliia Voroshilova
Iwona Biernacka
J. Luis Cagide Fajín
José Rui Marques
Luís Cunha Silva
Maria Manuel Bernardo
Marta Nunes
Mary Kalina Batista
Raquel Viveiros
Riccardo Concu
Tânia Vanessa Pinto
Víctor K. Fernández

PhD STUDENTS
Ana Catarina Pinho
Ana Pessoa
Ana Rita Caseiro
André D. Barbosa
Bruna Rijo
Carla P. Queirós
Carmen Montoya
Cátia Bonito
Clarinda Costa
Cláudia C. Ribeiro
Daniel Santos
Diana R. Morais
Diogo Dias
Fabiana Santos
Fábio M. Costa
Fernanda Dalto
Francisco M. Maligno
Gabriela Martins
Javier A. Fernández
José M. Campos
Kevin L. Oliveira
Luísa Fialho
Mariana R. Rocha
Mariana S. Lopes
Paulo José Neves
Pedro O. Pinto
Rita Pires
Rúbia S. Risso
Stéphanie Soares
Susana N. Ribeiro
Teresa M. Cordeiro
Tiago A. Silva

MSC STUDENTS
Ana Catarina Sousa
Bruna Pinheiro
Carla Sofia Baptista
Cláudia M. Sousa
Daniela Agostinho
Daniela M. Silva
Guilherme Costa
João Paixão
Luís Pinto Dias
Marlene Rajão
Nádia Figueiredo
Nuno Morgado
Thomas Pullert
Vanessa Caetano
Victor Silva

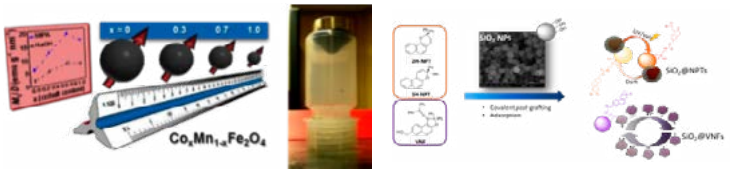
RESEARCH GRANTEES
Ana Isabel Soares
Bruno Silvano
Miguel Mateus

OTHER RESEARCHERS
Alexandre Viana
Joana Teixeira
José Dinis Silva
Rui Santos Costa

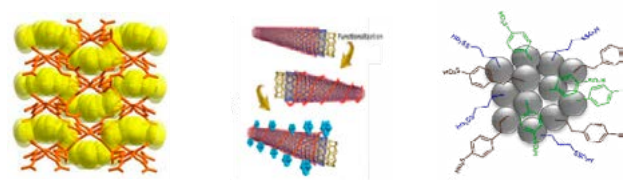
RESEARCH THEMES/
(BIO)MATERIALS ENGINEERING AND PRODUCTION

MatSusWell uses the long-term expertise in Materials Science to design and produce new advanced (nano)materials to support the different 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 small size and improved magnetic properties using water and organic bases as reaction media.[1,2]
- **Core-shell magnetic** nanomaterials with silica, TiO2 and gold coatings preparation using water as reaction medium or solvothermic methods.[3]
- **Noble metal nanoparticles** (Au, Ag, Ru) prepared using cost-effective reduction processes were immobilized onto silica and carbon nanomaterials.[4-6]
- **Hybrid silica nanoparticles** fabricated using water/organic bases and silylated naphthopyran/naphthofuran dyes (microwave-assisted synthesis).[7-9]



- **Mesoporous silica and/with metal oxides** based on TiO2 and tungstophosphoric acid.[10]
- **Carbon-based nanomaterials** (graphene, carbon nanotubes, carbon black) doping and functionalization using bottom-up (solvo- or hydrothermal methods) and top-down approaches (ball milling, ultrasound-assisted liquid exfoliation).[4,11]
- **Clays and nanosilicas** functionalized using cost-effective and sustainable silylation strategies.[12]
- **Multifunctional MOFs** preparation by hydrothermal, room temperature methods and microwave-assisted reactions.[13-16]
- **Oxometallic-based composites** including polyoxometalate preparation and functionalization using green and room temperature conditions and microwave-assisted reactions.[17]

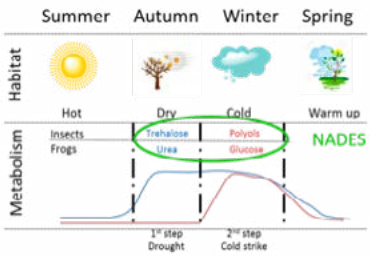


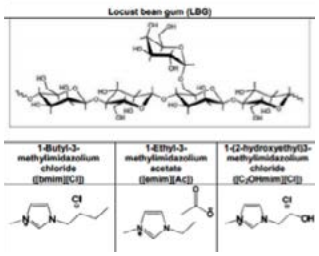
SELECTED PUBLICATIONS

1 C. Fernandes, et al. J. Mater. Chem. C. 2014, 2, 5818. doi:10.1039/C4TC00429A
2 C. Pereira, et al. J. Mater. Chem. B. 2015, 3, 6261. doi:10.1039/c5tb00789e
3 M. Freitas, et al. ACS Sensors. 2016, 1, 1044. doi: 10.1021/acssensors.6b00182
4 C. Fernandes, et al. Appl. Catal. A: Gen. 2014, 486, 150. doi:10.1016/j.apcata.2014.08.031
5 M. Rocha, et al. RSC Adv. 2015, 5, 5131. doi:10.1039/C4RA15865B
6 K. H. Liew, et al. ChemCatChem. 2017, 9, 1. doi:10.1002/cctc.201700649
7 T. V. Pinto, et al. Dalton Trans. 2015, 44, 4582. doi:10.1039/C5DT00090D
8 T. V. Pinto, et al. ACS Appl. Mater. Interfaces. 2016, 8, 7221. doi:10.1021/acsami.5b11983
9 T. V. Pinto, et al. Dalton Trans. 2017, 46, 9076. doi:10.1039/C7DT01376K
10 M. Caiado, et al. Appl. Catal. A: Gen. 2013, 451, 36. doi:10.1016/j.apcata.2012.11.007
11 S. L. H. Rebelo, et al. Phys. Chem. Chem. Phys. 2016, 18, 12784. doi:10.1039/C5CP06519D
12 A. F. Peixoto, et al. Micropor. Mesopor. Mater. 2016, 219, 145. doi:10.1016/j.micromeso.2015.08.002
13 L. Xu, et al. Cryst. Growth Des. 2013, 13, 1260. doi:10.1021/cg301725z
14 L. Xu, et al. CrystEngComm. 2014, 16, 10649. doi:10.1039/c4ce01722f
15 D. I. Alexandropoulos, et al. Chem. Commun. 2017, 53, 4266. doi:10.1039/c7cc01382e
16 D. I. Alexandropoulos, et al. Chem. Commun. 2016, 55, 1693. doi:10.1039/c5cc09385f
17 S. O. Ribeiro, et al. Fuel. 2016, 166, 268. doi:10.1016/j.fuel.2015.10.095

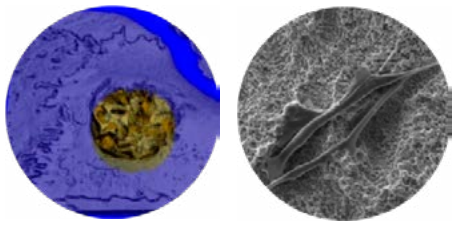
RESEARCH THEMES/
(BIO)MATERIALS ENGINEERING AND PRODUCTION

- **Cost-effective molecularly imprinted materials (MPI)** developed by combining molecular imprinting with supercritical fluid technology, using commercially available cheap monomers such as acrylates.[18-21]
- **Natural and therapeutic deep eutectic systems (NADES)** - new solvents from natural molecules (from sugars, aminoacids or organic acids) towards the development of greener and sustainable systems.[22]





- **Natural polymers extracted from plants and animals** for the production of bio inspired materials. Supercritical CO2 technology and methylimidazolium-based ionic liquids as alternative media in the preparation of biocompatible LBG gel matrices.[23-25]
- **Biocompatible materials** for skin, bone and tissue regeneration prepared using several polymers - PET, PLA, PLGA, PCL, PVA and modified chitosan; Ceramic materials prepared using calcium phosphates.[26-29]



- **Composite catalytic membranes** prepared from cross-linked PVA and calcium oxide.[30,31]
- **Biomass activated carbons or chars** with different textural and chemical surface properties prepared using different precursors - rice husk, sisal, potato peel and others.[32-35]

SELECTED PUBLICATIONS

18 R. Viveiros, et al. Chem. Eng. J. 2017, 308, 229. doi:10.1016/j.jiec.2017.06.012

19 R. Viveiros, et al. J. Clean. Prod. 2017, 168, 1025. doi:10.1016/j.jclepro.2017.09.026

20 A. N. C. Martins, et al. Ind. Crop. Prod. 2014, 60, 226. doi:10.1016/j.indcrop.2014.06.012

21 J. P. Ferreira, et al. RSC Adv. 2014, 4, 54948. doi:10.1039/c4ra11666f

22 A. Paiva, et al. ACS Sustain. Chem. Eng. 2014, 60, 3701. doi:10.1021/sc500096j

23 M. G. Ventura, et al. RSC Adv. 2015, 5, 107700. doi:10.1039/C5RA17314K

24 M. Bernardo, et al. Int. J. Environ. Sci. Technol. 2016, 13, 1989. doi:10.1007/s13762-016-1030-3

25 M. Araújo, et al. Int. J. Pharm. 2014, 469, 140. doi:10.1016/j.ijpharm.2014.04.051

26 P. I. Morgado, et al. Carbohyd. Polym. 2017, 159, 136. doi:10.1016/j.carbpol.2016.12.029

27 M. Araújo, et al. Mat. Sci. Eng. C. 2017, 77, 342. doi:10.1016/j.msec.2017.03.169

28 D. Mata, et al. J. Mater. Chem. B. 2015, 3, 1831. doi:10.1039/C4TB01628A

29 D. Mata, et al. J. Biomed. Nanotech. 2014, 10, 725. doi:10.1166/jbn.2014.1749

30 M. H. Casimiro, et al. Radiat. Phys. Chem. 2014, 94, 171. doi:10.1016/j.radphyschem.2013.05.058

31 T. F. Ceia, et al. Catal. Today. 2014, 236, 98. doi:10.1016/j.cattod.2014.02.052

32 D. Dias, et al. Waste Manage. 2017, 65, 186. doi:10.1016/j.wasman.2017.04.011

33 M. M. S. Bernardo, et al. Environ. Sci. Pollut. Res. 2017, 24, 22698. doi:10.1007/s11356-017-9938-9

34 M. K. S. Batista, et al. RSC Adv. 2016, 6, 45419. doi:10.1039/c6ra09006k

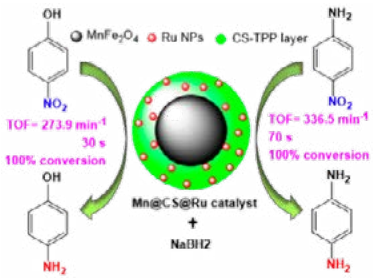
35 O. M. Couto Jr, et al. Can. J. Chem. Eng. 2015, 93, 68. doi:10.1002/cjce.22104

RESEARCH THEMES/
CATALYSIS FOR A SUSTAINABLE ENVIRONMENT

MatSusWell has a mature knowledge on catalysis & catalysts and is aware of the current Grand Challenges in this area: i) advanced design of novel catalysts, ii) understanding of catalysts from molecular to material scale and iii) expanding catalysis concepts (biorefinery, electro- and photocatalysis), directing the research towards the following topics:

i) Selective homogeneous and heterogeneous chemical catalysis

- **Reduction of nitroaromatics into aminoarenes** by recyclable noble metal-supported hybrid nanocatalysts using silica/chitosan-coated superparamagnetic nanoparticles or carbon nanomaterials as supports and gold or ruthenium nanoparticles as the active phase.[36-38]



- **Homogeneous and heterogeneous catalysts & catalysis for environmental-friendly oxidation reactions** for the synthesis of organic compounds with important pharmacological, environmental and industrial applications.[39-41]
- **Simultaneous desulfurization and denitrification of real fuels** by novel catalytically processes based on active polyoxometalate based composites,[42-46] in collaboration with Galp Energia.
- **Biomass valorization by esterification/transesterification/condensation reactions** into biofuels, bio-oil and bioproducts by carbon, silica and aluminosilicate based (nano)materials with sulfonic acid active sites.[47]

- **Biomass derived carbon catalysts** used in -pinene methoxylation reaction and in the hydrolysis of 1,4-glycosidic bond.[48]

SELECTED PUBLICATIONS

36 C. Fernandes, et al. Appl. Catal. A: Gen. 2014, 486, 150. doi:10.1016/j.apcata.2014.08.031

37 M. Rocha, et al. RSC Adv. 2015, 5, 5131. doi:10.1039/C4RA15865B

38 K. H. Liew, et al. ChemCatChem. 2017, 9, 1. doi:10.1002/cctc.201700649

39 C. Freire, et al. Sustainable Catalysis by Manganese Compounds: From Heterogeneous Molecular Complexes to Manganese-based (Nano)Materials, in Sustainable Catalysis: With Non-endangered Metals, Michael North Editor, RSC Green Chemistry Series Nº 38, The Royal Society of Chemistry, United Kingdom, 2016. ISBN:978-1-78262-056-3

40 C. M. Granadeiro, et al. Appl. Catal. A: Gen. 2013, 453, 316. doi:10.1016/j.apcata.2012.12.039

41 H. Gaspar, et al. Catal. Today. 2013, 203, 103. doi:10.1016/j.cattod.2012.04.018

42 S. Ribeiro, et al. Catal. Sci. Technol. 2013, 3, 2404. doi:10.1039/c3cy00287j

43 C. M. Granadeiro, et al. Catal. Sci. Technol. 2014, 4, 1416. doi:10.1039/c3cy00853c

44 C. M. Granadeiro, et al. Chem. Commun. 2015, 51, 13818. doi:10.1039/C5CC03958D

45 S. O. Ribeiro, et al. Fuel. 2016, 166, 268. doi:10.1016/j.fuel.2015.10.095

46 C. M. Granadeiro, et al. Catal. Sci. Technol. 2016, 6, 1515. doi:10.1039/c5cy01110h

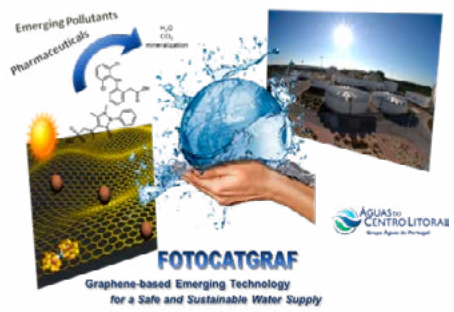
47 M. M. Aboelhassan, et al. New J. Chem. 2017, 41, 3595. doi:10.1039/c6nj04043h

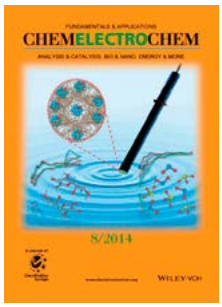
48 I. Matos, et al. Micropor. Mesopor. Mater. 2014, 199, 66. doi:10.1016/j.micromeso.2014.08.006

RESEARCH THEMES/
CATALYSIS FOR A SUSTAINABLE ENVIRONMENT

ii) Photocatalysis for clean and safe water supply

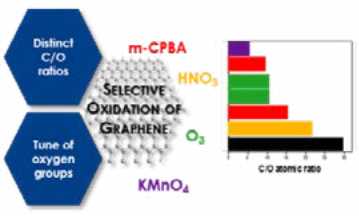
- Nanotechnology-enabled photocatalytic water treatment processes: doped graphene@semiconductor nanocomposites for the photodegradation of emerging pollutants in water/wastewater, in collaboration with Grupo Águas de Portugal.[39]
- Fenton-like photocatalysis for the degradation of emerging pollutants and textile dyes in water/wastewater using nanosize superparamagnetic transition metal ferrites as nanocatalysts.[39,49]





iii) Chemical sensors through electrocatalysis

- **Determination of biomolecules and contaminants** using POM@MOFs and POM@carbon materials (CNT, graphene) with multi-electrocatalytic properties.[50-54]
- **Oxidized graphene flakes with distinct oxygen contents and oxygen functionalities** to accomplish a full understanding of their surface chemistry and of their electrochemical behavior.[55]



SELECTED PUBLICATIONS

49 C. Pereira, et al. Magnetically Recyclable Nanocatalysts: Eco-friendly Solutions for Green Catalysis, Nanotech 2013, Vol. 1, Chapter 5: Nanomaterials for Catalysis, Washington DC, USA, 2013.
ISBN:978-1-4822-0581-7

50 D. M. Fernandes, et al. ACS Appl. Mater. Interfaces. 2013, 5, 13382.
doi:10.1021/am4042564

51 D. M. Fernandes, et al. J. Colloid Interface Sci. 2014, 432, 207.
doi:10.1016/j.jcis.2014.06.050

52 D. M. Fernandes, et al. ChemElectroChem. 2015, 2, 269.
doi:10.1002/celc.201402271

53 D. M. Fernandes, et al. Sensors Actuat. B: Chem. 2015, 218, 128.
doi:10.1016/j.snb.2015.05.003

54 D. M. Fernandes, et al. J. Solid State Electrochem. 2016, 21, 1059.
doi:10.1007/s10008-016-3463-5

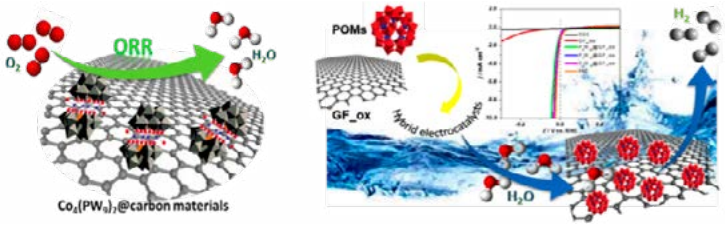
55 M. P. Araújo, et al. RSC Adv. 2017, 7, 14290.
doi:10.1039/C6RA28868E

RESEARCH THEMES/
RENEWABLE ENERGY & CLIMATE CHANGE MITIGATION

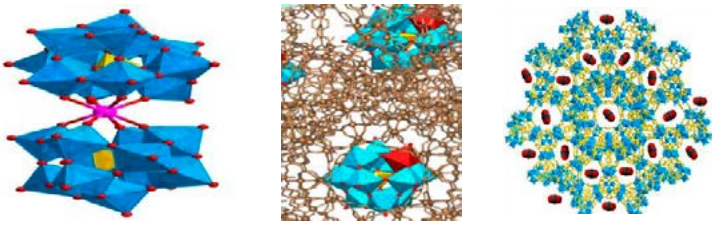
MatSusWell is committed with the transition to a Sustainable and Circular Economy based on renewable energy against the current linear economy based on fossil fuels and coal, which have limited availability and environmental impact (greenhouse gases effect), being considered the major cause for the global climate changes and air pollution. Consequently, research work has been developed in the following topics:

- **Energy efficiency - electrochromic (EC) materials and devices:** [Metal(salen)]-type polymeric films, composites with undoped and N-doped graphene, TiO_2 and WO_3 nanoparticles, and solid-state EC devices with multielectrochromic properties.[56-60]

- **Energy storage and conversion:** activated carbons from biomass and POM@carbon materials and mixed valence Co and Mn oxides@ graphene nanocomposites for application in electrochemical energy-related reactions - HER, OER and ORR.[61-63]



- **Gas adsorption separation and capture:** Porous MOF MIL-101 and composite materials of IL@MOF type combined with Matrimid to prepare mixed matrix membranes for the separation of CO2/N2 mixtures.



SELECTED PUBLICATIONS

56 M. Nunes, et al. ACS Appl. Mater. Interfaces. 2016, 8, 14231. **doi:10.1021/acsami.6b01977**

57 M. Nunes, et al. Langmuir. 2017, 33, 6826. **doi:10.1021/acs.langmuir.7b01380**

58 M. P. Araújo, et al. J. Colloids Interface Sci. 2017, 504, 790. **doi:10.1016/j.jcis.2017.06.023**

59 M. Nunes, et al. Electrochim. Acta. 2017, 238, 142. **doi:10.1016/j.electacta.2017.04.010**

60 M. Nunes, et al. Carbon. 2017, 120, 32. **doi:10.1016/j.carbon.2017.05.001**

61 M. Nunes, et al. RSC Adv. 2015, 5, 102919. **doi:10.1039/c5ra20874b**

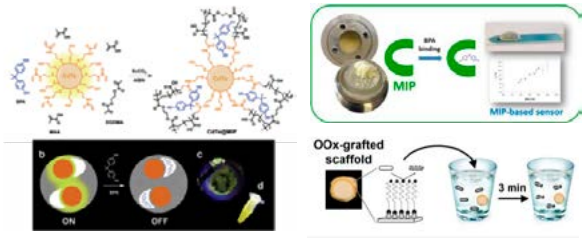
62 D. M. Fernandes, et al. ChemElectroChem. 2017, 4, 1. **doi:10.1002/celc.201701210**

63 C. Freire, et al. ChemCatChem. 2018, accepted. **doi:10.1002/cctc.201701926**

RESEARCH THEMES/
ENVIRONMENTAL PROTECTION AND REMEDIATION

Water, soil and air safety/availability are intimately linked to global health, energy production and economic development. Although their past treatments had a transformative impact, the air, soil and water quality and supply still faces major challenges, leading MatSusWell to identify the following intervening areas:

- **Engineered nanomaterials coupled with advanced air-curtains technology for sustainable indoor air safeguard** towards the concept of green buildings: interactive dark operating oxidizing composite materials able to generate adsorbed hydroxyl radicals.
- **Smart ultrasensitive MPI sensory particles** for molecular recognition to bisphenol A at very low concentrations.[64,65]
- **Antimicrobial polymers for anti-fouling applications and water treatment** using an eco-friendly strategy combining plasma surface activation and supercritical fluid technology, 2-oxazoline-grafted 3D surface with broad spectrum contact-active antimicrobial properties.[66]
- **Industrial collaboration with GEO - Ground Engineering Operations Soil Stabilization:** Water-soluble anionic acrylamide based polymers for stabilization of fluids during the preparation of molded stakes and walls.



- **Biomass activated carbons or chars** as adsorbents to remove liquid phase contaminants such as pharmaceutical compounds and heavy metals.[67-71]
- **Nanoporous and nanostructured adsorbents** for the treatment of serious health conditions associated with acute and chronic exposure to external radiation and uptake of heavy metals and radiation.[72,73]

SELECTED PUBLICATIONS

64 A. Lourenço, et al. RSC Adv. 2014, 108, 63338. **doi:10.1039/C4RA10179K**

65 S. Rebocho, et al. J. Supercrit. Fluids. 2018, 135, 98. **doi:10.1016/j.supflu.2018.01.006**

66 V. G. Correia, et al. Biomacromolecules. 2015, 16, 3904. **doi:10.1021/acs.biomac.5b01243**

67 M. Bernardo, et al. J. Colloid Interf. Sci. 2013, 409, 158 **doi:10.1016/j.jcis.2013.07.050**

68 D. Godinho, et al. J. Hazard. Mater. 2017, 321,173. **doi:10.1016/j.jhazmat.2016.09.006**

69 D. Dias, et al. Waste Manage. 2017, 65, 186. **doi:10.1016/j.wasman.2017.04.011**

70 A. S. Mestre, et al. Chem. Eng. J. 2016, 286, 538. **doi:10.1016/j.cej.2015.10.066**

71 A. S. Mestre, et al. Carbon. 2014, 77, 607. **doi:10.1016/j.carbon.2014.05.065**

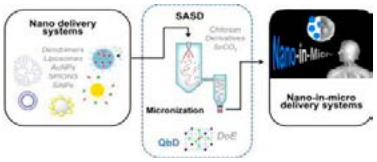
72 J. Madureira, et al. Water Sci. Technol. 2013, 67, 374. **doi:10.2166/wst.2012.544**

73 S. Gago, et al. Micropor. Mesopor. Mat. 2013, 180, 40. **doi:10.1016/j.micromeso.2013.06.001**

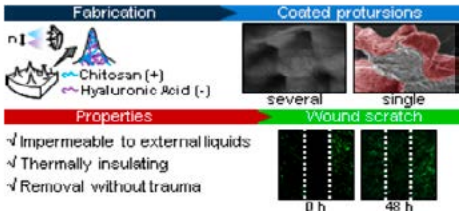
RESEARCH THEMES/
DRUG DELIVERY AND TISSUE REGENERATION

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 and pathological conditions:

- **Nano-enabled delivery systems** as polyurea (PURE-type) dendrimers for efficient cytosolic siRNA delivery.[74]
- **Polymer conjugates** - POxylation using oligo-oxazolines as a novel tool for next generation low cost and highly efficient nanotherapeutics.[75]
- **Nano-in-micro dry powder formulations** of POxylated dendriplexes and gold nanoparticle platforms with enhanced biocompatibility.[76-79]
- **Therapeutic deep eutectic systems (THEDES)** as new administration routes for anti-inflammatory agents, analgesics among other classes of API's.



- **Tailored membranes for wound healing** with striking topographies, tailored shapes and controlled drug release profiles produced using scCO2-assisted phase inversion[80,81] and electrospinning combined with layer-by-layer deposition.[82]



- **Innovative biomimetic biomaterials** for enhanced bone regeneration by developing "smart" scaffolds that are able to modulate cell response for enhanced regenerative outcome.[83-90]
- **Regenerative strategies for craniofacial and dental disorders** by developing integrated approaches engaging tissue engineered strategies that embrace the integrative use of cells, biomaterials, and mechanobiologic ques.[91-94]
- **Models of bone tissue metabolism and healing in physiological and pathologic conditions** (*in vitro*, *ex vivo* and *in vivo* models) for osteoporosis, diabetic-induced osteopenia and bone infectious diseases.

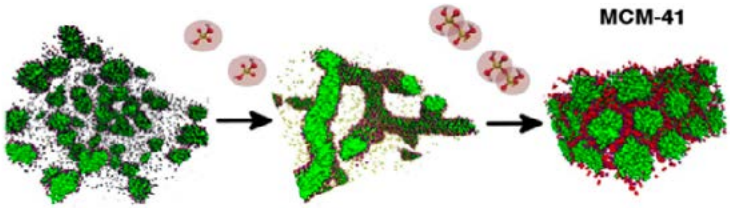
SELECTED PUBLICATIONS

74 R. B. Restani, et al. RSC Adv. 2014, 4, 54872. doi:10.1039/C4RA09603G
75 R. B. Restani, et al. Macromol. Biosci. 2015, 15, 1045. doi:10.1002/mabi.201500131
76 M. C. Silva, et al. Materials. 2017, 10, 74. doi:10.3390/ma10010074
77 R. B. Restani, et al. Part. Part. Syst. Charact. 2016, 33, 851. doi:10.1002/ppsc.201600123
78 A. S. Silva, et al. Int. J. Pharm. 2017, 519, 240. doi:10.1016/j.ijpharm.2017.01.032
79 M. Tavares, et al. J. Supercritical Fluids. 2017, 128, 235–243. doi:10.1016/j.supflu.2017.06.004
80 P. I. Morgado, et al. J. Membrane Sci. 2014, 469, 262. doi:10.1016/j.memsci.2014.06.035
81 P. I. Morgado, et al. Carbohydrate Polym. 2017, 159, 136. doi:10.1016/j.carbpol.2016.12.029
82 T. C. Reis, et al. Biomater. Sci. 2016, 4, 319. doi:10.1039/c5bm00211g
83 D. Santos, et al. J. Colloid Interface Sci. 2017, 504, 101. doi:10.1016/j.jcis.2017.05.032
84 S. Sequeira, et al. Ceramics Int. 2017, 43, 693. doi:10.1016/j.ceramint.2016.09.216
85 T. A. M. Valente, et al. ACS Appl. Mater. Interfaces. 2016, 8, 3241. doi:10.1021/acsami.5b10869
86 P. S. Gomes, et al. Biomed. Mater. 2016, 11, 045007. doi:10.1088/1748-6041/11/4/045007
87 A.Zomorodian, et al. Acta Biomater. 2013, 9, 8660. doi:10.1016/j.actbio.2013.02.036
88 C. Santos, et al. Int. J. Pharm. 2017, 516, 185. doi:10.1016/j.ijpharm.2016.11.035
89 M. Ribeiro, et al. Nanomed. Nanotech. Biol. Med. 2017, 13, 231. doi:10.1016/j.nano.2016.08.026
90 D. Mata, et al. Nanoscale. 2015, 7, 9238. doi:10.1039/C5NR01829C
91 B. Carvalho, et al. Sleep Med. 2017, 29, 92. doi:10.1016/j.sleep.2016.07.027
92 M. H. Fernandes, et al. J. Oral Maxillofac. Res. 2016, 7, e6. doi:10.5037/jomr.2016.7306
93 F. Costa, et al. J. Endodont. 2016, 42, 113. doi:10.1016/j.joen.2015.09.020
94 M. Ferreira, et al. Int. J. Pharm. 2017, 523, 241. doi:10.1016/j.ijpharm.2017.08.089

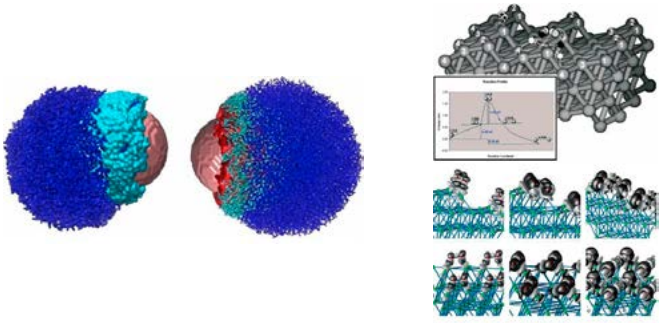
RESEARCH THEMES/
THEORETICAL AND COMPUTER MODELLING

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 and pathological conditions:

- **Theoretically modelling of nanostructured materials** by studying the formation of hexagonally ordered silica/surfactant mesophases, with a direct link to realistic experiments and demonstrating the validity of a co-operative templating mechanism.[95,96]



- **High-level quantum methods for the study of heterogeneous-catalysed reactions**, to elucidate mechanisms and derive reaction descriptors useful for the rational design of novel, more efficient catalysts namely for water gas shift reaction.[97-102]
- **Atomistic molecular simulations to study the structural properties of self-assembled monolayers** of alkylthiols on gold nanoparticles, and to disclose the growth mechanism of their coating in micro/nanofluidic processes.[103-105]
- **In silico modelling approach for predicting the cyto-/eco-toxicity of NPs** under diverse experimental conditions;[106-109] metal and metal oxide NPs, and toxicity assays targeting different endpoints (e.g., algae, bacteria, fungi, mammal cell lines, crustaceans, plants, fishes).



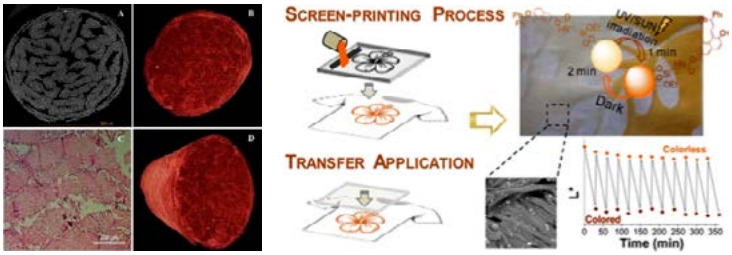
SELECTED PUBLICATIONS

95 G. Pérez-Sánchez, at al. Chem. Mater. 2016, 28, 2715. doi:10.1021/acs.chemmater.6b00348
96 S. Chien, et al. J. Phys. Chem. C. 2017, 121, 4564. doi:10.1021/acs.jpcc.6b09429
97 J. L. C. Fajin, et al. J. Catal. 2014, 313, 24. doi:10.1016/j.jcat.2014.02.011A
98 J. L. C. Fajin, et al. J. Phys. Chem. A. 2014, 118, 5832. doi:10.1021/jp411500j
99 J. L. C. Fajin, et al. RSC Adv. 2016, 6, 8695. doi:10.1039/c6ra01118g
100 J. L. C. Fajin, et al. J. Chem. Theor. Comput. 2016, 12, 2121. doi:10.1021/acs.jctc.6b00168
101 J. L. C. Fajin, et al. Phys. Chem. Phys. Chem. 2017, 19, 19188. doi:10.1039/c7cp02546g
102 J. L. C. Fajin, et al. Appl. Catal. B: Environ. 2017, 218, 199. doi:10.1016/j.apcatb.2017.06.050
103 V. Velachi, et al. J. Phys. Chem. C. 2015, 119, 3199. doi:10.1021/jp512144g
104 V. Velachi, et al. J. Chem. Phys. 2016, 144, 244710. doi:10.1063/1.4954980
105 D. Bhandary, et al. Langmuir. 2017, 33, 3056. doi:10.1021/acs.langmuir.6b04680
106 R. Concu, et al. Nanotoxicology. 2017, 11, 891. doi:10.1080/17435390.2017.1379567
107 F. Luan, et al. Nanoscale. 2014, 6, 10623. doi:10.1039/c4nr01285b
108 V. V. Kleandrova, et al. Environ. Sci. Technol. 2014, 48, 14686. doi:10.1021/es503861x
109 V. V. Kleandrova, et al. Environ. Int. 2014, 73, 288. doi:10.1016/j.envint.2014.08.009

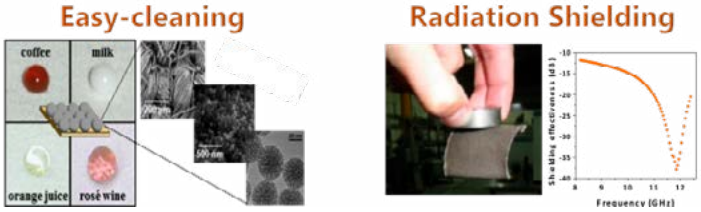
RESEARCH THEMES/
WEARABLE TECHNOLOGIES AND DEVICES

The European STOA identified wearables as one of the ten technologies which will change our lives in the next future. Wearable technologies can unlock benefits of data economy in numerous areas ranging from healthcare to manufacturing, from education to fashion, and from energy to security. In this context MatSusWell has been developing research work in the following topics:

- **Healthcare and medical devices:** Textile-based synthetic materials for tendon/ligament repair - innovative scaffolds for tendons/ligaments repair with enhanced mechanical performance and improved biocompatibility. A patent application is currently under submission.[110]



- **Smart textiles with enhanced photochromic properties under UV and/or sunlight exposure**, tunable color-switchable response and extended color palette range through the incorporation of silica nanoparticles functionalized with naphthopyran/naphthofuran dyes.[111]
- **Functional textiles with hydro/oleophobic properties, thermochromism, radiation protection and antistatic properties** through their coating/functionalization with silica nanoparticles, nanoclays, carbon-based nanomaterials and/or metal oxide nanoparticles.[112,113]



- **Smart textiles and wearable technologies towards IoT applications:** Design and production of smart energy storage textiles and wearable devices to power electronic devices and sensors integrated on clothes towards IoT applications.

SELECTED PUBLICATIONS

110 Smart structures for tendons and ligaments repair, Patent under submission.

111 T. V. Pinto, et al. ACS Appl. Mater. Interfaces. 2016, 8, 28935. doi:10.1021/acsami.6b06686

112 A. Monteiro, et al. Appl. Clay Sci. 2014, 101, 304. doi:10.1016/j.clay.2014.08.019

113 L. S. Ribeiro, et al. J. Mater. Sci. 2013, 48, 5085. doi:10.1007/s10853-013-7296-7

RESEARCH THEMES/
TECHNOLOGY TRANSFER AND ENTREPRENEURSHIP

MatSusWell research work has a strong emphasis on innovation by gathering fundamental and applied sciences and encompassing as the ultimate goal the scientific knowledge transfer and product & technology valorization through collaboration with Companies or entrepreneurship start-up projects.

i) Collaboration with companies and technological centers

- **Desulfurization of real fuels** – diesel, jet fuel and heavy fuel – by oxometallic porous materials in collaboration with Galp Energy – using cost-effective oxidative processes under sustainable conditions.
- **Selective and active bimetallic catalysts** to improve dry reforming of natural gas in micro channel reactors to monitor the CO2 reservoir in collaboration with GALP (PT and Brasil) and Petrogal Brasil, Brasilian National Agency of Petroleum.
- **Scaling-up of sustainable technologies** (pilot scale): graphene production by top-down strategies and biomass valorization by catalytic processes, in collaboration with Innovcat Lda (founded by members of MatSusWell).

- **New textile solutions for X-ray protection,** project TEXBOOST - LESS COMMODITIES MORE SPECIALITIES in collaboration with CITEVE and CENTI and three Portuguese Textile Companies.
- **Collaboration with Biosckin SA** - Molecular and Cell Therapies (cofounded and invested by members of MatSusWell) in the area of Regenerative Medicine.
- **Collaboration with Genetyca-ICM** (cofounded and invested by MatSusWell members) in the area of genetic tests.

ii) Entrepreneurship start-up projects

- **WEStoreOnTEX** entrepreneurship startup project focused on the creation of innovative textile-based technological solutions for energy storage on garments or accessories. The stored energy is used to power devices and sensors integrated on clothes for IoT applications.
- **PURECleanMIP** entrepreneurship project focused on the creation of innovative tailor-made purification solutions for the pharmaceutical industry. A patent was issued in collaboration with Hovione pharmaceutical company. A new provisional patent request was submitted.

HIGHLIGHTS

CLEAN FUELS BY COST-EFFECTIVE PROCESSES

Desulfurization of real fuels (diesel, jet fuel and heavy fuel) using cost-effective oxidative processes capable to operate under sustainable conditions (no use of toxic organic solvents) when catalyzed by oxometallic porous materials ((organo)silicas and metal-organic frameworks) have been performed. Structural catalyst improvement (performance, recycle capacity and robustness) and optimization of desulfurization process have been designed and showed to be crucial to achieved efficiency higher than 80%. The novel methodologies proposed are able to improve sustainability and cost-effectiveness of the actual industrial desulfurization process (hydrodesulfurization).

Efficient eco-sustainable ionic liquid-polyoxometalate desulfurization processes for model and real diesel

Applied Catalysis A: General, 2017, 537, 93.

FROM CATALVALOR PROJECT - A CATALYST FOR CHANGE - TO INNOVCAT SPIN-OFF

CATALVALOR project: A sustainable solution to solve the problems of biodiesel offering a disruptive technology based on a renewable, eco-friendly and reusable solid catalyst (X-CAT) combined with a simplified process to transform multiple feedstocks including low-grade (low-cost) fats/oils into biodiesel reducing simultaneously OPEX and CAPEX, turning the biodiesel market more competitive.

CATALVALOR project was selected for COHiTEC 2013 – turning science into business, a training program in technology commercialization. CATALVALOR project was the winner, in the most important national entrepreneurship competition in Portugal, category Industry - Acredita Portugal; and finalist in two other awards, Brisa Mobilidade and iUP25k (2015).

INNOVCAT Company (www.innovcat.pt) was created in 2015 to provide the continuity of CATALVALOR project. INNOVCAT is a spin-off of University of Porto focus on R&D, production and commercialization of solid catalysts and innovative functional materials.

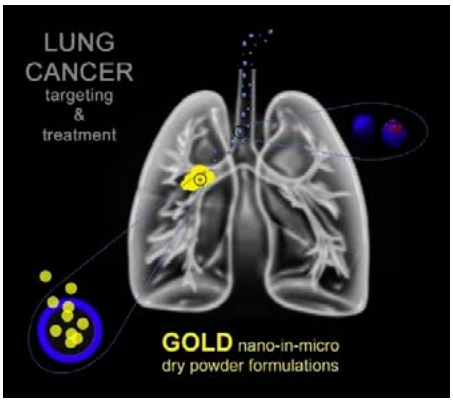
"Catalisadores heterogéneos, processo de preparação e sua aplicação no processo de produção de ésteres alquílicos de ácidos gordos"

Portuguese Patent application nº20171000020656

HIGHLIGHTS

ANTICANCER ULTRAFINE DRY POWDER

Proof-of-concept systems for the treatment of lung cancer were engineered using scCO2. The resulting ultrafine dry powders were able to reach the deep lung and showed optimal in vitro release profiles and biodegradation rates for the treatment of lung cancer. This work was part of A.S. Silva PhD thesis, entitled "Multifunctional nano-in-micro formulations for lung cancer theragnosis", and was distinguished as Best PhD Thesis Award 2016 from the International Society for the Advancement of Supercritical Fluids.

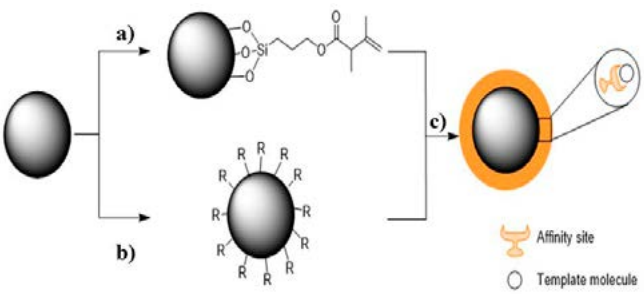


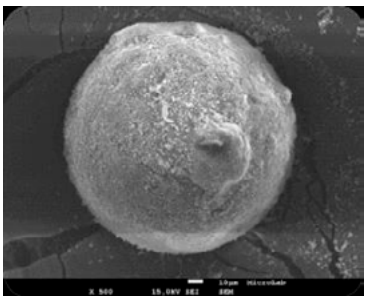
Aerosolizable gold nano-in-micro dry powder formulations for theragnosis and lung delivery

International Journal of Pharmaceutics, 2017, 519, 240-249.

A GRAVITY-DRIVEN API PURIFICATION PROCESS

Large core-shell affinity beads were developed using a green strategy by combining molecular imprinting and supercritical fluid technology. The cheap polymeric affinity materials produced could completely remove impurities from API solutions, with minimum loss of the active substance, by using a low-energy intensive gravity-driven process.





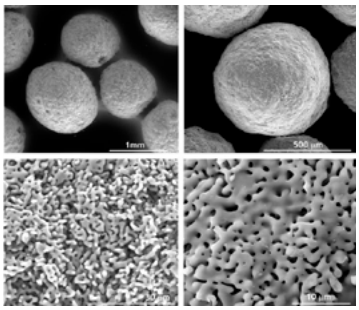
Green strategy to produce large core–shell affinity beads for gravity-driven API purification processes

Journal of Industrial and Engineering Chemistry, 2017, 54, 341–349.

HIGHLIGHTS

BONELIKE® - BIOACTIVE NANOSTRUCTURED SYNTHETIC BONE GRAFT FOR ENHANCED BONE REGENERATION

Bonelike® is a synthetic nanostructured bone graft with a chemical composition and structure similar to that of natural bone, revealing superior mechanical properties and improved bone regeneration, compared to other marketed bone substitutes. It has found a widespread application, being approved for dental, orthopedic and maxillofacial surgery applications, either as a filling material or employed within 3D biomodeling techniques. The biomaterial, with CE marking, is patent protected and commercialized by Biosckin SA – a company founded by members of the research group.

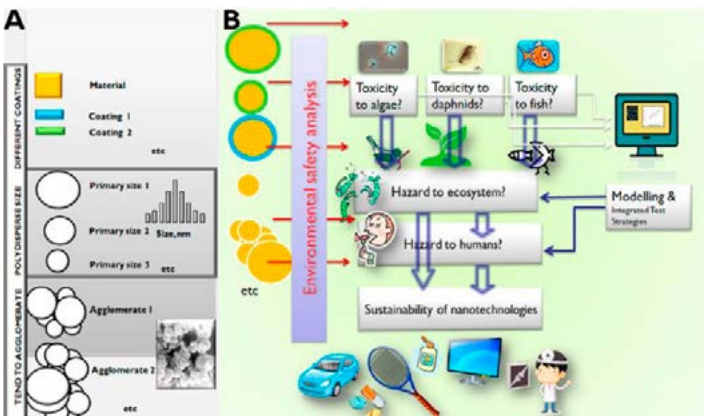


Sintered Hydroxyapatite Compositions and Method for the Preparation Thereof"

Worldwide Application PCT/GB00/01766, Nº: WO00/68164

IN SILICO PREDICTION OF THE (ECO-)TOXICITY OF NANOPARTICLES

We addressed the potential toxic effects of nanoparticles (NPs) to different ecosystems by means of a series of improved in silico-perturbation models, using data from different NPs characterised under diverse experimental conditions. We probed NPs ranging from solely metal-based to metallic oxide NPs, including silica-based NPs, whereas the toxicity assays targeted different endpoints – for instance: algae, bacteria, fungi, mammal cell lines, crustaceans, plants, fishes, among others. The resulting models showed an accuracy higher than 97%, and the structural information gathered from the in silico models per se shall aid the (eco-)toxicological assessment of new NPs at the design stage.



Probing the Toxicity of Nanoparticles: A Unified in Silico Machine Learning Model Based on Perturbation Theory

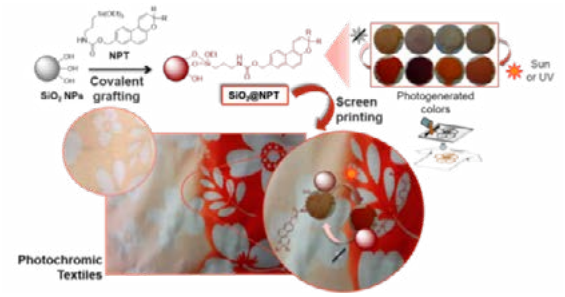
Nanotoxicology, 2017, 11, 891-906.

HIGHLIGHTS

HIGH-PERFORMANCE LIGHT-RESPONSIVE SMART NANOMATERIALS & TEXTILES

High-performance photoresponsive silica nanoparticles (SiO2 NPs) with high color contrast and tunable color-switching response under UV and/or sunlight were prepared by covalent grafting of silylated naphthopyrans (NPT). Smart photochromic cotton textiles were produced through the incorporation of the hybrid NPs by screen-printing. Both hybrids and textiles presented excellent performance, coloring in <1 min and bleaching in 2 min–2 h, with a wide color palette ranging from purple to red and high photostability for at least 12 UV/dark cycles. The most promising textiles were excellent competitors to other previously reported photochromic fabrics in terms of color contrast (ΔE=53.1), color/bleaching rate, photostability and washing fastness.

This was the first work on high-tech light-responsive textiles by screen-printing with hybrid SiO2 NPs as building blocks, being a step forward on the design of smart clothing with sensing and UV protection properties for fashion, sports and military.



Screen-Printed Photochromic Textiles through New Inks Based on SiO2@naphthopyran Nanoparticles

ACS Applied Materials & Interfaces 2016, 8, 28935.

WESTOREONTEX – WE POWER YOUR SMART WEARABLE

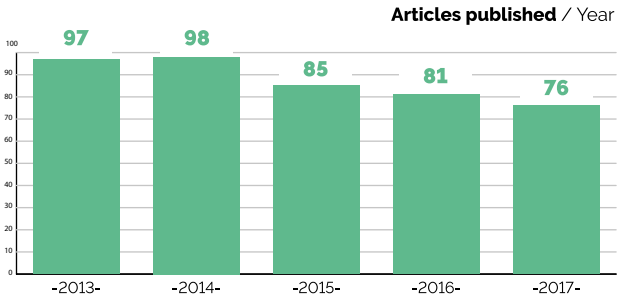
WEStoreOnTEX is an entrepreneurship startup project focused on the creation of innovative technological solutions in the areas of textiles and flexible electronics for energy storage on garments or accessories. The stored energy is used to power portable devices and sensors integrated on clothes. This technology is being implemented in the Textiles and Clothing areas, with the mission of boosting technological transfer of wearable energy storage technologies towards marketable products.

WEStoreOnTEX has been recognized by several entrepreneurship awards such as the Best Innovation Award of Exame Informática – The Technological Best in Portugal 2017, 2nd Place on the National Final of ClimateLaunchpad 2017 - Green Business Idea Competition, 1st Place in the Pitch Day of UPTEC School of Startups 2017, Award for BEST Energy Business in iUP25k Business Ideas Contest 2016 and 3rd Place in iUP25k Business Ideas Contest 2016. Incubated at UPTEC–Science and Technology Park of University of Porto.

www.uptec.up.pt/empresa/westoreontex

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION 2013-2017*



437 articles
3885 citations**
H-index: **59**

FUNDED PROJECTS *(Representative projects)*

- **Des.solve**
  ERC Consolidator Grant - grant 725034, Ana Rita C. Duarte (PI).
  Total funding: €1,877,006.00.
- **MOFsENS - Synthesis of metal-organic frameworks as optical gas sensors.**
  Supported by European Union /M-ERA.NET, Luís Cunha-Silva (PI).
  Total funding: € 533,625.00.
- **Graphene-based semiconductor photocatalysis for a safe and sustainable water supply: an advanced technology for emerging pollutants removal.**
  FCT UT Austin Program, UTAP-ICDT/CTM-NAN/0025/2014, Cristina Freire (PI).
  Total funding: €200,000.00.
- **UniRCell - Unitised Regenerative Fuel Cell for Efficient Renewable Energy Supply: from Materials to Device.**
  PAC Portugal 2020, Cristina Freire (Local PI).
  Total funding: € 59,904.71.
- **TEXBOOST - LESS COMMODITIES MORE SPECIALITIES. FEDER, COMPETE 2020, Riopele textile company.**
  Project Mobilizador nº 24523, Clara Pereira (Local PI).
  Total funding: €59,904,71.
- **CHARPHITE: Coal char as a substituting material of natural graphite in green energy technologies,**
  European Union / ERA-MIN, Cristina Freire (Local PI).
  Total Funding: € 88,412.00.

3 EU projects
2.1 M€

22 National projects
4.49 M€

3 Industry-financed projects
65 k€

INTERNATIONAL COOPERATION AND NETWORKING

- COST Action CM-1203, "Polyoxometalate Chemistry for Molecular Nanoscience (PoCheMoN)", 2012–2015
- SERP+ - International SERP-Chem master with Laboratoire de Chimie Physique, Université Paris-Sud, Paris, France
- Graphene & 2D Materials EUREKA cluster

- Stirring Committee member on the Division on Green and Sustainable Chemistry Division of EuCheMS
- Spanish-Portuguese Bilateral Cooperation, Instituto de Catálisis y Petroleoquímica, CSIC and Facultad de Ciencias, UNED, Madrid, Spain.

OUTREACH

- Organizing committee of ETE2017 – Workshop on Emerging Technologies for Energy: Towards a Circular Economy, Faculty of Sciences, University of Porto, Portugal, December 18–20, 2017 (joint with IFIMUP-IN, DFA-FCUP).
- Co-organizers of the Entrepreneurship Program for Researchers of the Chemistry and Biochemistry Department and of the Physics and Astronomy Department, Faculty of Sciences, University of Porto, Portugal, June 5–9, 2017 (joint organization with UPTEC and DFA-FCUP).
- Scientific committee of the national Scientix meeting, IST, Lisbon, Portugal, November 13–14, 2015. Scientix promotes and supports a Europe-wide collaboration among STEM (science, technology, engineering and maths) teachers, education researchers, policymakers and other STEM education professionals.
- Chair (A. Aguiar-Ricardo) of 2nd EuCheMS Congress on Green and Sustainable Chemistry, Lisbon, Portugal, October 4–7, 2015.
- Green Business Week – National Week for Green Growth, Lisbon Congress Centre, Lisbon, Portugal, March 1–3, 2016.
- Media appearance (TV) – Program "Mentes que Brilham" in Porto Canal – November 2016.
- Invited lectures in the Technological Specialization Course (CET) in Technical and Functional Textiles of CITEVE, in partnership with AFTEBI, January 23, 2014.
- Members of organizing committees and scientific advisory boards of international conferences: Euro CD 2017 - 5th European Conference on Cyclodextrin, UL, Lisbon, Portugal, October 2017; 8th Green Solvents Conference, Halle, Germany, October 16–19, 2016; 7th International Conference on Green and Sustainable Chemistry, Tokyo, Japan, July 5–8, 2015; 6th European Conference on Chemistry in Life Sciences, NOVA Rectory, Lisbon, Portugal, June 10–12, 2015; 2nd EuCheMS Congress on Green and Sustainable Chemistry, Lisbon, Portugal, October 4–7, 2015.
- Aguiar-Ricardo was appointed representative of Sociedade Portuguesa de Química at IUPAC – Chemistry and the Environment Division (2014-2015) and at the European Association for Chemical and Molecular sciences (EuCheMS) Working Party on Green and Sustainable Chemistry (Jan 2013-2016). Creation of an independent Division on Green and Sustainable Chemistry (DGSC) since 2016. A. Aguiar-Ricardo was recently appointed as President of DGSC for the term 2019-2021.


LABORATÓRIO ASSOCIADO
PARA A QUÍMICA VERDE


requimte
rede de química e tecnologia


U.PORTO


UNIVERSIDADE
NOVA
DE LISBOA


universidade
de aveiro

NanoPlat

NANOPLATFORMS

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

The Nanoplatforms group conveys expertise on 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 development of plasmonic, electrochemical and fluorescent (bio)sensors and their incorporation in miniaturized detection devices to enhance analytical automation. Other 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 [2018-2022]

The research activity of the Nanoplatforms group has attracted significant attention on 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


Ana Figueiras


Carla Vitorino

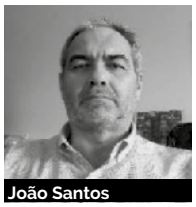

Clara Grosso


Cláudia Nunes


Eliana Souto

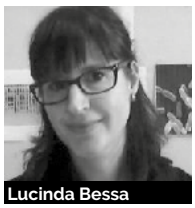

Eulália Pereira


Francisco Veiga


João Santos


João Sousa


Paula Gameiro


Lucinda Bessa


Lúcia Saraiva


Marieta Passos


★ Salette Reis


Sofia Lima

★ Group coordinator

RESEARCH TEAM

OTHER DOCTORATE RESEARCHERS

André Pereira
Edite Cunha
Luís Ribeiro
Paula Pinto
Pedro Fonte
Susana Costa

POST-DOCTORAL FELLOWS

Edson Cavalgante Filho
Catarina Pereira Leite
David Ribeiro
Fabíola Araújo
Lívio Nunes
Marina Pinheiro
Sandra Sofia Rodrigues
Sílvia Lopes
Susana Sousa

PhD STUDENTS

Ana Cláudia Santos
Ana Isabel Simões
Ana Marta Azevedo
Ana Rita Pinto
Ana Rita Fernandes
Ana Simões
Andreia Granja
Carla F. Sousa
Daniela Campos
Ivo A. Múrias
Joana Magalhães
João Albuquerque
João T. Bernardo
José Araújo
José Soares
Mafalda Patrício
Margarida Miranda
Maria Mendes
M. Céu Amaral
Maria Enea
Mariana Ferreira
Miguel P. Almeida
Ong Yong Sze
Virgínia Gouveia

MSc STUDENTS

Ana Joyce Coutinho
Cláudia Espinha
Daniela Resende
Domink Nowicki
Sara Cardoso
Sarah Pereira

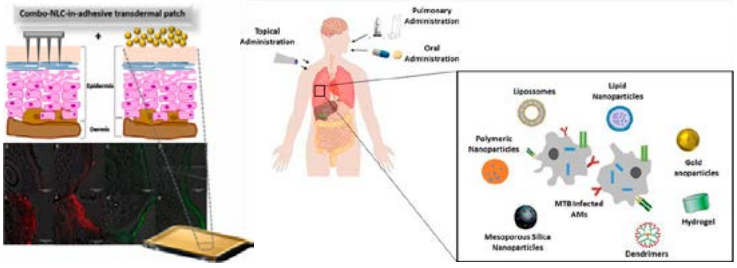
RESEARCH GRANTEES

Ana Filipa Neves
Ana Filipa Pinheiro
Ana Isabel Barbosa
Ana Miranda
André Lopes
André Vilaranda
Cátia Domingues
Diana F. Carvalho
Filipa Pinheiro
Joana Cardoso
João Almeida
Jorge Faria
Maria Ana Martins
Maria Inês Silva
Mariana Magalhães
Nuno Guedes
Rafael Martins
Sara Pinheiro
Sónia Guerra
Soraia Pinto

RESEARCH THEMES/
SMART MATERIALS AS SUSTAINABLE DELIVERY 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:

- Topical delivery of lipid nanoparticles-enriched hydrogels for psoriasis therapy. Collaboration with Centro Hospitalar do Porto.
- Multifunctional platform for the treatment of drug-sensitive and multi-drug resistant tuberculosis.
- Development of a dual-drug delivery system with the complement of biophysical studies of drug-membrane interaction to improve the current therapy against Helicobacter pylori.
- Design of a targeted nanotherapy approach for the upgrade of rheumatoid arthritis treatment. Collaboration with Centro Hospitalar do Porto.
- Targeting tumor cells through theranostic nanoparticles.
- Development of novel brain delivery systems loaded with bioactive phytochemicals for the treatment of neurodegenerative diseases.
- Cyclodextrins carriers to improvement drug bioavailability.
- Micelleplexes carriers development for cancer treatment.



SELECTED PUBLICATIONS

1 T. N. Pashirova, et al. ACS Appl. Mater. Interfaces. 2017, 9, 16922. doi:10.1021/acsami.7b04163

2 A. R. Neves, et al. Bioconjugate Chem. 2017, 28, 995. doi:10.1021/acs.bioconjchem.6b00705

3 C. Sousa, et al. Colloids Surf B: Biointerfaces. 2017, 158, 237. doi:10.1016/j.colsurfb.2017.06.050

4 P. Severino, et al. Eur. J. Pharm. Sci. 2017, 106, 177. doi:10.1016/j.ejps.2017.05.063

5 S. A. Costa Lima, et al. Mater Sci. Eng. C. 2017, 75, 1420. doi:10.1016/j.msec.2017.03.049

6 M. Mendes, et al. Mol. Pharm. 2017, 5, 2099. doi:10.1021/acs.molpharmaceut.7b00211

7 C. L. Seabra, et al. Int. J. Pharm. 2017, 519, 128. doi:10.1016/j.ijpharm.2017.01.014

8 M. C. Teixeira, et al. Prog. Lipid Res. 2017, 68, 1. doi:10.1016/j.plipres.2017.07.001

9 J. A. Loureiro, et al. Molecules. 2017, 22, 277 doi:10.3390/molecules22020277

10 F. Sousa, et al. Sci. Rep. 2017, 16, 3736. doi:10.1038/s41598-017-03959-4

11 D. B. Bittar, et al. Talanta. 2017, 174, 572. doi:10.1016/j.talanta.2017.06.071

12 A. C. Vieira, et al. Nanomedicine. 2017, 12, 2721. doi:10.2217/nnm-2017- 0248

13 A. C. Vieira, et al. Int. J. Pharm. 2017, 536, 478. doi:10.1016/j.ijpharm.2017.11.071

14 F. Andrade, et al. Nanomedicine. 2016, 11, 2305. doi:10.2217/nnm-2016-0045

15 J. Lopes-De-Araujo, et al. Pharm Res. 2016, 33, 301. doi:10.1007/s11095-015-1788-x

16 Vieira AC, et al. Int. J. Nanomedicine. 2016, 11, 2601. doi:10.2147/IJN.S104908

17 M. Pinheiro, et al. Drug Des. Devel. Ther. 2016, 10, 2467. doi:10.2147/DDDT.S104395

18 A. R. Neves, et al. J. Nanobiotechnol. 2016, 14, 1. doi:10.1186/s12951-016-0177-x

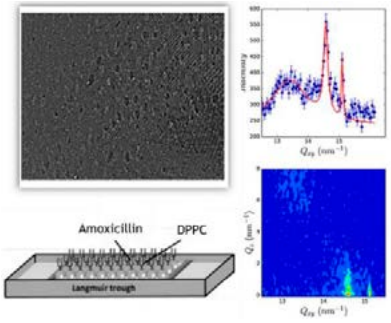
19 A. R. Neves, et al. J. Colloid Interface Sci. 2016, 463, 258. doi:10.1016/j.jcis.2015.10.057

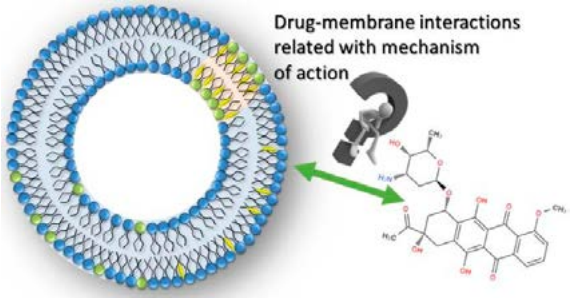
20 A. R. Neves, et al. J. Agric. Food Chem. 2015, 63, 3114. doi:10.1021/acs.jafc.5b00390

RESEARCH THEMES/
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 for 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;
- Cardiovascular and gastric toxicity related to the interaction between membrane lipids and conventional/recently developed NSAIDs;
- Acetylcholinesterase activity inhibition by drugs used for Alzheimer treatment using a 2D lipid model;
- Membrane-active peptides with improved selectivity toward bacterial cells;
- Pore formation and biophysical perturbations through a 2D amoxicillin-lipid membrane interaction approach;
- Pleiotropic action of natural compounds as a result of their interaction with different cell membrane lipids;
- Novel anticancer drugs activity through biophysical studies: applications in drug delivery systems;
- New methods and protocols based on biophysical techniques.





SELECTED PUBLICATIONS

21 P. V. Quelemes, et al. Carbohydr. Polym. 2017, 157:567. doi:10.1016/j.carbpol.2016.10.026

22 C. F. Sousa, et al. RSC Adv., 2017, 7, 10009. doi:10.1039/c6ra26466b

23 T. Moniz, et al. J. Inorg. Biochem. 2017, 175, 138. doi:10.1016/j.jinorgbio.2017.07.017

24 A. C. Alves, et al. Colloids Surf. B Biointerfaces. 2017, 160, 610. doi:10.1016/j.colsurfb.2017.09.058

25 A. C. Alves, et al. J. R. Soc. Interface. 2017, 14, 1. doi:10.1098/rsif.2017.0408

26 A. C. Alves, et al. Biochim. Biophys. Acta - Biomemb. 2017, 1859, 941. doi:10.1016/j.bbamem.2017.01.034

27 D. Lopes, et al. Biochim Biophys Acta - Biomemb. 2017, 1859, 803. doi:10.1016/j.bbamem.2017.01.031

28 D. Lopes, et al. Prog. Lipid Res. 2017, 65, 24. doi:10.1016/j.plipres.2016.12.001

29 A. C. Alves, et al. Biochim. Biophys. Acta - Biomemb. 2016, 1858, 2231. doi:10.1016/j.bbamem.2016.06.025

30 A.R. Neves, et al. Langmuir. 2016, 32, 12914 doi:10.1021/acs.langmuir.6b03591

31 A.R. Neves, et al. Soft Matter. 2016, 12, 2118 doi:10.1039/c5sm02905h

32 A.R. Neves, et al. Biochim. Biophys. Acta - Biomemb. 2016, 1858, 12 doi:10.1016/j.bbamem.2015.10.005

33 A.R. Neves, et al. J. Phys. Chem. B. 2015, 119, 11664 doi:10.1021/acs.jpcb.5b05419

34 C. F. Sousa, et al Int. J. Pharm. 2015, 495, 761. doi:10.1016/j.ijpharm.2015.09.037

35 C. Monteiro et al. Mol. Pharm. 2015. 12, 2904. doi:10.1021/acs.molpharmaceut.5b00113

36 M. Pinheiro, et al. Int. J. Pharm. 2014, 466, 190. doi:10.1016/j.ijpharm.2014.03.005

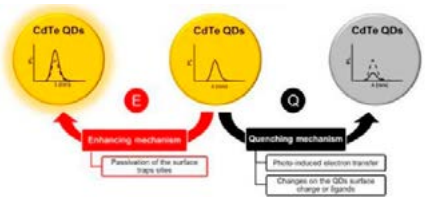
37 C. Nunes, et al. Pharm. Res. 2013, 30, 2097. doi:10.1007/s11095-013-1066-8

38 M. Pinheiro, et al. Phys. Chem. B. 2013, 117, 6187. doi:10.1021/jp403073v

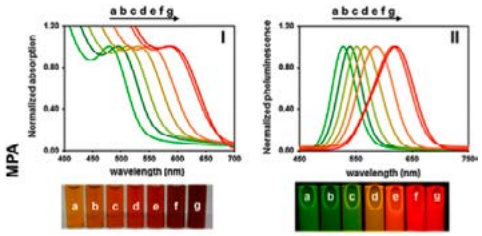
39 C. Pereira-Leite, et al. Eur. J. Pharm. Biopharm. 2013, 84, 183. doi:10.1016/j.ejpb.2012.12.005

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

The NanoPlatform group seeks to provide a strong contribution for 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 qantum dots (QDs) surface by means of functional groups or ligands, not only to assure the establishment of interactions with the target analyte, but also to guarantee that these interactions result in dramatic changes in the referred properties, fostering their application in sensing schemes.



The group is also entailed in the preparation and applications of ultra-sensitive and low cost substrates based on surface-enhanced Raman spectroscopy (SERS) and on the synthesis of nanoparticles that can enhance the Raman signal and provide additional functionality. This is being achieved by means of the optimization of the optical properties by developing new synthetic methods of plasmonic nanoparticles and by resorting to enhance bioconjugation methods.



Another research areas are 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 of a disposable sensor device for the screening of poisonous mushrooms.

SELECTED PUBLICATIONS

40 M. J. Oliveira, et al. Sci. Rep. 2017, 7, 2480. **doi:10.1038/s41598-017-02484-8**

41 A. Patil, et al. J. Mol. Struct. 2017, 1143, 495. **doi:10.1016/j.molstruc.2017.04.094**

42 D. S. M. Ribeiro, et al. J. Mater. Sci. 2017, 52, 3208. **doi:10.1007/s10853-016-0610-4**

43 D. B Bittar, et al. Talanta. 2017, 174, 572. **doi:10.1016/j.talanta.2017.06.071**

44 Rodrigues, S. S. M., et al. Coordin. Chem. Ver. 2017, 330, 127. **doi:10.1016/j.ccr.2016.10.001**

45 G. C. S. de Souza, et al. RSC Adv. 2016, 6, 8563. **doi:10.1039/C5RA23133G**

46 J. Jimenez-Lopez, et al. J. Lumin. 2016, 175, 158. **doi:10.1016/j.jlumin.2016.02.036**

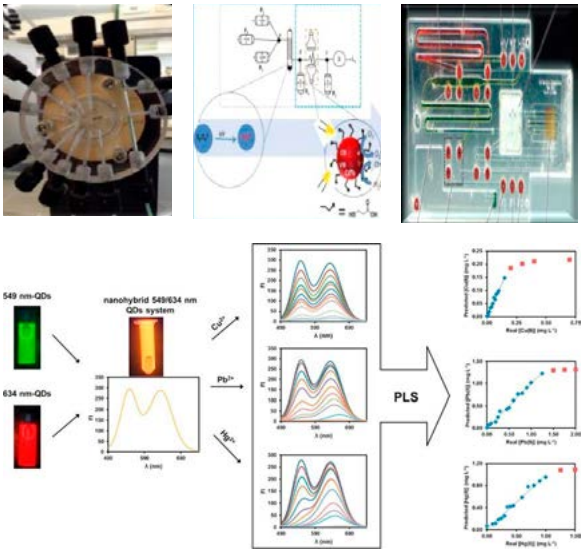
47 L. Soares, et al. Analyst. 2014, 139, 4964. **doi:10.1039/c4an00810c**

48 P. Quaresma, et al. RSC Adv. 2014, 4, 3659. **doi:10.1039/C3RA46762G**

49 L. Soares, et al. Analyst. 2014, 139, 4964. **doi:10.1039/c4an00810c**

RESEARCH THEMES/
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 type 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 applications as rapid screening of wound biomarkers for monitoring the infection status, real time information about the toxicity and environmental impact of nanomaterials and, food components control will be pursued. During the development of the multipurpose nanoplatforms several technological aspects will be taken in account, such as kinetics of (bio)molecular interaction, techniques of immobilization, simplification of assay procedures, and system miniaturization.



SELECTED PUBLICATIONS

50 D. B. Bittar, et al. Talanta. 2017, 174, 572. doi:10.1016/j.talanta.2017.06.071

51 D. Costa, et al. Microchem. Journal 2017, 134, 98. doi:10.1016/j.microc.2017.05.010

52 S. Costa, et al. ChemSusChem. 2017, 10, 2321. doi:10.1002/cssc.201700261

53 S. Rodrigues, et al. Coord. Chem. Rev. 2017, 330, 127. doi:10.1016/j.ccr.2016.10.001

54 A.Azevedo, et al. Chemosphere. 2017, 173, 351. doi:10.1016/j.chemosphere.2016.12.138

55 S. Costa, et al. J. Hazard Mater. 2016, 309, 165. doi:10.1016/j.jhazmat.2016.02.005

56 R. Ribeiro, et al. Talanta. 2016, 150, 20. doi:10.1016/j.talanta.2015.12.009

57 E. Cunha, et al. Talanta. 2015, 141, 293. doi:10.1016/j.talanta.2015.04.028

58 S. Costa, et al. J. Hazard Mater. 2015, 284, 136. doi:10.1016/j.jhazmat.2014.10.049

59 M. Passos, et al. Anal. Chim. Acta. 2015, 889, 22. doi:10.1016/j.aca.2015.05.052

60 S. Rodrigues, et al. ChemPhysChem. 2015, 16, 1880. doi:10.1002/cphc.201500159

61 M. Passos, et al. Talanta. 2014, 133, 45. doi:10.1016/j.talanta.2014.04.089

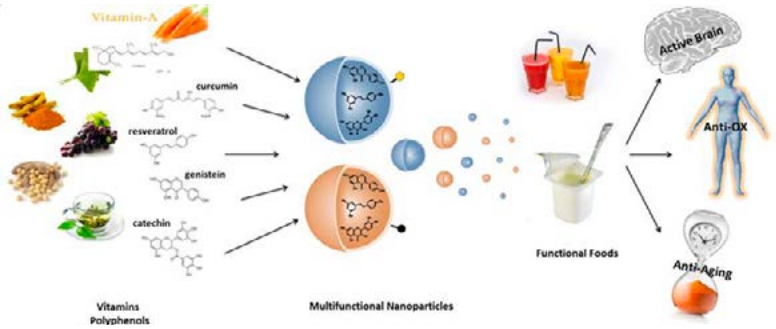
62 M. Passos, et al. RSC Adv. 2014, 4, 59697. doi:10.1039/C4RA09748C

63 M. Carvalho, et al. New J. Chem. 2014, 38, 2856. doi:10.1039/c4nj00158c

RESEARCH THEMES/
FUNCTIONALIZED NANOPLATFORMS AS DELIVERY SYSTEMS FOR FOOD APPLICATIONS

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 that also improve their oral bioavailability. Research is focused on two main topics:

- Design of novel nutraceutical nanoformulations using bioactive phytochemicals. To achieve these purposes, it is planned the rational design, preparation and modelling of different nanomaterials taking into account their future applications as nutraceutics.
- Development of new nanomaterials for antibiofilm applications. A major concern in the food industry is the formation of bacterial biofilms on abiotic surfaces, leading to significant economic and health problems. NanoPlatforms group will engage the development of new nanomaterials for antibiofilm applications, targeting specific features intrinsic to biofilms endurance. Gold and silver nanoparticles with be functionalized and their properties tuned and optimized, being subsequently tested against a multitude of mono and multispecies biofilms.



SELECTED PUBLICATIONS

30 A. Granja, et al. Food Chem. 2017, 237, 803. doi:10.1016/j.foodchem.2017.06.019

31 I. Frias, et al. Drug Des. Devel. Ther. 2016, 10, 3519. doi:10.2147/DDDT.S109589

32 P. Fonte, et al. Pharm. Res. 2016, 33, 2777. doi:10.1007/s11095-016-2004-3

33 A. Granja, et al. Nutrients. 2016, 8, E307. doi:10.3390/nu8050307

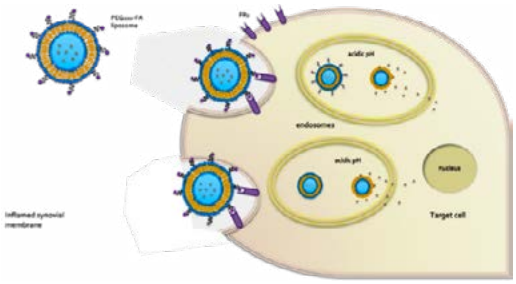
34 P. Fonte, et al. Int. J. Pharm. 2016, 503, 163. doi:10.1016/j.ijpharm.2016.03.011

35 A. R. Neves, et al. Nutrients. 2016, 8, 131. doi:10.3390/nu8030131

36 P. Fonte, et al. J. Control. Release 2016, 225, 75. doi:10.1016/j.jconrel.2016.01.034

HIGHLIGHTS

TARGETING FOR TREATMENT APPROACHES USING MULTIFUNCTIONAL PLATFORMS



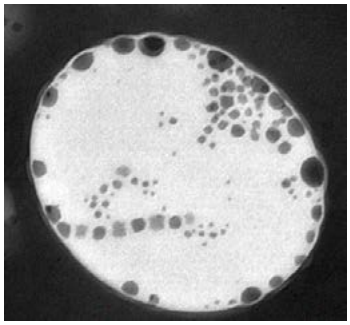
Multifunctional nanospheres for co-delivery of methotrexate and mild hyperthermia to colon cancer cells

Materials Science and Engineering: C Mater Biol Appl. 2017, 75, 1420.

Multifunctional platforms have been successfully developed as proof-of-concept for treatment approaches reaching pre-clinical trials and some are ready for clinical trials. This has been achieved by a rational design approach, driven by the optimization of the processes in a way to be financially competitive, easily scaled-up and optimized according to the pathophysiological characteristics of the targeted disease and administration route. In this field we have accomplished:

- pH sensitive nanoparticles to improve the treatment of tuberculosis. *In vivo* results demonstrates that a promising approach was developed and the *in vitro* data demonstrated an efficient strategy to increase infected macrophages internalization.
- Hybrid nanoparticles to target cancer. Multifunctional nanospheres able to provide a combinatorial therapeutic response through hyperthermia and targeted uptake from colorectal cancer were successfully developed and show *in vitro* evidences of improved efficacy compared with conventional therapies.
- Multifunctional nanoparticles as theranostic approaches for chronic inflammatory conditions. Promising formulations are in ex-vivo trials using human samples, either with synovial tissue or with skin biopsies to treat rheumatoid arthritis and psoriasis, respectively.

MULTIPLE LIPID NANOPARTICLES: THE NEW GENERATION OF LIPID NANOPARTICLES



Multiple Lipid Nanoparticles (MLN), a New Generation of Lipid Nanoparticles for Drug Delivery Systems: Lamivudine-MLN Experimental Design.

Pharmaceutical Research, 2017, 34, 1204-16.

A new type of lipid nanoparticles, the multiple lipid nanoparticles (MLN), was developed. An optimized methodology, based on a quality by design approach, was used. MLN have characteristics between nanostructured lipid carriers (NLC) and multiple emulsions (W/O/W), but without the outer aqueous phase. MLN present large and multiple aqueous vacuoles, which are achieved without the use of any organic solvents, enabling the incorporation of high amounts of both hydrophilic and lipophilic molecules. As MLN are obtained as a semisolid product, they do not require additional water evaporation or separation steps that are often necessary in most formulations, which simplifies the scale-up of this kind of formulation. The designed MLN are suitable for the delivery of drugs and bioactive compounds, due to their low toxicity and high biocompatibility. Additionally, the administration route can be either topical (as a semisolid), or oral (after resuspension).

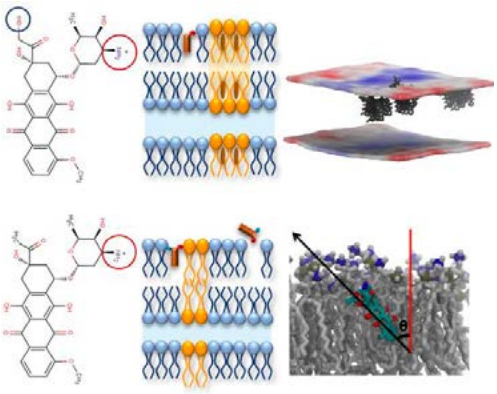
HIGHLIGHTS

READY-TO-USE NANOPLATFORMS TO DRUG DISCOVERY AND DEVELOPMENT

Ready-to-use nanoplatforms that enable the study of drug-membrane interactions and cellular uptake mechanisms have been successfully designed and exploited. The outcomes have been revealing an undiscussable relation between the interactions of the drug molecules with membrane lipids and both therapeutic and toxic effects.

The validation of these nanoplatforms for drug discovery and development was achieved with the most clinically relevant drugs used in cancer diseases. Particularly, the results regarding the combination of anthracyclines-membrane interplay leads to the idea that, when designing and developing new drugs, the different membrane characteristics should be taken into account. In fact, the different properties of cell membranes can modulate anthracyclines behavior, even conditioning their use depending on the type of cancer.

Thereby, these nanoplatforms can and should be incorporated in the preclinical phase of anticancer drugs' development. They allow to predict the pharmacokinetic properties of novel compounds, to clarify their mechanisms of action and toxicity and allow the selection of the best candidates for in vivo evaluation.



Influence of doxorubicin on model cell membrane properties: insights from in vitro and in silico studies

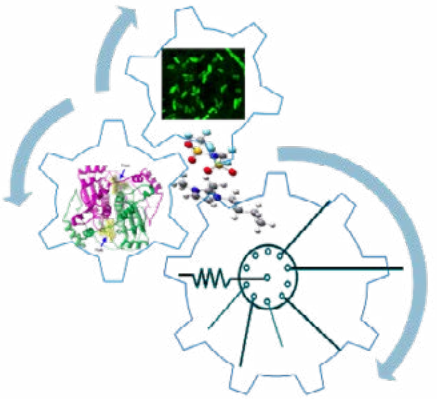
Scientific Reports, 2017, 7, 6343.

NOVEL AND MINIATURIZED (BIO)ASSAYS FOR (ECO) TOXICITY SCREENING

A generic tool for rapid screening of the (eco)toxicity of chemicals and materials was developed based on a battery of miniaturized (bio)assays, as a part of their sustainable synthesis in the early stage of their development.

Molecular and cellular tests are useful to clarify the impact of particular structural elements and to guide their modification to reduce their hazardous potential. The evaluation of toxicity by means of enzymes with important biological functions or whole cell presents additional advantages such as simplicity of laboratory implementation and data interpretation as well as reduction of costs and duration of the assays.

With downscaling of conventional procedures in micro conduits, rigorous control of the reaction conditions in terms of time and volumes are attained with advantages regarding assay´s robustness. Thus valuable tools are proposed for the multidimensional assessment of the risk associated to their use.

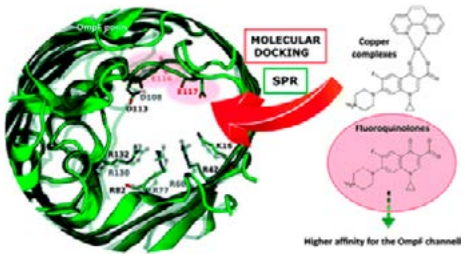


Toxicity assessment of ionic liquids with Vibrio fischeri: An alternative fully automated methodology

Journal of Hazardous Materials, 2015, 284, 136-142.

HIGHLIGHTS

ANTIBIOTIC-PORIN INTERACTIONS AN IN VITRO BIOPHYSICAL STUDY



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

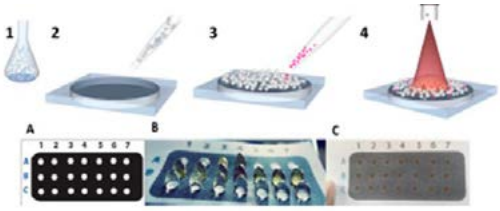
RSC Advances 2017, 7, 10009-100019.

Biological studies of the uptake of fluoroquinolones and fluoroquinolone-derivatives were performed in several bacterial strains that have a series of porin mutants which lack one or several major outer membrane proteins (OmpF, OmpC, lamB, OmpR). Based on the biological experiments, the in vitro biophysical study of antibiotic-porin interactions using purified porins incorporated into liposomes has been performed. Characterization of the liposome/proteoliposome systems and bacteria, in the presence and absence of compounds, was carried out by fluorescence techniques, light scattering and AFM.

Biophysical properties such as fluidity of bacterial membranes has been characterized in a multitude of bacterial strains, from Gram-negatives to Gram-positives, and both susceptible/reference strains and multidrug-resistant clinical isolates, also in the presence and absence of antibiotics.

To make the most of the bacterial collection that has been constructed mostly during the last year, antimicrobial susceptibility testing has been performed to assess the potential antimicrobial activity of diverse extracts and compounds, such as antimicrobial peptides and cationic polymers.

LOW-COST ULTRASENSITIVE SENSORS PLATFORMS FOR PORTABLE DEVICES



Office paper decorated with silver nanostars - an alternative cost effective platform for trace analyte detection by SERS

Scientific Repor ts, 2017, 7, 2480.

To provide reliable and efficient analytical tools for a variety of health, food and environmental challenges, several electrochemical, surface-enhanced Raman spectroscopic and fluorescent (bio)sensors were successfully developed.

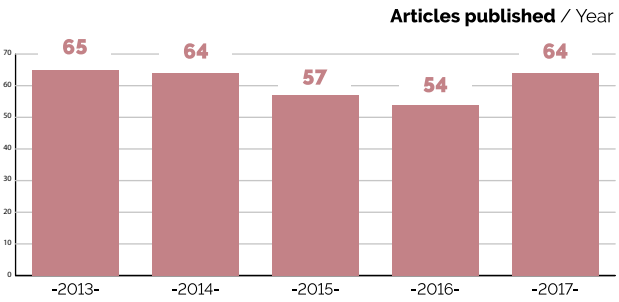
The excellent performing characteristics (selectivity, sensitivity, linear working range, precision, accuracy, etc.) and the small size of these sensors will enable their inclusion in portable and/or disposable devices, resulting in cost effective sensing strategies for point-of-care or in situ applications.

We have accomplished a low-cost SERS (Surface-enhanced Raman spectroscopy) substrates for point-of-care portable sensors, using silver nanostars drop-casted on hydrophilic wells patterned on paper, were also implemented. A low limit of detection for rhodamine-6G has been achieved, with good signal uniformity and stability.

The optimization of the aqueous synthesis of new fluorescent nanoprobes to prepare gram-amounts of nanomaterials with improved selectivity and surface reactivity, capable of inclusion into portable sensing devices was also achieved. The developed fluorescent nanoprobes were assayed in the determination of various metal ions in distinct samples demonstrating a high efficiency for monitoring Hg(II) levels.

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION 2013-2017*



304 articles
2595 citations**
H-index: **54**

FUNDED PROJECTS *(Representative projects)*

- "PAIRED: Magnetically and photochemically actuated bioactive nanowires for remotely controlled drug delivery"
  M-ERA-NET/0004/2015, Eliana Souto (PI)
  Total funding: € 123,000.00.
- "MAGNAMED - Novel magnetic nanostructures for medical applications"
  H2020-MSCA-RISE-2016, Cláudia Nunes (local PI)
  Total funding: € 67,500.00.
- "Flavonoids for Brain Disorders: Engineering Polymeric Nanoparticles to Improve Drug Delivery",
  FCT IF/01332/2014, Clara Grosso (PI)
  Total funding: € 22,000.00.
- "Upgrading rheumatoid arthritis treatment through a targeted nanotherapeutic approach"
  FCT IF/00293/2015, Cláudia Nunes (PI)
  Total funding: € 48,000.00.
- "Development and characterization of smart micelleplexes for lung cancer therapy",
  FCT, PTDC/CTM-BIO/1518/2014, Francisco Veiga (PI)
  Total funding: € 95.076,00.
- "Dual nanostructured lipid carriers as a multifunctional platform for brain tumor therapy"
  FCT, PTDC/CTMNAN/2658/2014, Carla Vitorino (PI),
  Total funding: € 180.206,00.

5 EU projects
2.5 M€

12 national projects
5.99 M€

INTERNATIONAL COOPERATION AND NETWORKING

- COST Action MP1302, "NanoSpectroscopy", 2013-2017.
- COST Action TD1402, "RADIOMAG - Multifunctional Nanoparticles for Magnetic Hyperthermia and Indirect Radiation Therapy", 2014-2018.
- COST Action CM1307, "Targeted chemotherapy towards diseases caused by endoparasites", 2014-2018.
- COST Action CA16124, "Brillouin Light Scattering Microspectroscopy for Biological and Biomedical Research and Applications", 2017-2020.
- COST Action TD1305, "Improved Protection of Medical Devices Against Infection" (IPROMEDAI), 2014-2018.
- Brazilian-Portuguese Bilateral Cooperation under a FAPESP Thematic Project (2013/08166-5), 2013-2018, University of São Paulo, Brazil.
- Brazilian-Portuguese Bilateral Cooperation financed by CNPq, Federal University of Piauí, Brazil

OUTREACH

- Summer in Project for high school students: "Decovering nanotechnology: applications in health and nutrition", Junior University, University of Porto, 3-14 July 2017.
- Organizing committee of the summer course: "Membrane Biophysics: Impact of Lipids on Health, Disease and Therapy", Porto, 24-28 July 2017.
- Organizing and scientific committee of the "International Conference Optical NanoSpectroscopy IV", Lisbon, 28-31 May 2017.
- Organization of Hands-on workshop on "Preparation and characterization of lipid nanoparticles for biomedical application", III AEICBAS Biomedical Congress, Porto, 20 March 2015.
- Reis S. "The power of nanopharmaceutics to cure deadly diseases". International Innovation, 185 – Catalysts for care, ISBN 2054-6254.
- Audio slides on publications in Journal of Colloid and Interface Science and Biochimica et Biophysica Acta.


LABORATÓRIO ASSOCIADO
PARA A QUÍMICA VERDE


requimte
rede de química e tecnologia


U.PORTO


UNIVERSIDADE
NOVA
DE LISBOA


universidade
de aveiro

4FOOD

FOOD QUALITY AND TECHNOLOGY

OVERVIEW & OBJECTIVES

RESEARCH OVERVIEW

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 in vitro and tissues; 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 [2018-2022]

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;
- Explore the agricultural biodiversity to uncover 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;
- Develop nutritious and safe processed products;
- Assess 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 the environment, agrochemicals, packaging materials and formed during processing and estimate the bioaccessibility of those contaminants;
- Evaluate of new endocrine disruptors on human reproduction;
- Develop human cells based assays for testing the effects of food bioactive/toxic compounds.

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 and will contribute to strength 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 Rita Cabrita


Angelina Pena


André Pereira


André Pereira


Beatriz Oliveira


Bela Franchini


Catarina Mansilha


Celeste Lino


Fátima Martins


Fernando Ramos


Helena Costa


Hileia Souza


Isabel Mafra


Isabel Ferreira


Ivonne Delgadilo


Joana Oliveira


Jorge Saraiva


José A. Silva


José Fernandes


Liliana Silva


Luís Cruz


Luís Guido


Pilar Gonçalves


Miguel Faria


Manuel Coimbra


Nuno Mateus


Olga Viegas


Olívia Pinho


Rita Alves


Sara Cunha


Sílvia Rocha


Sofia Duarte


Susana Casal


Victor Freitas

★ Group coordinator

RESEARCH TEAM

OTHER DOCTORATE RESEARCHERS

Ada Rocha
Ana Paula Vale
Carla Barbosa
Dulcineia Wessel
Joana Amaral
Jorge Barbosa
Luís Cunha
Manuel Alves
Margarida Maia
M. Conceição Manso
Sónia Soares
Sonia Losada-Barreiro
Susana Fonseca
Tânia Tavares
Vitor Martins

POST-DOCTORAL FELLOWS

Ana Luísa Fernandes
André Pereira
Ângela Fernandes
Armindo Melo
Bárbara Teixeira
Carla Pereira
Cláudia Pereira Passos
Edgar Pinto
Elisabete Alexandre
Elisabete Coelho
Filipe Coreta Gomes
Filomena Raposo
Francisca Rodrigues
Iva Fernandes
Joana Costa
Joana Sousa
Maria Rosa Gregório
Natércia Teixeira
Sofia Reis
Sónia Barreiro
Susana Soares
Zita Martins

PhD STUDENTS

Adriana Santos
Alexandra Nascimento
Álvaro Lemos
Ana Ribeiro
Ana Soraia Silva
Andreia Ferreira
Carla Santos
Carlos Pinto
Catarina Ribeiro
Caterina Villa
Cátia Martins
Cristina Caleja
Diana Santos
Élia Maricato
Elsa Brandão
Filipa Pimentel
Guido Lopes
Hana Scepankova
Hélder Oliveira
João Santos
João Trigo
Júlio Machado Jr.
Lígia Rodriguez
Liliana Fidalgo
Liliana Grazina
Luana Fernandes
M. Virgínia Mota
Margarida Rodrigues
M. Angélica Rocha
Maria Antónia Nunes
Maria Mota
Marlene Costa
Martin Vojtek
Mauro Santos
Rebeca Cruz
Ricardo Dias
Ricardo Duarte
Rita Bastos
Rita Inácio
Rita Lopes

RESEARCH GRANTEES

Ana Carolina Amaral
Ana Sofia Évora
Ana Sofia Sousa
Carina Costa
Diana Melo
Jéssica Marques
Joana Azevedo
Juliana Peixoto
Luís Ferraz
Mafalda Silva
Marta Guimarães
Michele Fajardo
Paula Araújo
Pedro Fontes
Rui Silva
Telmo Francisco
Vasco Teixeira

OTHER RESEARCHERS

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

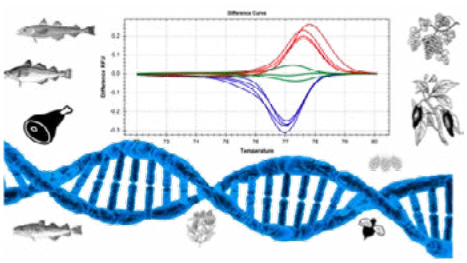
RESEARCH THEMES

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, pommegranate, 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).

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;
- Exploiting DNA-barcoding and high-resolution melting analysis for species identification in foods, herbal medicines and plant food supplements.



SELECTED PUBLICATIONS

1 L. Fernandes, et al. J. Food Compos. Anal. 2015, 39, 13. doi:10.1016/j.jfca.2014.11.006

2 E. Pinto, et al. J. Food Compos. Anal. 2015, 37, 38. doi:10.1016/j.jfca.2014.06.018

3 S. Soares, et al. J. Agr. Food Chem. 2016, 64, 7823. doi:10.1021/acs.jafc.6b02659

4 E. Brandão, et al. Food Chem. 2017, 228, 427. doi:10.1016/j.foodchem.2017.02.027

5 J. R. L. Guerreiro, et al. ACS Sens. 2016, 1, 258. doi:10.1021/acssensors.5b00054

6 A. Baptista, et al J. Food Meas. Charact. Food Measure 2017, 11, 442. doi.org/10.1007/s11694-016-9412-2

7 E. Pinto, et al. J Agric, Food Chem. 2015, 63, 440. doi.org/10.1021/jf505453s

8 N. Costa, et al. Food Control 2016, 64, 128. doi.org/10.1016/j.foodcont.2015.12.010

9 G. R. Lopes, et al. Food Res. Int. 2016, 89, 989. doi.org/10.1016/j.foodres.2016.01.018

10 D. P. Leão, et al. Food Chem. 2017, 225, 146. doi.org/10.1016/j.foodchem.2017.01.027

11 C. Tomás, et al. Food Control 2017, 71, 255. doi:10.1016/j.foodcont.2016.07.004

12 T. J. R. Fernandes, et al. Food Control 2017, 82, 8. doi.org/10.1016/j.foodcont.2017.06.016

13 C. Villa, et al. Food Chem. 2017, 229, 680. doi.org/10.1016/j.foodchem.2017.02.136

14 S. Soares, et al. Food Control 2015, 48, 130. doi.org/10.1016/j.foodcont.2014.02.035

15 L. Grazina, et al. Food Control 2017, 73, 1053. doi.org/10.1016/j.foodcont.2016.10.020

16 L. Meira, et al. LWT - Food Sci. Technol. 2017, 75, 408. doi.org/10.1016/j.lwt.2016.08.061

17 B. Martín-Fernández, et al. Food Chem. 2016, 211, 383. doi.org/10.1016/j.foodchem.2016.05.067

18 C. L. Manzanares-Palenzuela, et al. Sensors & Actuators: B. Chemical, 2016, 222, 1050. doi.org/10.1016/j.snb.2015.09.013

19 J. Costa, et al. Food Chem. 2015, 173, 257. doi.org/10.1016/j.foodchem.2014.10.024

20 J. Costa, et al. Food Chem. 2017, 231, 340. doi.org/10.1016/j.foodchem.2017.03.154

RESEARCH THEMES

ALLERGENS, ADDITIVES AND CONTAMINANTS

- Assessment of trace levels of food allergens based on DNA markers (tree nuts, fish, crustaceans, gluten-containing cereals);
- 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);
  - "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.
- Assessment of mycotoxins (e.g. ochratoxin A, aflatoxins and zearalenone) and plant toxins (e.g. cyanogenic glycosides) in agricultural products.;
- 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.

SELECTED PUBLICATIONS

21 A. M. P. T. Pereira, et al. Sci. Total Environ. 2017, 603-604, 226. doi:10.1016/j.scitotenv.2017.06.022

22 A. Melo, et al. Chemosphere 2016, 161, 19. doi: 10.1016/j.chemosphere.2016.06.088

23 N. Costa, et al. Food Control 2016, 64, 128. doi:10.1016/j.foodcont.2015.12.010

24 S. C. Cunha, et al. Environ. Res. 2015, 143, 65. doi:10.1016/j.envres.2015.05.003

25 S. C. Cunha, et al. J. Chromatogr. A 2015, 1414, 10. doi:10.1016/j.chroma.2015.07.099

26 S. C. Duarte, et al. World Mycotoxin. J. 2015, 8, 121. doi:10.3920/wmj2014.1707

27 H. M. Oliveira, et al. LWT-Food Sci. Technol. 2017, 84, 674. doi:10.1016/j.lwt.2017.06.035

28 R. Cruz, et al. TrAC Trends Anal. Chem. 2017, 87, 129. doi.org/10.1016/j.trac.2016.12.005

29 M. H. Petrarca, et al. Food Chemistry 2016, 212, 528. doi.org/10.1016/j.foodchem.2016.06.010

30 S. C. Cunha, et al. Food Control 2016, 63, 15. doi.org/10.1016/j.foodcont.2015.11.006

31 A. M. P. T. Pereira, et al. Chemosphere 2016, 144, 2507. doi.org/10.1016/j.chemosphere.2015.10.100

32 M. Gelormini, et al. JMIR Res. Protoc 2015, 4, e98. doi.org/10.2196/resprot.4096

33 L. Molina-Garcia, et al. Food Anal. Meth. 2015, 8,1436 doi.org/10.1007/s12161-014-0014-5

34 L. A. T. Santos, et al. Food Control 2015, 47, 141. doi.org/10.1016/j.foodcont.2014.06.046

35 G. Vandermeersch, et al. Environ. Res. 2015, 143, 29. doi.org/10.1016/j.envres.2015.06.011

36 S. C. Cunha, et al. Environ. Res. 2015, 143, Part B, 65–71. doi.org/10.1016/j.envres.2015.05.003

37 N. M. C. Ribeiro, et al. Food Control 2015, 57, 147. doi.org/10.1016/j.foodcont.2015.03.043

38 A. M. P. T. Pereira, et al. J. Toxic. Environ Health A 2015, 78, 959. doi.org/10.1080/15287394.2015.1036185

39 S. C. Cunha, et al. Food Chem 2017, 232, 501. doi.org/10.1016/j.foodchem.2017.04.006

40 Silva, et al, Environ. Pollut. 2016, 213, 432. doi:10.1016/j.envpol.2016.02.022.

RESEARCH THEMES

IMPROVEMENT OF ANIMAL FEEDING AND NUTRITION

- Evaluation and valorization of under exploited feeds towards increased sustainability of animal production;
- Understanding rumen function to improve ruminant nutrition and production;
- Modulation of feeding strategies to increase animal nutrient efficiency use, animal health and welfare;
- Mitigation of ruminant methane emissions and nitrogen excretion;
- Feeding strategies to produce healthier foods of animal origin;
- Identification of new biomarkers and development of non-invasive techniques to study the rumen function.

PROCESSING HEALTHIER, APPEALING AND SAFER FOODS

- Optimization of traditional (grilling, barbecueing, 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);
- Development of microencapsulation techniques using different materials to stabilize food ingredients, extend food shelf-life and control taste;
- Microbial fermentation at sub lethal pressure levels for use in novel products production.

SELECTED PUBLICATIONS

41 I. M. Valente, et al. Talanta 2017, 167, 747. doi:10.1016/j.talanta.2017.01.091

42 S. C. Q. Magalhães, et al. Ind. Crop. Prod. 2017, 95, 286. doi:10.1016/j.indcrop.2016.10.033

43 F. Ferreres, et al. Food Chem. 2017, 214. doi:10.1016/j.foodchem.2016.07.129

44 O. A. Rego, et al. Ital. J. Anim. Sci. 2016, 15, 76. doi:10.1080/1828051X.2016.1141330

45 P. Amaro, et al. J. Anim. Feed Sci. 2015, 24, 3. doi:10.22358/jafs/65647/2015

46 A. R. J. Cabrita, et al. J. Appl. Phycol. 2016, 28, 3135. doi.org/10.1007/s10811-016-0839-y

47 H. M. Oliveira, et al. LWT - Food Sci. Technol. 2017, 84, 674. doi.org/10.1016/j.lwt.2017.06.035

48 A. R. J. Cabrita, et al. Algal Res. 2017, 24, 290. doi.org/10.1016/j.algal.2017.04.024

49 S. C. Q. Magalhães, et al. Food Chem. 2017, 215, 177. doi.org/10.1016/j.foodchem.2016.07.152

50 E. Salas-Leiton, et al. Aquac. Nut. 2018, 24, 131. doi.org/10.1111/anu.12541.

51 L. Fernandes, et al. Food Bioprocess Technol. 2017, 10, 799. doi:10.1007/s11947-017-1887-2

52 A. Sousa, et al. LWT-Food Sci. Technol. 2015, 60, 22. doi:10.1016/j.lwt.2014.08.026

53 A. Fernandes, et al. Food Chem. 2016, 209, 17. doi:10.1016/j.foodchem.2016.04.018

54 R. N. Pereira, et al. LWT-Food Sci. Technol. 2016, 74, 493. doi:10.1016/j.lwt.2016.07.074

55 G. Pancrazio, et al. Meat Sci. 2016, 121, 382. doi:10.1016/j.meatsci.2016.07.009

56 M. M. C. Sobral, et al. LWT - Food Sci. Technol. 2017, 85, 316. doi.org/10.1016/j.lwt.2016.11.055

57 I. Gonçalves, et al. Carbohydr. Polym. 2017, 175, 628. doi.org/10.1016/j.carbpol.2017.08.029

58 S. R. Monteiro, et al. Food Res. Int. 2017, 102, 14. doi.org/10.1016/j.foodres.2017.09.066

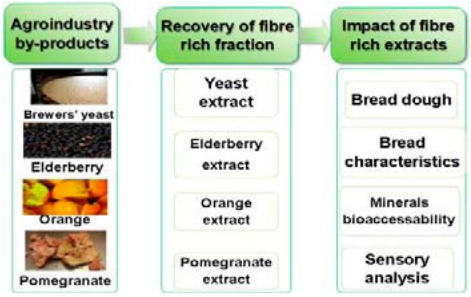
59 A. S. P. Moreira, et al. Food Chem. 2017, 227, 422. doi.org/10.1016/j.foodchem.2017.01.107

60 M. C. Santos, et al. Innov. Food Sci. Emerg. Technol. 2016, 33, 76. doi.org/10.1016/j.ifset.2015.11.018

RESEARCH THEMES

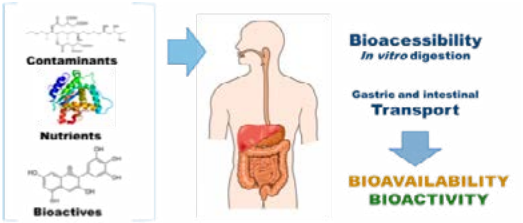
FOOD SUSTAINABILITY

- Valorization of compounds recycled from agro-industrial wastes (brewer's spent grain and spent yeast, fruit peels and pomace, coffee silverskin and spent coffee, 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 development of new and profitable ingredients;
- Optimization of the extraction of valuable compounds from plant cell walls, yeasts and marine animals;
- Formulation of new appealing processed products, toward 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.



FOOD AND HEALTH

- 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.
- Impact of malnutrition on the pathophysiology mechanisms of fetal programming of hypertension.



SELECTED PUBLICATIONS

61 R. Cruz, et al. Food Res. Int. 2015, 73, 190. doi:10.1016/j.foodres.2014.11.018

62 J. Oliveira, et al Tetrahedron Lett. 2016, 57, 1277. doi:10.1016/j.tetlet.2016.02.026

63 L. Cruz, et al. Food Funct. 2016, 7, 2754. doi:10.1039/c6fo00466k.

64 M. Costa, et al. Food Chem. 2015, 175, 233. doi:10.1016/j.foodchem.2014.10.016

65 J. Almeida, et al. J. Agric. Food Chem. 2016, 64, 5274. doi:10.1021/acs.jafc.6b01468

66 Z. E. Martins, et al. Eur. Food Res. Technol. 2017, 243, 1973. doi:10.1007/s00217-017-2903-5

67 Martins, et al. J. Food Sci. 2017, 82, 2183. doi:10.1111/1750-3841.13837

68 C. P. Passos, et al. Food Chem., 2017, 231, 114. doi.org/10.1016/j.foodchem.2017.03.105

69 J. C. Raguzzoni, et al. Carboh. Polym. 2016, 150, 369. doi.org/10.1016/j.carbpol.2016.05.024

70 S. C. Pinto, et al. Enzyme Micro. Technol. 2015, 79, 8. doi.org/10.1016/j.enzmictec.2015.07.002

71 E. Vieira, et al. Eur. Food Res. Technol. 2016, 242, 1975. doi:10.1007/s00217-016-2696-y

72 E. F. Vieira, et al. J. Agric. Food Chem. 2016, 64 , 7335. doi:10.1021/acs.jafc.6b02719

73 F. M. Peixoto, et al. J. Funct. Food 2016, 24, 373. doi:10.1016/j.jff.2016.04.021

74 J. C. Machado, et al. J. Funct. Food. 2017, 36, 255. doi:10.1016/j.jff.2017.07.006

75 S. Soares, et al. RSC Adv. 2015, 5, 12664. doi:10.1039/c4ra13403f

76 I. Fernandes, et al. Food Funct. 2017, 8 , 2030. doi:10.1039/c7fo00329c

77 H. Oliveira, et al. J. Agr. Food Chem. 2015, 63, 7685. doi:10.1021/acs.jafc.5b00412

78 R. Dias, et al. RSC Adv. 2015, 5, 32151. doi:10.1039/c5ra02968f

79 M. Segade, et al. J. Funct. Food 2016, 23, 637. doi:10.1016/j.jff.2016.03.024

80 R. Novoa-Carballal, et al. Carbohydr. Polym., 2017, 157, 31-37. doi:10.1016/j.carbpol.2016.09.050

81 V. M. R. Martins, et al. Carbohydr. Polym. 2017, 157, 176. doi.org/10.1016/j.carbpol.2016.09.079

82 T. R. Dias, et al. J. Nut. Biochem. 2016, 37, 83. doi.org/10.1016/j.jnutbio.2016.07.018

HIGHLIGHTS

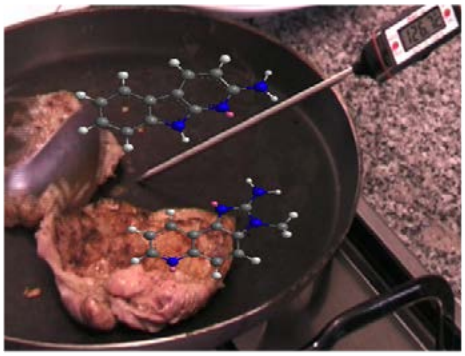
NEW SAFE SEAFOOD GUIDES AVAILABLE FOR CONSUMERS, INDUSTRY STAKEHOLDERS AND POLICYMAKERS

The EU-funded ECsafeSEAFOOD project has published three safe seafood guides that aim to help consumers, industry stakeholders and policymakers understand the benefits and risks associated with seafood consumption. Each guide includes recommendations to help reduce possible risks associated with seafood contamination from the specific stakeholder's perspective.

http://www.ecsafeseafood.eu/

ANTIOXIDANT RICH SEASONINGS AND MARINADES REDUCE FORMATION OF CARCINOGENIC COMPOUNDS IN COOKED MEAT

The consumption of grilled meat entails a high intake of carcinogenic compounds, namely polycyclic aromatic hydrocarbons (PAHs) and heterocyclic aromatic amines (HAs). Both form when meat like beef, pork or fish is cooked at high temperatures, especially coal fired barbecue that can get up to lofty temperatures of 300 degrees Celsius and produce lots of smoke. The formation of both contaminants can be highly reduced using antioxidant rich seasonings and beer marinades, which are efficient mitigation strategies.



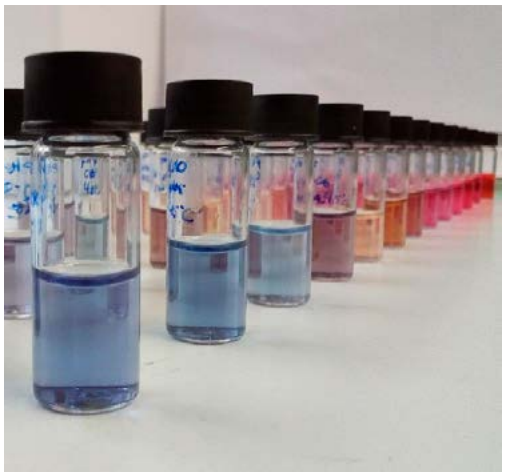
Influence of red wine pomace seasoning and high-oxygen atmosphere storage on carcinogens formation in barbecued beef patties.

Meat Science, 2017, 125, 10-15.

HIGHLIGHTS

NEW ANTHOCYANIN-BASED COLORANTS

Novel pyranoanthocyanin pigments with unique chromatic features and natural anthocyanins acylated with fatty acids were synthetized starting from food Industry by-products aiming to use them as colorants for new technological applications in lipid-based foods and in cosmetics.
This approach allows to use natural pigments with appealing colours (from orange to bluish hues) in lipophilic matrices including dairy products, cosmetic oils and emulsions and skin care products.

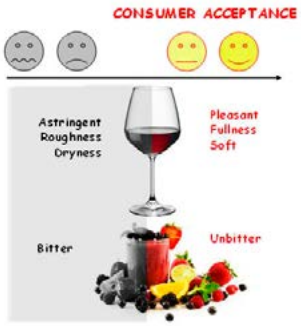


Malvidin-3-glucoside-fatty acid conjugates: from hydrophilic towards novel lipophilic derivatives

Journal of Agricultural and Food Chemistry, 2017, 65, 6513-6518.

IMPROVING THE TASTE OF HEALTHY FOODS

The impact of different food polyphenols on food astringency and bitterness was correlated with their interaction with salivary proteins, bitter taste receptors and oral cells. Novel approaches have been made to better comprehend the molecular mechanisms responsible for the bitter taste of phenolic-containing foodstuffs. Hence, the bitter taste of foods containing health promoting nutraceuticals such as polyphenols could be modulated during processing aiming to improve their final acceptance by the consumer.



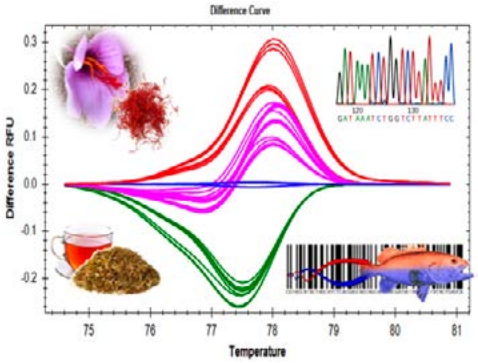
Study of human salivary proline-rich proteins interaction with food tannins

Food Chemistry, 2018, 243, 175-185.

HIGHLIGHTS

DNA BARCODING COUPLED WITH HIGH RESOLUTION MELTING (HRM) ANALYSIS FOR FOOD AUTHENTICATION

Bar-HRM analysis is a innovative, simple, fast, reliable, cost-effective and high throughput DNA-based approach for the authentication of highly valued seafood, spices, and herbal medicines. With the application of this technique, it was possible to distinguish *Gadidae* fish species and *Penaeidae* shrimps from its adulterants and the spice Crocus sativus (saffron) from closely related species. It was also applied to differentiate two medicinal plants *Hypericum androsaemum* (Hipericão do Gerês) and *Hypericum perforatum*.

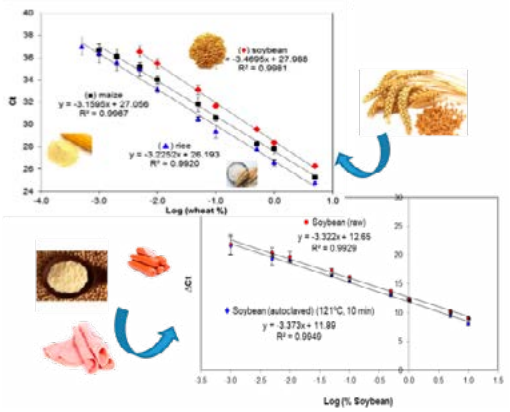


HRM analysis targeting ITS1 and matK loci as potential DNA mini-barcodes for the authentication of Hypericum perforatum and Hypericum androsaemum in herbal infusions

Food Control, 2016, 61, 105–114.

PCR ASSAYS FOR THE QUANTITATIVE ANALYSIS OF FOOD ALLERGENS ARE AFFECTED BY MATRIX, GENE MARKER AND PROCESSING

The quantitative performance of real-time PCR approaches was studied and compared for soybean and wheat detection. The new models allowed the detection of wheat and soybean down to 5 and 10 mg/kg, respectively. Gene maker and matrix greatly affected the assay performance of wheat quantification. However, thermal processing did not affect the normalised quantitative performance of soybean. Normalised real-time PCR assays can be new alternative accurate and sensitive tools for allergen quantification.



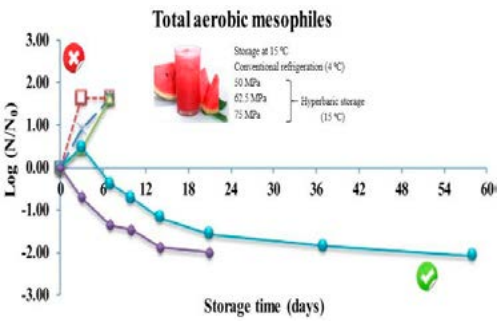
Matrix-normalised real-time PCR approach to quantify soybean as a potential food allergen as affected by thermal processing

Food Chemistry, 2017, 221, 1843–1850.

HIGHLIGHTS

QUASI ENERGETICALLY COSTLESS EXTENSION OF FOODS SHELF LIFE BY HYPERBARIC STORAGE

Whereas refrigeration (RF) increased the microbial loads of raw watermelon juice (a highly perishable food), hyperbaric storage (HS) at 62.5/ 75 MPa (15 °C) not only was able to control microbial growth, but showed additionally a reduction of initial microbial loads, by at least 2.5 log CFU/mL, while pH and color values did not change. Furthermore, the combination of a lower temperature with HS showed further beneficial effects to control microbial development, even for a lower pressure (50 MPa/10 °C). Hyperbaric storage increased watermelon juice shelf-life for at least 58 days, compared to 3 to 5 days under refrigeration.

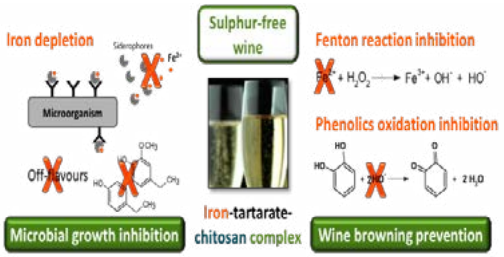


Extension of raw watermelon juice shelf-life up to 58 days by hyperbaric storage.

Food Chemistry, 2017, 231, 61-69.

POLYSACCHARIDE-BASED FILMS FOR REPLACEMENT OF THE USE OF SULPHUR DIOXIDE IN LIQUID FOODS

A novel approach using chitosan-genipin films was developed as a sustainable method for wine preservation at industrial scale with no additional costs. White wines were produced without addition of sulphur dioxide as preservative. The wines produced using the films had lower susceptibility to browning, with organoleptic characteristics comparable with those prepared using sulphur dioxide. The formation of iron-tartrate-chitosan complexes promotes the decrease of iron and other metal availability, minimizing oxidation reactions, as well as inhibiting microbial growth. The overall volatile character of the wines was maintained. The application of chitosan-genipin films was successfully extended to the production of vinegars.

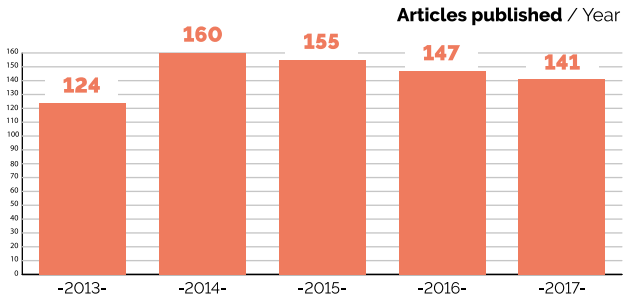


Wine preservation using chitosan-genipin films as an alternative to sulphur dioxide

Green Chemistry, 2016, 18, 5331-5341.

GROUP IN NUMBERS

SCIENTIFIC PRODUCTION 2013-2017*



727 articles
5732 citations**
H-index: **70**

FUNDED PROJECTS *(Representative projects)*

- "SEAFOODTOMORROW",
  Horizon 2020, GA 773400, Sara Cunha (local PI)
  Total funding: € 209,325.00
- "FOODINTEGRITY - Ensuring the Integrity of the European food chain"
  FP7-KBBE-2013-single-stage, No 613688, Isabel Mafra (Local PI)
  Total funding: € 81,440.00
- "FoodNanoSense - Qualidade e Segurança Alimentar: uma abordagem (nano) tecnológica".
  NORTE-01-0145-FEDER-000011. Isabel Ferreira (PI)
  Total funding: € 3,153,322.67
- "ECsafeSEAFOOD - Environmental contaminants in seafood: safety assessment, impact and mitigation strategies"
  FP7-KBBE-2012.02.4-01, project nº 311820, Sara Cunha (Local PI)
  Total funding: € 174,040.00
- IBERPHENOL - Research cooperative within the scope of polyphenols and its industrial applications
  0377_IBERPHENOL_6_E, European Fund for Regional Development – INTERREG Spain-Portugal, Nuno Mateus (PI).
  Total funding: € 208,592.97
- GMOsensor - Monitoring Genetically Modified Organisms in Food and Feed by Innovative Biosensor Approaches
  FP7 PEOPLE-2013-IRSES, Marie Curie actions nº 612545), Isabel Mafra (Local PI)
  Total funding: € 60,900.00

7 EU projects
1.5 M€

19 national projects
8.38 M€

22 industry-financed projects
2 M€

INTERNATIONAL COOPERATION AND NETWORKING

- COST Action FA1402, "ImpARAS: Improving Allergy Risk Assessment Strategy for New Food Proteins", 2014-2018
- COST Action MP1206, "Electrospun Nano-fibres for bio inspired composite materials and innovative industrial applications", 2013-2017
- FEEDcities - Food Environment Description in cities from Central Asia and Eastern European countries, WHO registration 2015/591370 and 2017/698514
- WHO - International Agency for Research in Cancer - IARC Monographs on the Evaluation of Carcinogenic Risks to Humans – Participation in the interdisciplinary working groups of expert scientists that evaluate the weight of the evidence that an agent can increase the risk of cancer, 2016-2017
- Cooperation in Science & Technology Portugal-Morocco CNRST/FCT (FCT/6460/6/6/2017/S), 2017-2018
- Cooperation in Science & Technology Portugal-Serbia (FCT/10971/22/6/2015/S), 2015-2016
- Sino-Portuguese Programme of Cooperation in Science & Technology (Ref. 441.00) in collaboration with Wuhan Polytechnic University, P.R. China, 2014-2016
- "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

OUTREACH

- The project FoodNanoSense funding from FCT has been published in several communication media including the TV channel "Porto Canal", the journal "Jornal de Notícias", in the websites related to the University of Porto "FCUP news" and "Portal U.Porto".
- The World Health Organization-Europe in collaboration with University of Porto published a report on the situation of trans fatty acids in Portugal.
- MobFood: "Mobilização de conhecimento científico e tecnológico em resposta aos desafios do mercado agroalimentar", Projeto Nº 24524 liderada por PRIMOR, SA, consórcio composto por 21 empresas e 24 entidades de ENESII.
- ValorMar: "Valorização integral dos recursos marinhos: potencial, inovação tecnológica e novas aplicações", Sistema de Incentivos Programa PORTUGAL 2020. Liderado pela SONAE CENTER SERVIÇOS II SA, consórcio composto por 31 entidades, 18 empresas e 13 entidades de ENESII.


LABORATÓRIO ASSOCIADO
PARA A QUÍMICA VERDE


requimte
rede de química e tecnologia


U.PORTO


UNIVERSIDADE
NOVA
DE LISBOA


universidade
de aveiro

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 WELLBEING

NanoPlat
NANOPLATFORMS

4FOOD
FOOD QUALITY AND TECHNOLOGY

LAQV requimte
LABORATÓRIO ASSOCIADO PARA A QUÍMICA VERDE

2013/2018
ACTIVITY REPORT
& HIGHLIGHTS

04

Post-Graduation

MASTER PROGRAMS | MSC

Biochemistry
FCUP

DIRECTOR:
Paulo Correia de Sá (ICBAS-UP)

LOCAL COORDINATOR:
Paula Gameiro (LAQV)

Biochemistry
UAveiro

DIRECTOR:
Rita Ferreira (LAQV)

Bioorganic Chemistry
FCT/UNL

COORDINATOR:
Paula Branco (LAQV)

Biotechnology
FCT/UNL

COORDINATOR:
Susana Barreiros (LAQV)

Chemistry
UAveiro

DIRECTOR:
Helena Nogueira (UAveiro)

LOCAL COORDINATOR:
Diana Pinto (LAQV)

Conservation and Restoration
FCT/UNL

DIRECTOR:
Joana Lia Ferreira (LAQV)

Food Science and Technology
FCUP

DIRECTOR:
Victor Freitas (LAQV)

Gastronomic Sciences
FCT/UNL

COORDINATOR:
Paulina Mata (LAQV)

Membrane Engineering (Erasmus Mundus)
FCT/UNL

COORDINATOR:
Isabel Coelhoso (LAQV)

Quality Control
FFUP

DIRECTOR:
Beatriz Oliveira (LAQV)

DOCTORAL PROGRAMS | PHD

Sustainable Chemistry

DIRECTORS:
Manuel Nunes da Ponte (LAQV), 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:
Mário Barbosa (ICBAS-UP)

VICE-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)

Chemical and Biochemical Engineering

PDEQB

COORDINATOR:
José Paulo Mota (LAQV)

Food Sciences

DPFD

COORDINATOR:
Marco Gomes da Silva (LAQV)

Materials Chemistry

ChemMat

DIRECTOR:
Manuel Leite de Almeida (IST/ULisboa)

LOCAL COORDINATOR:
Cristina Freire (LAQV)

Medical Biochemistry and Biophysics

M2B-PhD

DIRECTOR:
Miguel Castanho (FM/ULisboa)

LOCAL COORDINATOR:
Victor Freitas (LAQV)

Chemistry

UAveiro

COORDINATOR:
Augusto Tomé (LAQV)

Chemistry

Nova.Lisboa

COORDINATOR:
Marco Gomes da Silva (LAQV)

Chemistry |UPorto

DIRECTOR:
Victor Freitas (LAQV)

Biochemistry

UAveiro

COORDINATOR:
Francisco Amado (LAQV)

LAQV requimte
LABORATÓRIO ASSOCIADO PARA A QUÍMICA VERDE

2013/2018
ACTIVITY REPORT
& HIGHLIGHTS

05

Scientific Platforms

BIOLOGICAL AND CHEMICAL ANALYSIS

This facility is devoted to the comprehension of cellular and molecular mechanisms, from 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
- Isothermal Titration Calorimetry - TA™ Nano ITC
- MicroScale Thermophoresis - Nano Temper Technologies™ Monolith NT.115
- Flow Cytometry - Attune™ Acoustic Focusing Cytometer

UPORTO

- Langmuir Trough with Brewster Angle Microscopy - KSV-NIMA KN-1006 trough with Nanofilm_Ultrabam (Accurion GmbH)
- Langmuir Trough with Polarization-modulation infrared reflection-absorption spectroscopy (PM-IRRAS) - KSV-NIMA KN-1002 trough with KSV-NIMA PM-IRRAS spectrophotometer
- Isothermal Titration Calorimetry - MicroCalTM iTC200
- Differential Scanning Calorimetry - MicroCalTM VP-DSC

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 ultra-fast 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

The Computer cluster Facility has its own cluster of computers with the following characteristics:

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
- 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
- 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

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. The NMR facility of FCT NOVA, hosted in the Chemistry Department, pioneered in Portugal in the use of NMR for the determination of protein structures. Currently, we still support many research projects focused on the determination of protein structure and dynamics but most of the research being conducted is related to the study of molecular interactions and molecular recognition in a wide range of chemical and biochemical systems. The facility is also strongly committed to providing NMR routine services to support in-house synthesis and chemical (bio) engineering research groups. The Magnetic Resonance facility of LAQV-UPORTO is part of the Structural Analysis Laboratory of the University of Porto Materials Center (CEMUP). The three spectrometers available provide routine services to support in-house researchers, graduate and post-graduate students as well as external users. The NMR facility at University of Aveiro hosted at the chemistry department is constituted by 5 NMR spectrometers and allows to cover a wide range of applications, from comprehensive characterization of the chemical structure, conformations and configurations of synthetic and natural molecules to metabolomics analysis for biochemical characterization. However, there is also spectrometers devoted to solid-state NMR using high-resolution methods to study small molecules, inorganic materials and inorganic-organic hybrid materials

EQUIPMENT

FCT NOVA

- 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 HR-MAS 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)

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)

MAGNETIC RESONANCE (CONT.)

- Magnet: BRUKER AVANCE III - 400 MHz, Solid-state NMR spectrometer (wide-bore), 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/15N-2H, 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

UPORTO

- 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 HR-MAS 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)

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 post-graduate students as well as external users.

EQUIPMENT

U. Aveiro

- Q-EXACTIVE (Thermo) with a Thermo Scientific Nanospray Flex Ion Source coupled with an 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

UPORTO

- LTQ-Orbitrap XL (Thermo) with an ESI source coupled to an ACCELA 600 HPLC system
- Thermo Scientific EasyNanospray Ion Source coupled with an nano LC Thermo Scientific™ UltiMate™ 3000
- BRUKER UltrafleXtreme MALDI-TOF/TOF-MS
- Shimadzu Nexera UHPLC coupled to LCMS-8040 ESI-QqQ-MS

ELECTRON MICROSCOPY

The electron microscopy network laboratory consist is a focal point of the Portuguese Electron Microscopy Network. It is hosted at the Universities of Aveiro and Porto and are available to be used by students, faculty and staff members of the LAQV-Aveiro.

EQUIPMENT

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.

UPORTO

- XPS Kratos Axis Ultra HSA

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 – 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, High-performance 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 PIXcel-1D 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

PILOT PLANT

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, involving membrane processes or supercritical CO2 extraction or fractionation.

EQUIPMENT – FCT NOVA

Solid / Supercritical Fluid Pilot plant

- 5 AISI 316 Extractors (up to 500 bar and 80 °C; Volume capacity: 4 with 1800 cm3 + 1 with 3800 cm3)
- 2 AISI 316 Cyclones (up to 450 bar; Volume capacity: ca. 200 cm3)

SFE pilot plant for liquid mixtures

- 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)

Microfiltration and Ultrafiltration Membrane units

Stainless steel 316 membrane units, including several flat lab scale rigs (membrane area up to 150 cm2) and pilot units (membrane area up to 7.6 m2), prepared for operation with hollow fibre modules and spiral wound modules. These units are fully equipped, with pressure transducers, flowrate mass controllers and on-line data acquisition and storage. The pilot units are mobile, making possible their operation at the field.

Nanofiltration and Reverse Osmosis Membrane units

Identical to the microfiltration and ultrafiltration equipment described (also lab and pilot scale units), equipped with spiral wound modules, and feed and pressure pumps, allowing for operation up to 20 bar in the case of the nanofiltration units and up to 80 bar in the reverse osmosis units.

LAQV requimte
LABORATÓRIO ASSOCIADO PARA A **QUÍMICA VERDE**

LAQV
2013-2018 ACTIVITY REPORT & HIGHLIGHTS

PORTO
Setembro 2018