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The Centro de Química e Bioquímica was founded in 2001 aiming at developing internationally competitive science, particularly at the frontier of chemistry and biochemistry. The multidisciplinary teams working in the experimental and theoretical labs within CQB involve approximately sixty PhD members and more than one hundred collaborators, most of them PhD and Master students. The lively and youthful atmosphere of the Faculdade de Ciências extends to CQB and is further amplified by the large number of international collaborations and programs (students from ERASMUS, IAESTE and others).

We conduct fundamental research disseminated by recognized peer-reviewed scientific journals, and the high number of citations reflects its relevance to the scientific community worldwide.

CQB research is organized in two thematic lines, which are aligned with the Societal Challenges defined in Horizon 2020 EU, the priorities for the regional development of the Lisbon area, and take advantage of the consolidated skills of CQB members:

**Chemistry and Biochemistry for a Clean Environment**

**Healthy Life: Molecular Interventions and Regulation Mechanisms**

I invite you to read these pages, visit our website and know more about us and our research!

Lisbon, November 15, 2015

Maria José Calhorda
(CQB coordinator)
# Index

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Mission

The mission of CQB is grounded on three pillars: to investigate challenging problems in chemistry and biochemistry, to train the next generation of highly skilled chemists and biochemists, and to create social, economic and cultural value from scientific knowledge.

CQB has....

- Excellence in scientific production
- Research goals aligned with EITHealth, H2020 and the Strategic Priorities for the Region of Lisbon, namely those concerning the Smart Specialization
- Networking in EIP AHA, EITHealth – INNOStar, COST programs, Soft Matter@PT Network, Health Cluster Portugal, Colleges “Brain” and “3F (Farm, Food, Forestry)” at ULisboa.
- A collaborative culture, as attested by joint programs with industry and academia at the national and international level
- Privileged interactions with society
We are

61 Integrated Members (IM)

& 115 Students

University Staff 56%

Post Doc 29%

FCT Investigators 15%

Visiting students (Erasmus/Bilateral) 21%

PhD Industry 3%

PhD 23%

Undergraduates 22%

MSc 31%
We are

12 Research Groups

AAM  Adsorption and Adsorbent Materials
CC   Carbohydrate Chemistry
EMBS Environmental and Biological Mass Spectrometry
E    Enzymology
ITC  Inorganic and Theoretical Chemistry
IE   Interfacial Electrochemistry
MB   Molecular Biophysics
ME   Molecular Energetics
RB   Redox Biology
SST  Separation Science and Technology
SSC  Solid State Chemistry
SR   Structure and Reactivity
In 2014, publications included
• 27% with international collaborations
• 18% with internal collaborations
• 15% in Top 10% journals*
• 65% in Top 25% journals* (Q1)

*by impact factor and subject area

In 2015
• 80 papers in International peer reviewed journals
• 3 Book Chapters

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- 623 Publications 2008-2012  
  ~104 / year
- 246 Publications 2013-2014  
  123 / year

• Hundreds of oral & poster presentations in international conferences each year
• Organization of national and international conferences
Achievements - Investigador FCT

7 successful applications in the 2012, 2013 and 2014 calls

CQB receives a comparatively large number of applications which have a higher degree of success than the national average rate in this highly competitive program.

Researchers and projects

2012 Call
- Carla D. Nunes, Developing Grant: Innovative Concepts in Asymmetric Catalysis
- Rodrigo F. M. de Almeida, Developing Grant: Tackling Membrane Lipid Organization to Understand and Refine Drug Mechanisms of Action

2013 Call
- Ana S. Viana, Starting Grant: Novel Nanotestructured Electrodes towards Optimal Biosensing
- Nuno M. Xavier, Starting Grant: Synthesis of Nucleotide Mimics as Potential Antitumor Agents Targeting Cyclin-dependent Kinases

2014 Call
- Gonçalo Costa, Starting Grant: Revealing Amyloid Fibril Formation through the ions of Mass Spectrometry
- Olinda Monteiro, Starting Grant: Titanate nanotubes photosensitization by narrow bandgap semiconductor nanoparticles
- Paulo Costa, Starting Grant: Halogen Bonds in (Bio)chemical Systems: a Theoretical Approach for ‘Real World’ Applications

FCT investigator program is a researcher-centered, highly competitive scheme, aimed at providing 5-year support for the most talented and creative researchers, capable of carrying out independent research and becoming leaders in their fields. info: www.fct.pt
Achievements - Papers


Top 10%


Achievements - Papers

Key Scientific Articles classified by GLOBAL MEDICAL DISCOVERY


[\text{Ru}^{4+}(\eta^5-C_5H_5)(\text{bipy})(\text{PPh}_3)]^+, a promising large spectrum antitumor agent: cytotoxic activity and interaction with human serum albumin.


Scientific Articles recommended by


ISI highly cited paper - Top 1% in Pharmacology and Toxicology

Achievements - Papers

ISI highly cited paper - Top 1% in Biology and Biochemistry


2 scientific dissemination papers written by young CQB researchers, 2013

- Therapeutic properties of nitric oxide
  Moisés Luzia Pinto

- Rafts in our cells: a new role for lipids in the molecular organization of life
  Rodrigo F. M. de Almeida

These papers were chosen after a selection process with only 1% successful applications around Europe and were published in 2013:

- The Permanent Platform for European Excellence – Atomium Culture (sponsored by the European Commission)
- “El País” (Spanish newspaper)
- “Il sole 24 Ore” (Italian newspaper)
Achievements - Prizes

Second Prize of the Crystals in Art Competition
The British Association for Crystal Growth 2014

Crystals of 4’-hydroxyacetophenone (polymorph I)
by Carlos Bernardes

Infusions to reduce blood cholesterol and improve digestion

Food & Nutrition Awards 2014:
L. Serralheiro and P. L. Falé, CQB won 2nd Honorable Mention in the category of Research & Development

Project awarded under Programa de Estímulo à Investigação,
Fundação Calouste Gulbenkian

Sara Realista, CQB PhD student, won the prize in the area of Chemistry, with the project: "Smart polymer switches for green CO2 capture“, March 2014.

To distinguish and stimulate research of highly promising young researchers (under 26 years), to help achieving the scientific goals of the project.
Achievements - Images

Cover of ChemCatChem 2014, 6


Image displayed in 2015 at the Homepage of the Sociedad de Biofísicos Latino Americanos (SOBLA)

Participation in National & International organizations

Participation in editorial boards of international scientific journals

- Editor of the Royal Society of Chemistry Book Series Specialist Periodical Reports entitled Carbohydrate Chemistry – Chemical and Biological Approaches (A. P. Rauter)
- Associate Editor of Mediterranean Journal of Chemistry (A. P. Rauter)
- Associate Editor of Frontiers in Cell and Developmental Biology (F. Antunes)
- Associate Editor of RSC Advances (P.D. Vaz)
- Advisory Board of Journal of Chemical Thermodynamics (M. Minas da Piedade)
- Advisory Board of European Journal of Organic Chemistry (A. P. Rauter)
- Editorial Board of Journal of Carbohydrate Chemistry (A. P. Rauter)
- Editorial Board of Drug Design Methodologies and Modern Medicinal Chemistry (A. P. Rauter)
- Editorial Board of Frontiers in Membrane Physiology and Biophysics (R. F. M. de Almeida)
Participation in National & International Organizations

Participation in decision-making bodies and in International and National Organizations, Committees and Divisions

- *Sociedade Portuguesa de Química*, President (M.J. Calhorda)
- IUPAC Division (VIII) of Chemical Nomenclature and Structure Representation, Titular member (A. P. Rauter)
- IUPAC Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS) (Associate member) and Division VIII representative in ICTNS (A. P. Rauter)
- IUPAC Division (III) of Organic and Biomolecular Chemistry, Associate member and Secretary (A. P. Rauter)
- Chief Operational Officer of the LisbonLiving+ Consortium and member of its Executive Committee (2013-Sept.2014), established for the application to the EIT KIC on Healthy Life and Active Ageing EITHealth (A. P. Rauter)
- FCUL Sponsor of the FCT-PhD Program Catalysis and Sustainability (CATSUS) (M.J. Calhorda)
- Steering Committee of the Technology Transfer Unit of the University of Lisbon UL-INOVAR (2009-2013) (A. P. Rauter)
- International Society of Electrochemistry, National Representative (J. Correia)
- International Carbohydrate Organisation National Representative (A. P. Rauter)
- Rede Nacional de Espectrometria de Massa (M. H. Florêncio: Coordinator)
- Rede Procura: Associação Portuguesa de Proteómica (A. Ferreira, Member of Audit Committee Board and C. Cordeiro, Secretary of the General Council)
- *Conselho Geral da Universidade de Lisboa* (H. Florêncio)
- *Autoridade da Segurança Alimentar e Económica*, ASAE (H. Florêncio)
CQB Networking

The European Innovation Partnership on Active and Healthy Ageing (EIP AHA), Action Group A3

- Prevention of functional decline and frailty
- More than 70 consortia and institutions
- CQB belongs to the FCUL consortium

CQB activities and deliverables:

- Interactive website to educate the general public (functional foods for disease prevention)
- e-learning courses
- Chemical and biological approaches towards innovative molecular entities and functional food ingredients
- Understanding the mechanisms of frailty and ageing
- Novel high-added products from biomass
CMST COST Action CM1302 - European Network on Smart Inorganic Polymers (SIPs), 2013-2017, MC and WG2
CMST COST Action CM1307 - Targeted chemotherapy towards diseases caused by endoparasites (2014-2018), WG
CMST COST Action CM1402 - From molecules to crystals - how do organic molecules form crystals? (Crystallize) (2014-2018), MC and WG1, WG2, and WG4
FA COST Action FA1403 – Inter individual variation in response to consumption of plant food bioactives and determinants involved (POSITIVe) (2014-2018), MC
BMBS COST Action BM1102 - Ciliates as model systems to study genome evolution, mechanisms of non-Mendelian inheritance, and their roles in environmental adaptation (2011-2015),MC
TD COST Action TD1402 - Multifunctional Nanoparticles for Magnetic Hyperthermia and Indirect Radiation Therapy (RADIOMAG) (2014-2018), MC
TD COST Action TD1305- iPROMEDAI: Improved Protection of Medical Devices Against Infection (2014-2018), WG

MC- Management committee
WG- Working Group
CQB Networking

EIT-KIC/IVE/0051/2013

The European Institute of Innovation and Technology (EIT) has launched an application to a Knowledge and Innovation Community (KIC) on Healthy Life and Active Ageing

- FCT approved the project EIT-KIC/IVE/0051/2013 to prepare the application
- CQB is one of the founders of the consortium LisbonLiving+ built within this project. This consortium involves Industry, Governmental bodies and Academia partners.

7th Sino-Portugal Scientific and Technological Cooperation, 2013-2015

- The Construction of Novel Sensitive Biosensing Interfaces for Tumor Marker and BOD Detection.
Smart Specialization

Collaboration with Laboratório de Polícia Científica da Polícia Judiciária

Identification of new psychoactive substances marketed as recreational drugs in Portugal.

Contracts and research projects with national and international Industries, collaboration with high-tech SMEs, and governmental bodies, to develop:

- New materials to monitor/ remove/ degrade priority pollutants in complex matrices (e.g. drinking water) with much higher efficiency and lower cost than current procedures.
- Innovative procedures for the recovery of Pt-group metals from hydrometallurgical chloride leaches.
- Correlations of traditional knowledge with scientific evidence for Portuguese flora, as a source of functional foods and nutraceuticals.
- The energetic valorization of olive-mill wastewaters and of cork industry by-products.
- Development and application of new active substances with phytopharmaceutical use.
- The identification of bioactive compounds in marine fauna and flora resources.
- Partnerships to assess biological activities towards causative bacterial agents of global health threats.
- Collaboration with PARALAB and NETZSCH on testing the Premium Differential Scanning Calorimeter, DSC 204 F1 Phoenix
- Contract between Laboratórios Atral S.A. and CQB for analytical services
- Collaboration with Autoridade de Segurança Alimentar e Económica
CQB was involved in launching three start-up companies:

- Adsorfoam, SA. Filtering media for improving indoor air quality
- Sea4Us. New marine leads
- BioMimetx. Bio-additives for marine antifouling paints

**CQB Patents 2013-2015**

- Two-Component Natural Polymeric Water-Based Glues obtained from Derivatives of Cork. WO 2015034383 A1, 2015.


- Colas Naturais de Base aquosa, de dois componentes, obtidas a partir de Derivados de cortiça (Water-based natural glues obtained from cork derivatives). PT107143, 2013.

- Utilization of olive bagasse as acetylcholinesterase inhibitor for cholinergic diseases. PT105914B, 2013.

- Applications of antioxidant and antiproliferative natural products from alfarroba biomass. PT105731B, 2013.

- New C-glycosylpolyphenol antidiabetic agents, effect on glucose tolerance and interaction with beta-amyloid. Therapeutic applications of the synthesized agent(s) and of *Genista tenera* ethyl acetate extracts containing some of those agents. WO201313247OA2, 2013 (Pending Patent).

- Compostos derivados de açúcar inibidores de espécies de *bacillus*, processo de obtenção e respectivas utilizações. PT105475, 2011. (Pending Patent)
Outreach Activities

changer CQB organizes annual meetings open to the academia and society, such as the CQB day and workshops, to stimulate joint research and enhance public visibility.

changer Set-up of a website (in Portuguese, 2012) to provide the general public with scientific information about antioxidants http://antioxidantes.fc.ul.pt/

changer Involvement in “Ciência Viva”: Action European Researchers Night
changer Talks, demonstrations and quizzes on FCUL Open Days and Futurália
changer Radio/TV broadcasts to comment scientific discoveries

CQB day – September 2015
Outreach Activities

- Porque é que o Space Shuttle não anda a gasolina?
  Video presentation on the frame of *Saber Porquê*, O Programa o Mundo na Escola, promoted by Ministério da Educação e Ciência (www.mundonaescola.pt)

- Trabalho experimental em Química no Ensino Secundário- Novos programas, novos desafios a partir de 2015/16; *Short training/updating courses* for secondary school teachers

- Olimpíadas da Química Júnior, organized by SPQ

- A Tabela Periódica no Dia Mundial do Ambiente

- Erasmus +
  - Staff mobility for teaching and training activities, La Sapienza University, Rome, Italy, May 2015
  - International Week, University of Foggia, Italy, June 2015
Thematic Lines

Chemistry and Biochemistry for a Clean Environment
Coordination: Carla D. Nunes
(FCT Principal Investigator)

Healthy Life: Molecular Interventions & Regulation Mechanisms
Coordination: Rodrigo F. M. de Almeida
(FCT Principal Investigator)

MCM-41-Mo is an agent for rhodamine B degradation

Aligned with H2020 Societal Challenges
Aligned with Lisbon area regional priorities
Overview and goals

*Chemistry and Biochemistry for a Clean Environment* focuses on the European societal challenges to develop methodologies that ensure a clean and healthy environment. To achieve this, new ways of identifying, assessing, preventing, controlling, or efficiently removing contaminants, thereby reducing human health risks, will be addressed. In parallel, we create selective and environment friendly catalyst for industrial relevant processes.

CQB has the expertise to synthesize and characterize new molecules and materials able to degrade contaminants, to adsorb pharmaceutical remains, to obtain heterogeneous and homogeneous catalysts to improve industrially relevant reactions.
Overview and goals

These efforts combined with those purveying analytical methods development and biochemists conducting research oriented to the evaluation of their impact on human health will contribute to improve the cleanliness of the environment.

The support of groups with expertise in computational studies, determination of properties and characterization of molecules and materials will significantly improve the knowledge needed to live in a Clean Environment, one condition at the heart of the idea of Healthy Ageing!

These potentialities will lead to the creation of environment-friendly and decontamination technologies, new methods for decontamination control and residual hazard assessment, and for evaluation of their impact on human health.
Chemistry and Biochemistry for a Clean Environment

Key publications

2015


Development of tertiary thioamide derivatives to recover palladium(II) from simulated complex chloride solutions, O. Ortet, A.P. Paiva, Hydrometallurgy, 2015, 151, 33–51.


2014


Chemistry and Biochemistry for a Clean Environment

New projects- FCT 2015

- Multifunctional Luminescent Spin Labile Hybrid Materials
  PTDC/QEQ-QIN/3414/2014
- Overcoming environmental problems associated with antifouling agents: synthesis of Nature inspired nontoxic biocides and immobilization in polymeric coatings
  PTDC/AAGTEC/0739/2014

New projects- Environment Policy & Governance projects, EU 2015

- LIFE-Impetus: Improving current barriers for controlling pharmaceutical compounds in urban wastewater treatment plants.
  LIFE 14 ENV/PT/000739

Ongoing projects

- CO₂ Mitigation and Production of Methanol by Reforming of CH₄
  FCT Project PTDC/AAG-TEC/3324/2012
- BIONANOMINE: Bio-synthesis of nanosized semiconductors using mine wastes as material sources and environmentally friendly applications
  PTDC/AAG-TEC/2721/2012
- Antifouling compounds for the biofouling control in aquaculture (ECOFOULESS)
  OF/6923/2014/DPA/DRAPALG
- MAROC – Morphology-Activity Relationship in Oxidation Catalysis
  FCT Project EXPL/QEQ-QIN/1137/2013
- Smart polymer switches for green CO₂ capture
  Fundação Gulbenkian- Estímulo à Investigação
- Materiais de carbono para degradação de compostos farmacêuticos em fase aquosa em processos avançados
  CRUP Action Portugal-Spain E11/11
Healthy Life: Molecular Interventions & Regulation Mechanisms

Overview and goals

Promotion of a healthy life and an active ageing is a societal challenge in Europe, aiming at a better quality of life and providing social and economic benefits.

The synergies afforded by the multidisciplinary research team of CQB provide optimal conditions to be at the forefront of this research area.

Several chemistry oriented labs are proficient in synthesizing or obtaining from natural sources novel molecules with potential high-value bioactive properties. On the other hand, biochemists are conducting research on the biological mechanisms underpinning health and disease.

The preventive and therapeutic properties of new molecules obtained by chemists can, therefore, be investigated in the framework of the most advanced and updated biochemical knowledge.

Marine Natural Products
The combined efforts of several labs in this thematic line will be directed towards the promotion of healthy habits in the general population and catalyzing novel collaborations with the business world.

In summary, with this thematic line we aim at providing key scientific contributions to a fast incorporation of chemical and biochemical knowledge into the society, thus effectively contributing to a healthier and more active life!

*Salvia sclareoides*, medicinal plant for the prevention of neurodegenerative impairments
Healthy Life: Molecular Interventions & Regulation Mechanisms

Key publications

2015

The extracellular matrix modulates H$_2$O$_2$ degradation and redox signaling in endothelial cells, A. Baguão, F. Vilas-Boas, A. Pena, C. Peneda, F. C. Santos, A. Jerónimo, R.F.M. de Almeida, C. Real; Redox Biology; 2015, 6: 454


2014


Healthy Life: Molecular Interventions & Regulation Mechanisms

New projects- FCT 2015

- Sphingolipid organization in the plasma membrane of Saccharomyces cerevisiae. Implication in antifungal mode of action and fungal resistance. PTDC/BBB-BQB/6071/2014
- Biomimetic/nanobioconjugates flexible platforms for sensitive immunosensing PTDC/CTM-NAN/0994/2014
- Anion transmembrane transport promoted by drug-like molecules: building a library of anion carriers inspired in Ataluren (PTC124) PTDC/QEQ-SUP/4283/2014

Ongoing projects - European Projects, Commitments and QREN

- Personalised ICT Supported Service for Independent Living and Active Ageing, FP7-ICT-2013-10, Project Nr. 610359, 2013 - 2016
- Diagnostic and Drug Discovery Initiative for Alzheimer’s Disease, FP7-PEOPLE-2013-IAPP, Project Nr. 612347, Industry-Academia Partnerships and Pathways (IAPP), 2014 – 2018
- Healthy ageing with innovative functional foods/leads for degenerative and metabolic diseases (INOVAFUNAGEING), approved in the “Invitation for Commitments to the Strategic Implementation Plan of the European Innovation Partnership on Active and Healthy Ageing (EIP AHA) – Action A3”, 2012-2015
Adsorption and Adsorbent Materials

The main goal of the Adsorption and Adsorbent Materials (AAM) group is to develop porous materials and explore their potentialities as adsorbents, catalysts or catalysts supports or as matrixes for drug delivery systems. Different products are under study, e.g. carbon materials which are usually obtained from sub products of agricultural or industrial activities or by template methodologies; natural-clay based solids and metal-organic frameworks. Polyurethane matrixes with different compositions, and physical properties (e.g. hydrophobicity), are also developed to be used as supporting adsorbent materials.

Applications of these porous materials include the separation of alkenes from alkane/alkene mixtures, the purification (upgrade) of biogas and natural gas by removing carbon dioxide and nitrogen. Special interest has been given to the use of carbon materials as adsorbents for the removal of emergent pollutants (e.g. pharmaceutical compounds) from water.

Additionally, functionalization of porous materials with transition metal complexes using different methodologies for encapsulation is a hot topic within AAM group. The main goal is to obtain heterogeneous complexes which are catalytic active in the homogeneous phase.

Regarding catalysis the group has also interests in the modification of zeolites structures aiming the improvement of their performance in refining and petrochemical processes as well as catalysts supports.

In the drug delivery systems frame, adsorption and release of nitric oxide was evaluated, by storing this compound in porous materials aiming a slow release which could be very helpful for therapeutic applications.

http://adsorption.fc.ul.pt/
Hierarchical zeolites to higher performance catalysts


Zeolites are crystalline materials with a wide range of applications, especially as heterogeneous catalysts. However, the microporous nature of these materials limits its application in the presence of large molecules with industrial interest. The development of hierarchical zeolites (micro + mesopores) aims to increase molecular diffusion and the access to the active sites, extending the range of application for these materials in refining, petrochemistry and fine chemistry reactions.
From biomass to carbon materials to enhance water treatment technologies

Water contamination with pharmaceutical compounds is a reality worldwide and scientists and governmental entities consider that this kind of contamination may require legislative intervention. In fact, pharmaceutical compounds appear in a Watch List in the 2013/39/EU directive and, for now, activated carbons which are non-specific adsorbents, appear as the best available decontamination technology for the removal of the pollutants that have a recalcitrant behaviour in conventional water treatment plants.

The biomass-derived activated carbons developed in the Adsorption and Adsorbent Materials group of CQB outperform commercial samples in the ability to remove even the most recalcitrant pharmaceuticals from water.


Processo de produção de carvão activado a partir de material de cortiça
Nitric oxide (NO) is a small endogenous molecule with particularly interesting effects on biological systems, despite its toxicological potential. The delivery of nitric oxide in controlled amounts to the human body is an attractive therapeutic alternative for a large number of pathologies. NO is involved in neurological functions in synaptic plasticity, neurotransmission, learning, and memory, in addition to having a primary role in non-specific immunity and platelet aggregation inhibition.

NO is a gas at room temperature and pressure, unlike more common drug molecules that are usually in a solid or liquid state. Because of the limited utility of genuine NO gas in many experimental systems and the short half-life of NO in vivo, compounds that have the capacity to release NO have been researched. More recently, nanoporous materials were explored for their ability to act as NO delivery platforms, particularly for topical applications in dermatology, wound healing, and organ conservation.
Carbohydrate Chemistry

Based on a sustainable model, starting from sugars or from natural resources towards new drug candidates / functional food ingredients for pharmaceutical / food industries, the Carbohydrate Chemistry Group aims to provide economic and social benefits in terms of prevention of functional decline and ageing, nutrition, health and biosecurity.

Strategic areas:
- New approaches towards healthy ageing included in the activities of the European Innovation Partnership on Active and Healthy Ageing Action Plan 3 on prevention of functional decline
- Sustainable Chemistry for Functional Molecules
- Therapeutics and mechanisms of action

Research is based on:
Generation of new molecular entities by:
- Design and synthesis
- Environmentally friendly methodologies
- Isolation from natural resources (plants, algae) and structure elucidation

Polyphenols chemistry and society
- Functional foods
- Biomass residues valorization
- Cultural heritage

Challenges:
- New leads for degenerative (cancer) and amyloid diseases (Alzheimer's disease, diabetes)
- Sugar-based bactericides towards biosecurity
- Functional foods for a healthy ageing

http://carbohydrate.cqb.fc.ul.pt/
Highlight

New synthetic approaches for bicyclic sugars

Potent and selective BChE inhibitor

Stereoselective reactions
Wittig olefination as key step
Olefin stereocontrol based on sugar protection
Reaction regiocontrol based on solvent selection

Structure optimization for bioactivity

Alzheimer’s Disease
Selective inhibitor of BChE
CANCER

Projects
Diagnostic and Drug Discovery Initiative for Alzheimer’s Disease
FP7-PEOPLE-2013-IAPP

Total synthesis and stereochemical elucidation of Miharamycins A and B.
Carbohydrate-based generation of analogues and bioactivity studies
POCI/PPCDT/QUI/59672/2004

Colaborations:

Fellowships
“New synthetic strategies and structural optimization of the sugar moiety from a selective butyrylcholinesterase inhibitor”
SFRH/BD/90359/2013
Potential nucleotide mimetics


- New nucleotide-like derivatives intended to inhibit disease-associated enzymes possessing catalytic sites binding either nucleotides or functional groups mimicking partial structures contained in nucleotides.
- Efficient synthetic approaches for molecules based on new structural frameworks for nucleoside/nucleotide mimicry.
- Biological targets focused: CDKs, cholinesterases and carbonic anhydrases

Collaborations: Palacký University & AS CR (Czech Republic); Universität Halle-Wittenberg, Faculdade Farmácia UL
Highlight

INFECTION | Tackling antimicrobial resistance and Biosecurity

Antimicrobial resistance is an increasingly serious threat to global public health as new resistance mechanisms emerge and spread globally.

Research on new antibacterial agents with new mechanisms of action is becoming urgent.

Dodecyl glycoside displaying selective antimicrobial activity against *Bacillus anthracis* and *Bacillus cereus* (25 µM)


Alkyl deoxy glycosides also significantly inhibit *Enterococcus faecalis*;
Surface properties showed that headgroup structure is determinant for the aggregation/adsorption balance.


- Generation of a small library of deoxy hexopyranosides against *Bacillus* species
- Tuning alkyl glycoside bioactivity through structural features (D,L series), deoxygenation pattern and anomeric configuration. Surface activity is necessary but not sufficient for antimicrobial activity. Compounds target cell membrane acting with a new mechanism of action


A multidisciplinary project involving organic synthesis, physical chemistry, computational chemistry, biophysics and biology for the generation of a new family of antibiotics with a new mechanism of action

Patent *Sugar derivatives having tensioactive and antimicrobial activity* A. P. Rauter *et al.* WO 2012095792 A1
(submission: 10-01-2012, pub. date: 19-07-2012)

Projects
New drugs from sugars against infection caused by pathogenic *Bacillus* species (FACIB), QREN Diagnostic and Drug Discovery Initiative for Alzheimer’s Disease, FP7-PEOPLE-2013-IAPP

In collaboration with:
Highlight

Genista tenera for diabetes and Alzheimer´s disease prevention

Genista tenera is a plant endemic to Madeira Island and is used in traditional medicine to control diabetes.

8-β-D-glucosylgenistein, the main component of the EtOAc extract:
- Is not toxic towards human lymphocytes
- Normalizes blood glucose levels of STZ-induced diabetic Wistar rats
- Increases glucose-induced insulin secretion
- Inhibits human islet amyloid polypeptide (hIAPP) fibrillization
- Interacts with Amyloid β 1-42 (Aβ1-42) polypeptides
- Exhibits a common binding epitope to both hIAPP and Aβ.

Exploiting the Therapeutic Potential of 8-β-D-Glucopyranosylgenistein: Synthesis, Antidiabetic Activity, and Molecular Interaction with Islet Amyloid Polypeptide and Amyloid β-Peptide (1–42)


Projects:
- New antidiabetic agents from Genista tenera: Isolation, structural characterization, synthesis and mechanisms of action, funded by FCT
- From a multitarget antidiabetic glycosyl isoflavone towards new molecular entities against Diabetes and Alzheimer’s disease: generation of lead series and target assessment, PhD grant funded by FCT
- Diagnostic and Drug Discovery Initiative for Alzheimer’s Disease” Industry and Academia Partnerships and Pathways (IAPP); FP7-PEOPLE-2013-IAPP
- PERsonalised ICT supported Service for Independent Living and Active Ageing”, FP7-ICT-2013-10
Highlight

**Salvia sclareaoides** for neurodegenerative disease prevention

*S. sclareaoides* extracts

< potent inhibition of acetylcholinesterase (AChE), the enzyme that hydrolyzes the neurotransmitter acetylcholine

A. P. Rauter et al., *Fitoterapia* 2007, 78, 474

AChE inhibition is a standard therapy to treat patients with Alzheimer’s disease (AD) (e.g. donepezil, rivastigmine, galantamine). A new binding site of AChE for the major component rosmarinic acid (binding site B) was discovered


Rosmarinic acid also interacts with Aβ1-42. Aromatic protons are mostly involved in the binding

A. P. Rauter et al, *Chem Asian J.* 2013, 8, 596

*S. sclareaoides* interacts also with AD toxic oligomers, removes amyloid fibrils to form amorphous aggregates, and prevents normal Prion protein to convert to Prion infectious isoform


Projects:

Diagnostic and Drug Discovery Initiative for Alzheimer's Disease, Industry-Academia Partnerships and Pathways (IAPP), FP7-PEOPLE-2013-IAPP

Study of Salvia species crop production aiming at the evaluation of their constituents for the potential control of Alzheimer's disease, funded by FCT

In collaboration with:
Challenges and solutions for the prevention of frailty

Multimodal service (screening, monitoring and training services) containing nutrition, physical and cognitive modules, supported by an interoperable ICT infrastructure offering intelligent decision support systems and gamification.

The Portuguese team: Nutriageing website

Nutrition literacy

- How much should I eat?
- What type of fat should I choose?
- Is fiber important for a healthy nutritional status?
- How much water do I need to drink?
- Calcium and salt intake, how much?
- How important is antioxidants intake?
- What are functional foods? What is their role in disease prevention?
- How foods and drugs interact?

Videos: Chef is discussing with experts!

Vegetable gardens growing ingredients, condiments.....

Discussing video topics and functional food ingredients with Livia Sarkadi, EuCheMS Executive Board, expert in Food Science

Collaborations:
INSA, Portugal
Auckland University, Australia
Budapest University of Technology and Economics, Hungary
University Milano Bicocca, Italy
Networking within FCUL and CQB groups

Website funding:
IUPAC 2013-054-2-300
The main long-term objective of the Environmental and Biological Mass Spectrometry group is to explore the potentialities of advanced mass spectrometry and spectroscopy in order to investigate at molecular level, the structure, reactivity and energetics of compounds with, mainly, environmental and biological interest.

Advanced mass spectrometry, ‘Hyphenated’, tandem MS, high resolution (FTICR MS) and spectroscopic techniques, applied to environmental, biochemical/biological, conservation and forensic sciences, enable the structural characterization of compounds, even at trace level, and in complex matrices (as for example degradation products of emerging contaminants in the aquatic environment), of particular importance to the elucidation of chemical and biochemical reaction mechanisms and to the development of decontamination processes encompassed in the strategic area entitled Sustainable Chemistry for Functional Molecules and Materials, defined for CQB. These advanced analytical capabilities are also of major importance and a key issue for characterization and properties evaluation of bioactive molecules that can potentially contribute for the development of novel therapeutic agents and medicines and for evaluation of the effectiveness and safety of these molecules.

Theoretical methodologies are also applied as a support for rationalization of molecular ion structure, mechanisms and gas-phase thermochemistry data.

https://www.fc.ul.pt/pt/unidade/grupo-de-espectrometria-de-massa-ambiental-e-biológica
Cardiovascular diseases are among the highest cause of death in EU including Portugal. The high cholesterol level in the blood can be mentioned as being among the main causes of these diseases. The first and most simple action to reduce cholesterol level is to decrease its ingestion in the diet. When this action is not enough, drugs start to be prescribed. Herbal teas, or infusions, used for a wide range of purposes can also be used to diminish cholesterol in the blood. Although these compounds cannot be sold with claims for health benefits, it is well known that they are sold and consumed in order to improve people's health. Functional foods, among which are herbal teas, of natural origin, have been the subject of our studies. In our laboratory we have long been studying “teas” from plant origin, to determine their composition by mass spectrometry techniques and also in what concerns their initial and final biochemical activity after the gastro-intestinal digestion. The results of these studies, besides highlighting the components of those mixtures, which is important for their quality control, also show that the infusions can have beneficial effects to health and can be used, for example, for lowering cholesterol in the bloodstream and to facilitate the digestive process.


Enzymes are the core of life. It is our mission to unravel enzyme function and structure, exploring the exquisite complexity of life through a systems biology approach. Our final goal is to shape the rules of life to our defined purposes such as changing enzyme specificity, rewiring pathways and creating novel functional macromolecular structures.

Our research comprises the role of protein glycation, the glyoxalase pathway and protein-protein interaction networks in transthyretin amyloidosis as well as a systems biology approach to human infectious diseases, namely leishmaniasis and pneumococcal diseases. We are seeking enzymes and pathways towards novel therapeutic opportunities against these human pathogens.

Our tools are a combination of computational methods, mostly implemented through in house designed software, biochemical and molecular biology techniques, as well as advanced analytic tools, including FTICR-MS, enabling research in metabolomics and proteomics. We are continuously improving these tools and expanding the scope of its applications, most notably in the field of mass spectrometry, with the development of native MS, top down proteomics and 2DFTICR-MS.

We spawned and support a biotech start-up, BioMimetx, dedicated to deliver innovative solutions for the control of biological proliferation, most notably, biofouling in marine environments.

http://enzymology.fc.ul.pt/
Our group combines complementary experimental and computational approaches to chemistry and biochemistry.

We develop new organometallic complexes and materials (porous solids, nanoparticles and ionic liquids) to obtain new homogeneous and heterogeneous catalysts, aiming at improving (enantio)selectivity in industrially relevant reactions. We also immobilize bioactive compounds to get new non-leaching bioactive polymeric materials to protect surfaces against biofouling. Functional nanomaterials and devices of magnetic molecules based on spin crossover to provide polymeric, amphiphilic or nanocrystalline environments are being synthesized, as well as materials for electrochemical CO$_2$ reduction. Bioactive natural products are isolated in the quest for new drug leads from Portuguese marine organisms. New psychoactive substances marketed as recreational drugs in Portugal are identified by NMR.

We use Quantum Chemistry to study mechanisms of organometallic reactions, to calculate the properties of molecules and materials in order to improve functionalized materials, and to understand in detail the interactions between bioactive metal complexes and polyoxometalate derivatives with biomolecules and materials. With the help of molecular modeling and simulation, we are interested in the study of the dynamic properties of membranes and proteins, their pH-dependence and relation with disease. Additionally, the modeling of non-conventional bonds (such as halogen bonds) in (bio)chemical systems aiming at drug design is also pursued.

http://intheochem.fc.ul.pt/
Inorganic and Theoretical Chemistry

Experimental Approaches
Computational Studies

Inorganic molecules and materials for energy and magnetism
Antifouling molecules and materials for biofouling prevention
Ionic liquids in biphasic catalysis with molybdenum complexes
The role of hydrophobic interactions in a molecular disease
Mechanisms/properties of transition metal derivatives
Halogen bonding in (bio)chemical systems

Hybrid Materials for selective catalytic processes
Identify new abuse drugs by NMR to prevent health risks
pH effects on membranes and proteins
In silico nanobio solutions for medicine and materials

Carla Nunes
Elisabete Silva
Helena Gaspar
Marta Saraiva
Paulo Martinho

Adrià Gil
Maria José Calhorda
Miguel Machuqueiro
Nuno Galamba
Paulo Costa

The 2000 Nobel Prize was awarded jointly to Alan J. Heeger, Alan G. MacDiarmid and Hideki Shirakawa for the discovery that plastic is able to conduct electricity after being conveniently modified. Since then, researchers and their groups have developed efforts to find new polymeric materials with conducting properties. Our work aimed at the preparation of polymers incorporating metal ions in their polymeric backbone. This modification additionally confers both chemical and morphological properties opening possibilities to fine-tune materials for target applications.
Non-Releasing biocidal coatings: A new strategy for biofouling prevention

Biofouling, a spontaneous colonization of surfaces in contact with water by aquatic organisms, is a global problem in water management systems of several industrial activities, and is responsible for serious environmental and economic consequences. For instance, its accumulation on hulls of ships can lead to drag friction increases up to 40% and subsequent power penalties of up to 86% at cruising speed; when occurring in cooling circuits of power plants, it can lead to efficiency losses of about 5%. The main strategy to combat this biofouling relies on chemical control. However, this strategy has revealed to be harmful for the aquatic ecosystems, mainly owing to the ecotoxicity and cumulative effect of the applied bioactive agents. Therefore, rigid international regulations have been issued (BPD EU Regulation, 2012), and more are expected to come in a near future. New strategies, which can combine more efficiency against biofouling and non-toxic properties for the aquatic systems, are sought.

Our Group developed a new antifouling environmental friendly strategy based on the covalent bonding of biocides in polymeric coatings (e.g. silicone based). This non-releasing biocide strategy evidenced an effective biocide immobilisation, with promising coatings’ antifouling performance, up to 6 months to date, on seawater submerged coated surfaces with biocidal silicone based coatings.

The problem:

Biofouling ON A SHIP HULL

The potential solution:

Biofouling ON A SHIP HULL

Highlight

The problem:

Biofouling ON A SHIP HULL

The potential solution:

Biofouling ON A SHIP HULL


Biofouling ON A SHIP HULL

BIOCORROSION ON A SHIP HULL

With immobilised biocides

Without biocides

6 months of exposure in Atlantic seawater (Peniche, Portugal)
In the last decade, more than 450 new psychoactive substances (NPS) appeared in the market of drugs of abuse. The fast dissemination of these new drugs in the internet created an emerging need for developing new analytical methodologies for their rapid identification. Since May 2014, a team of researchers of FCUL, led by Helena Gaspar, researcher at the Centro de Química e Bioquímica, works in collaboration with the Laboratório de Policia Científica da Polícia Judiciária in the identification and quantification of NPS in products seized by the Portuguese police. Recently, this team has identified, for the first time in Europe, a new synthetic cathinone, 4F-PBP. The results have already been published in the journal Forensic Science International 2015. This outcome highlights the importance of the academia in supporting the resolution of current problems in our society, as the control of NPS’s trade.

The work developed by the group of FCUL consists in the isolation and structural characterization of NPS, by means of NMR spectroscopy and Mass Spectrometry, from products supplied by the LPC, or in their synthesis, allowing not only their toxicological evaluation, but also the supply of NPS standards to forensic laboratories, to be used in routine analyses.

Polylactide (PLA), a biodegradable thermoplastic polyester derived from lactic acid, is a renewable resource, currently attracting attention for applications ranging from biomedical to food packaging and device applications. It is considered a promising alternative to petrochemical-based plastics and the fast growth of its production capacity (150,000 tons/year currently) suggests it will be a high volume commodity material in the near future. In collaboration with an experimental team, we used a computational approach to calculate the energy of all the intermediates and transition states of the full mechanism of the ring opening polymerization (ROP) of lactide catalyzed by a binuclear Zn(II) complex in mild conditions. We identified the determining steps and the cooperative role of the two zinc centers. Indeed, detailed knowledge of the reaction will allow the optimization of the process, namely improving the catalyst (cheaper, more active), and the reaction (environmentally friendlier).
Since the incorporation of cisplatin in chemotherapy, the interest in the application of metal systems in medicine has grown rapidly. One step beyond was the incorporation of phenanthroline (phen) ligand in metal complexes, these systems showing significant antitumoral activity. Within the interactions of coordination complexes with DNA, intercalation is an important binding mode and the intercalative capacity of molecules is influenced by the planarity of ligand, type of donor atom, and metal coordination geometry. Thus the aim of this work was the comprehension and rationalization of the interaction of phen with DNA strands by means of computational techniques. The results showed that intercalation produces important changes of geometric parameters of the base pairs. For the systems containing guanine and cytosine, hydrogen bond interactions are more important than stacking interactions, whereas for the systems with adenine and thymine these stacking interactions become competitive. Moreover, the contribution of dispersion forces is the most important contribution to explain the interaction. Nevertheless, this contribution is necessary but not sufficient to stabilize the Pauli repulsion contribution originating between electrons of different fragments having the same spin. Thus, charge transfer contribution (small) and the electrostatic contribution (more important) play an important role to stabilize the intercalator and compensate Pauli repulsion. In fact, the values of the electrostatic contribution are roughly similar to the values of the interaction energy.

Biological membranes are complex systems that have recently attracted significant scientific interest. Experimental techniques are very limited in measuring the physicochemical processes near membranes. On the other hand, computational methods are very useful since they allow us to study the molecular details of several lipid bilayer disorders, associated with diseases like the Barth syndrome. The presence of many charged lipids, render these membranes sensitive to pH. The protonation states of lipids and the ion distribution close to the bilayer are two of the main challenges in biomolecular simulations of these systems. In this work, we proposed a new method based on the Poisson–Boltzmann equation to estimate the ion concentration near a lipid bilayer that avoids the need for neutrality at the microscopic level. This new methodology allows for an increased realism in our molecular simulations and can have an important contribution in future studies.
Interfacial Electrochemistry

Interfacial Electrochemistry Group research is focused on interfacial phenomena involving high performance modified electrodes and semiconductor nanomaterials, to develop new platforms for (photo)electrocatalytic, energy production, (bio)sensing and protective purposes. This is achieved by a careful and precise combination of materials (conducting polymers, self-assembled monolayers and nanostructures) and preparation methods (electrochemical, chemical coupling/adsorption, modification/sensitization).

In catalysis and sensing is extremely advantageous and challenging to have active centres stably immobilized preserving their identity and function. Association of electrochemical and surface sensitive characterization techniques greatly contributes to elucidate about structure, properties and reactivity relationships. Benefits arise from the use of functionalized electrodes, since reactive entities properties can be tailored and modulated by electric potential application.

Additionally, the materials evaluation in energy production and environmental remediation processes, are studied in the IEG group. Another research line, is the evaluation of the effect of bioactive chemicals and proteins on biomimetic supported lipid bilayers, mainly by high resolution imaging.

http://electro.fc.ul.pt/

Electronically conducting polymers (or conducting plastics) are well known electrochromic materials. They undergo reversible colour modifications according with the electrical potential they are submitted. On the other hand, some metalloporphyrins like the iron-porphyrin - that we can find in hemoglobin – are very sensitive to the presence of oxygen, which induces redox transformations in the molecule. Incorporating the iron porphyrin into a polyaniline (conducting polymer) matrix, resulted in a high sensitive oxygen sensor. In a cooperative work of the Centre of Chemistry and Biochemistry from Ciências and the Chinese Academy of Sciences, a novel oxygen sensor for Biochemical Oxygen Demand assessment with dual transduction was developed. The interaction of the dissolved gas with the porphyrin provokes a spontaneous adjustment of the intrinsic electric potential of the polymer causing the modification of the optical properties of the material. In this way, both the electric signal and the optical response of the polymer reflect to the presence and amount of dissolved oxygen. The optical monitoring of the electrode is performed by TIRIE (Total Internal Reflection Imaging Ellipsometry) which is a technique highly sensitive to changes of the dielectric properties of the samples. The combined electrochemical and optical signals strongly corroborate each other, allowing the normalization of the readings in repetitive measurements using the same modified electrode.
The use of nanocrystalline semiconductors as photocatalysts, on the treatment of industrial wastewaters, has generated great interest, due to their unique physicochemical properties.

In particular this project aims TNTs manipulation by surface sensitization processes, through the synthesis of nanocomposite materials combining titanate nanofibers (TNF) with nanocrystalline ZnS and Bi$_2$S$_3$, in order to obtain nanocomposite materials with new and improved photocatalytic performances. The TNF were produced via hydrothermal synthesis and sensitized with the semiconductor nanoparticles, through a single-source precursor decomposition method. ZnS and Bi$_2$S$_3$ nanoparticles were successfully grown onto the TNF’s surface and Bi$_2$S$_3$–ZnS/TNF nanocomposite materials with different layouts. The samples’ photocatalytic performance was first evaluated through the production of the hydroxyl radical using terephthalic acid as model molecule. All the tested samples show photocatalytic ability for the production of this oxidizing specie, very important in the photodegradation of organic pollutants. Afterwards, the samples were investigated for the removal of methylene blue. Methylene blue is an industrial dye, used often as model pollutant in photocatalytic degradation studies. From the nanomaterials materials studied, the nanocomposites with best adsorption ability were the ZnS/TNF and Bi$_2$S$_3$–ZnS/TNF. The most promising results, for the complete pollutant removal, were obtained considering a sequential combination of an adsorption-photocatalytic degradation process using the Bi$_2$S$_3$ZnS/TNF powder as a highly adsorbent and photocatalyst material.
A platform to study membrane nanodomains and redox processes of bioactive molecules in different lipid environments

Supported lipid bilayers (SLB) are a very useful model system of biological lipid membranes to study membrane-related phenomena, since it allows the use of a great variety of very sensitive surface techniques. In particular, if SLB are prepared on metallic surfaces, electrochemical and optical methods can be employed expanding their applications, namely on biosensing. There has been a great effort in the development of SLB on gold surfaces, though most of the studies only concern single-component or single-phase lipid systems, then failing to mimic the mammalian plasma membrane. This work results from a close collaboration with the Molecular Biophysics group and is focused on the design of planar, continuous and stable multicomponent lipid platforms on gold with distinct phase behavior. Such lipid interfaces enable to detect, with high sensitivity, redox processes of molecules interacting with membranes, such as ubiquinones, flavonoids, and cathecolamine hormones or proteins.

Currently, we are developing lipid-based biointerfaces for immunosensing, which combine a number of important characteristics in a biosensor, namely: biomimetic environment, ability to block nonspecific interaction with serum proteins, a robust arrangement regarding a continuous flow of buffer solutions (even in the presence of surfactant), and high sensitivity.
The main goal of our group is to advance the state-of-the-art of membrane lipid domains, providing means for improved assessment of their involvement in drug mechanisms of action, pointing directions to develop new drugs/drug-formulations.

Biological membranes are organized into (micro)domains consisting of regions with different lipid and protein composition, properties and functions. Furthermore, several pathologies, including cancer and neurodegenerative conditions, are characterized by specific alterations in lipid composition and hence membrane biophysical properties. Moreover, the molecular mechanism of action of many drugs involves at some point their effect on membrane lipid organization (the membrane-lipid therapy principle). Thus, fundamental research on membrane domains in both physiological and pathological situations will take place in parallel with the study of compounds that can potentially promote health and prevent functional decline.

Several molecular biophysical approaches are used to tackle the complex interactions between these agents and biomembranes, proteins and DNA, with potential benefits for society. We use design-and-synthesis approaches to develop new compounds, bio-inspired and from natural origin, namely, essential oils from aromatic and medicinal plants, seeking the valorization of Portugal and CPLP countries natural resources.

In addition, we address the following important topics:
• Development of synthetic receptors for chiral resolution of drugs and for the transmembrane transport of anions.
• Research of natural pesticide for control of insect vectors of human pathogens (e.g. malaria and dengue).

http://bmn.cqb.fc.ul.pt/
Dengue has recurrent epidemics in Latin America and occurred recently in Cape Verde and Madeira Island. The lack of anti-viral treatment or vaccine makes the control of mosquito vectors a high option to prevent virus transmission. The use of plants for insect control has increased worldwide, with particular emphasis on search of essential oils (EOs) obtained by hydrodistillation.

The present study evaluated the potential use of Foeniculum vulgare (fennel) EO in the control of the dengue vector Aedes aegypti. EOs isolated from fennel aerial parts collected in Cape Verde and from a commercial fennel EO of Portugal were analyzed by NMR, GC and GC-MS. trans-Anethole (32 and 30%, respectively), limonene (28 and 18%, respectively) and fenchone (10% in both cases) were the main compounds identified in the EOs isolated from fennel from Cape Verde and Portugal, respectively.

The larvicidal activity of the EOs and its major constituents were evaluated, using WHO procedures, against third instar larvae of Ae. aegypti for 24 h. Pure compounds, such as limonene isomers, were also assayed. The lethal concentrations LC$_{50}$, LC$_{90}$ and LC$_{99}$ were determined by probit analysis using mortality rates of bioassays. A 99% mortality of Ae. aegypti larvae was estimated at 37.1 and 52.4 μL L$^{-1}$ of fennel EOs from Cape Verde and Portugal, respectively. Bioassays showed that fennel EOs from both countries displayed strong larvicidal effect against Ae. aegypti, the Cape Verde EO being as active as one of its major constituents, (-)-limonene.

These results suggest the potential application of fennel EO as a possible natural larvicidal for the control of the major dengue mosquito vector.
Biological membranes are generally believed to exist in a fluid regime, where a liquid disordered (ld) phase with low lipid packing and fast lateral diffusion of molecules coexists with a liquid ordered (lo) one displaying higher lipid packing and slightly slower lateral diffusion.

In recent years, however, our studies have challenged the dogma that another lipid phase, the gel or solid ordered phase, is not physiologically relevant, due to the very slow lateral diffusion of its components. We have proved that gel domains are present in the plasma membrane of growing yeast cells through the use of fluorescent probes that exhibit different fluorescence parameters in each lipid phase [1]. This finding is now supported by independent studies in other laboratories.

More recently, in an attempt to understand the formation and properties of gel domains in biomembranes, we undertook a series of experiments using a common glycerophosphospholipid, the phosphatidylcholine (POPC) and phytoceramide, the backbone of the complex sphingolipids found in plants and fungi, also present in several human tissues such as skin [2]. Our findings using fluorescent probes and liposome suspensions pointed to the formation of POPC : phytoceramide stoichiometric complexes (with stoichiometries 3:1 and 1:2) that display unique biophysical properties [2]. Experiments using atomic force microscopy in supported lipid bilayers, confocal fluorescence microscopy in giant liposomes and X-ray scattering in multibilayers corroborated the supramolecular organization of the lipids into complexes. Interestingly, the fluorescent parameters (anisotropy and lifetimes), exhibited by fluorescent probes in liposome suspensions [2] were identical to the ones obtained for living yeast cells [1], which show that the gel domains identified in vivo may share important properties with the stoichiometric complexes formed in the POPC/phytoceramide mixtures.
Recently, our group has contributed with a hypothesis/theory paper, proposing a model “whereby seeds comprised of oligomerised proteins and/or lipids would serve as crystal nucleation centers for the formation of diverse gel/crystalline nanodomains”, the nanodocks model [3]. Moreover, we presented a book chapter, where the literature reports pointing for the formation of highly ordered lipid domains in vivo was critically reviewed [4]. The relevance that ordered domains may play in the organization and function of biomembranes, and their implication in drug modes of action, and antidrug mechanisms of resistance, both in infectious agents and in cancer cells, were discussed.


Molecular Energetics

Understanding the relationships between thermochemical information and the structure and dynamics of molecules and complex molecular systems (e.g. crystals, living cells) is the main long-term objective of the Molecular Energetics group.

The thermodynamic stability of molecules, as measured by standard enthalpies of formation and “bond strengths”, can, for example, be rationalized by investigating the relationships between those properties and bond lengths and angles, steric and electronic parameters, activation energies, etc.

The energetics of intermolecular interactions regulates phenomena such as the dissolution of a solute in a solvent and the structural organization of molecules in crystals. By probing these interactions it is possible, for example, to understand many aspects of polymorphism occurrence and to elucidate the role of solvents in chemical reactivity. Monitoring the production of heat by living organisms can also provide important clues about their adaptation to environmental changes.

The research carried out at the Molecular Energetics group relies on a variety of experimental techniques, such as X-ray diffraction, microscopy, reaction and combustion calorimetry, Calvet-drop microcalorimetry, flow-calorimetry, time-resolved photoacoustic calorimetry, differential scanning calorimetry, thermogravimetry, crystallization reactors, and Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR-MS), along with quantum chemical methods and molecular dynamics simulations. The group has a long tradition in instrument building and database development.

http://molenergetics.fc.ul.pt/
One of the most interesting features of nanomaterials is the change in properties that normally accompanies a decrease in particle size. Using calorimetric experiments and atom-atom pair potential calculations, we were able to show, for the first time, that the stability of sodium chloride, the most abundant salt on earth, considerably decreases (>30%) with the decrease of the crystal size up to the single molecule dimension. The decrease is particularly steep for crystal sizes below ~100 nm. The results further suggested that the cohesive energy within each crystal layer varies from site to site, with the energy differences between adjacent sites decreasing on moving from the periphery to the centre of the crystal. As expected, the atoms at the outmost surface layer exhibit the lowest cohesive energies.
Cubane is a unique molecule for its extraordinary C8 cage, where all the sp3 hybridized carbon atoms have C–C–C bonds angles of 90°. It is therefore one of the most strained compounds known and, until its synthesis in 1964, there was doubt that such a molecule could even hold together. But cubane turned out to be a surprisingly stable molecule, since no kinetically viable paths exist for its thermal decomposition. The synthesis of cubane was driven by the curiosity and fascination of organic chemists in obtaining the molecular equivalent of a platonic solid. Nevertheless, its derivatives have many important potential applications, such as in high-energy fuels, explosives and propellants (e.g., octanitrocubane), and as an intermediates in pharmaceutical preparations. Because the cubane frame is rigid, substituents will have precise spatial relationships to each another. This offers fascinating substituent positioning possibilities for the synthesis of novel pharmaceuticals. To assess viable synthetic pathways, knowledge on the energetics of the cubane molecule and its reactive intermediates is needed. In general, this kinetic modeling requires “chemical accuracy” of about ±4 kJ mol⁻¹. We used high-accuracy state of the art computational methods to determine the enthalpies of formation of cubane and related compounds.
The Redox Biology group research focuses on hydrogen peroxide (H$_2$O$_2$), the main cellular oxidant now considered a key redox regulator. The long-term goal is to understand signalling pathways and molecular mechanisms by which H$_2$O$_2$ regulates physiological processes that, when unbalanced, lead to disease.

H$_2$O$_2$, is continuously produced intracellularly, as a by-product of aerobic metabolism, and extracellularly as a result of phagocyte activation. Our group uses an interdisciplinary approach, as the team is composed of people with a strong background in molecular biology, free radical biochemistry, cell biology and mathematical modeling, with a combination of both experimental and mathematical modelling approaches to study cellular redox regulation by hydrogen peroxide and its involvement in physiological cellular processes and in disease.

The group expects to establish quantitative and cause/effect relationships between H$_2$O$_2$ levels and regulation of gene expression, organelle dynamics and disease. These studies will allow to identify molecular targets of H$_2$O$_2$ with possible therapeutic use in diseases, such as cancer and inflammation, and in aging.

In addition, we aim at assessing the biological effects of emerging contaminants at sub-lethal concentrations. Our efforts will be focused on the biological adaptation induced by contaminants. For that we will use our know-how on H$_2$O$_2$ adaptation acquired over the last decade.

http://redox.fc.ul.pt/
Hydrogen peroxide (H₂O₂), a reactive oxygen species (ROS), is a ubiquitous oxidant present in all aerobic organisms. Since its first identification in a living cell, H₂O₂ was considered a toxic by-product of aerobic metabolism, something that cells had to remove. If H₂O₂ detoxification catalyzed by catalases and peroxidases was not adequate, H₂O₂ would diffuse and oxidize biological targets causing cellular malfunctions, i.e. oxidative stress, responsible for several pathologies and aging. Starting in the 90s this paradigm of hydrogen peroxide as toxic started to change to a paradigm where hydrogen peroxide acts in cellular regulation and is involved in cellular signalling – redox signalling – through the oxidation of thiols in proteins that act as redox sensors. Nowadays, redox biology is an established field and the essential regulating role played by H₂O₂ in vivo with important implications in health and disease is unquestionable. In this work it was shown that the complexity of redox regulation increases along the phylogenetic tree and that H₂O₂ modulates gene expression at all steps from transcription to protein synthesis. Also, some of the unanswered questions regarding our understanding of redox-dependent regulation of gene expression were addressed:

- What makes a good H₂O₂ sensor?
- What are the common chemical and kinetic principles that govern H₂O₂ signaling?
- Is it possible to obtain an integrative view of H₂O₂ regulation of transcription factors?
The Separation Science & Technology (SS&T) group is composed by two research laboratories, namely, the Chromatography & Capillary Electrophoresis Lab. and the Hydrometallurgical Separations Lab. The common goal of our group is the development of new approaches to implement chemical separation techniques. The research work carried out by our group is based on two different research lines:

- The Chromatography and Capillary Electrophoresis line involved on the development of new analytical methodologies to monitor trace levels of several classes of emergent compounds (e.g. EDC’s, PPCP’s, POP’s, DBP’s, etc.) from many type of priority matrices. Most of our analytical work has been focused on the implementation of novel sorption-based microextraction methodologies in combination with modern instrumental systems, in particular as analytical alternatives to monitor environmental, pharmaceutical, food, forensic and biological samples.

- The Hydrometallurgical Separations line focuses research on the development and characterization of new functional organic molecules to efficiently and selectively recover metal species from feed industrial complex aqueous solutions, and / or effluents. One of the aims is to contribute to the decontamination of the environment, through innovative processes for the hydrometallurgical recycling of end-of-life materials, and profiting from the economic value several metals in industrial wastes have.

http://sepscitech.fc.ul.pt/
The main goal of the Solid State Chemistry group is related to the preparation and characterization of environmental / energy / biocompatible materials with high economic and social benefit. Solid State Chemistry Group interests are focused on functional inorganic materials, namely binary and ternary oxides. These materials can be designed, tailoring its properties and improving its functionality through solid state chemistry, solution chemistry, hydrothermal and/or electrochemical synthesis routes.

Applications of these materials include:

**Environment protection** – Development of new catalysts for toxic pollutants and pharmaceutical drugs degradation, by means of photocatalysis or photoelectrocatalysis processes. The group combines different materials composition with specific methods of synthesis to design the catalyst surface, which is crucial to improve the catalytic activity.

**Energy conversion** – The manufacture and improvement of photoanodes for dye-sensitised solar cells (DSSC) is an area where the SSC group has been working. The main objective of our work is the enlargement of metal oxide based nanostructures that maximize the electron transport, enhancing the power conversion efficiencies of the DSSC device, using low-cost and soft processing methods.

**Biomedicine** – One of the biomedical applications of magnetic iron oxide nanoparticles is magnetic hyperthermia for cancer therapy, a technique which allows to destroy cancer cells, also increasing the efficiency of chemo- or radiotherapy. Our group is particularly interested in the development of new biocompatible materials with magnetic properties suitable to make them good candidates for magnetic hyperthermia for cancer therapy.

http://ssc.ciencias.ulisboa.pt/
Highlight

New materials for wastewater treatment


The removal of organic pollutants and pharmaceutical drugs from wastewater is currently one of the major concerns in environmental control. In order to address these problems, considerable efforts have been devoted to develop techniques more effective than the conventional processes to eliminate these pollutants.

Removal of organic pollutants:
For the first time the growth of immobilized CaMn$_3$O$_6$ nanorods (NRs) by RF magnetron sputtering onto quartz glass substrates was carried out. It was found that the immobilized CaMn$_3$O$_6$ NRs exhibit much higher photocatalytic activity than the TiO$_2$ films on the degradation of Rh6G under visible light irradiation. This study further revealed that the high catalytic efficiency of CaMn$_3$O$_6$ NRs probably arises as a result of the complex interaction between the double chains of edge-shared MnO$_6$ octahedra, the mixture between Mn$^{3+}$ and Mn$^{4+}$, and/or the higher surface-to-volume ratio (surface morphology) afforded by the nanorods geometry, together with a process of dye self-sensitization. Furthermore, it is reported here the importance of this new nanostructured material in obtaining active visible-light photocatalysts.

Pharmaceutical drugs degradation:
Photoactive annealed Ti/Zn-TiO$_2$ electrodes were successfully prepared and used for the first time on the photoelectrochemical degradation of Ibuprofen. We demonstrated that Ibuprofen was efficiently degraded probably due to high area of the films, as a consequence of their morphology: ZnO needle-shaped grains.
Tailoring one-dimensional nanostructured metal oxides and their application in energy conversion technology

**Highlight**

The general use of solar energy harvesting is still limited by two significant challenges, conversion efficiency and cost. Among novel PV technologies, the highest efficiency was attained, up to now, with solid-state perovskite solar cells (PSC) with an overall efficiency of 20%.

The manufacture and improvement of electron-transporting materials for PSC is an important subject which has been developed in recent years by our group, contributing to the progress of new technologies for applications in energy conversion.

Our principal aim is to develop metal oxides based nanostructures that maximize the electron transport, enhancing the power conversion efficiencies of the solar cells device, using low-cost and soft processing methods, combining electrochemical-chemical deposition routes.

This work is developed in straight collaboration with DEGGE/FCUL, CEFITEC/FCT/UNL and CIDETEC.


Synthesis of magnetic nanoparticles for magnetic hyperthermia

Hyperthermia studies of ferrite nanoparticles synthesized in the presence of cotton

Magnetic hyperthermia therapy can be a valuable aid in cancer treatment, with less harmful side effects to the patient. It relies on the heat released by magnetic nanoparticles under the influence of an alternate magnetic field. Magnetite \((\text{Fe}_3\text{O}_4)\) and maghemite \((\gamma\text{-Fe}_2\text{O}_3)\) are by far the most explored nanoparticles for hyperthermia applications, but other ferrites, nanocomposites and core@shell structures are also being investigated, in order to improve their ability to act as nano-heaters, making them useful for magnetic hyperthermia.

The Solid State Group from CQB, working in straight collaboration with BiolISI - Biosystems and Integrative Sciences Institute, has been especially involved in the search of new synthesis and processing methods that can improve the magnetic properties of the nanoparticles. We intend to pursue this route since, in spite of the large efforts deployed by various research groups, the thermal efficiency of biocompatible nanoparticles have not yet reached the threshold required to allow regular efficient clinical use of magnetic hyperthermia.
The major long term goal of the Structure and Reactivity group (SRG) is the development of rigorous and well-validated quantitative structure-property/activity relationships (QSPR/QSAR) to interpret and predict biological and physicochemical phenomena, as well as to assist in the design, synthesis and assessment of new molecules.

The group’s expertise in structural characterization of either newly synthesized molecules (designed on the basis of various QSAR methodologies) or of isolated compounds from natural sources (e.g., marine invertebrates from Portuguese exclusive waters), has also been focused on the evaluation of antimicrobial activities, in particular antitubercular activities against wild and resistant strains, or on the identification of new leads to target cancer and Central Nervous System disorders (e.g., IDO, β-amyloid and TAU proteins), within the scope of several collaborations.

Also central to the group’s work is the structural and physicochemical characterization of conventional and/or non-conventional solvents and their mixtures, for solvent tuning in dynamic and equilibrium processes, in view of greener future applications in synthetic, separation and/or CO₂ capture processes.

SRG integrates researchers with diverse backgrounds and skills ranging from Physical to Organic Chemistry. It has a consolidated know-how in spectroscopic characterization, in the study of solute and solvent effects and in the accurate evaluation of kinetic, thermodynamic, interfacial and solvatochromic properties, as well as in the use of statistical and machine learning techniques such as Multiple Linear Regressions and Neural Networks.

http://structreact.fc.ul.pt/
Isoniazid (INH) is still one of the two most effective antitubercular drugs and is included in all recommended multitherapeutic regimens. Because of the increasing resistance of Mycobacterium tuberculosis to INH, new INH-based compounds have been proposed to circumvent this problem. The KatG enzyme is known to activate INH, leading to a potent antitubercular drug. The S315T enzyme mutant is very common and interferes with this “drug production” process. In this work, we present a detailed comparative molecular study of the interactions between the normal enzyme or its S315T mutant form and either INH or INH-C10, a new acylated INH derivative. Our results indicate that the aliphatic tail in INH-C10 brings the compound closer to the active site. INH-C10 is able to counterbalance most of the conformational restrictions introduced by the mutation, which are thought to be responsible for the decrease in INH activity in the mutated strain. Therefore, INH-C10 appears to be a very promising lead compound and a new hope against tuberculosis.
2015 PUBLICATIONS
**Publications**

**Thermochemistry of 1-alkylimidazoles**  
J. Vitorino, F. Agapito. C. E. S. Bernardes, M. E. Minas da Piedade  
J. Chem. Thermodyn., 2015, 80, 59-64. IF: 2.679, Q1

**Size Matters: An Experimental and Computational Study of the Influence of Particle Size on the Lattice Energy of NaCl**  
S. Range, C. E. S. Bernardes, R. G. Simões, M. Eppl, M. E. Minas da Piedade  
J. Phys. Chem. C 2015, 119, 4387-4396. IF: 4.772, Q1

**Gas Phase Affinity Scales for Typical Ionic Liquid Moeities by Cooks Kinetic Method**  
J. Vitorino, J. P. Leal, M. E. Minas da Piedade  

**Benchmark Thermodynamic Properties of Methyleneisoles: Experimental and Theoretical Study**  
V. N. Emel’yanenko, K. V. Zaitseva, F. Agapito, J. A. Martinho Simões, S. P. Verevkin  
J. Chem. Thermodyn., 2015, 88, 155-162. IF: 2.679, Q1

**The Thermochromy of Cubane 50 Years After Its Synthesis: A High-Level Theoretical Study of Cubane and Its Derivatives**  
F. Agapito, R. C. Santos, R. M. Borges dos Santos, J. A. Martinho Simões,  

**Evaluation of the OPLS-AA Force Field for the Study of Structural and Energetic Aspects of Molecular Organic Materials**  
C. E. S. Bernardes, A. Joseph  

**Kinetics and Mechanism of the Thermal Dehydration of a Robust and Yet Metastable Hemihydrate of 4-Hydroxyisonicotinic Acid**  
A. Joseph, C. E. S. Bernardes, A. S. Viana, M. F. M. Piedade, M. E. Minas da Piedade  

**Benchmark Thermochromy of Methylbenzonitriles: Experimental and Theoretical Study**  
K.V. Zaitseva, V.N. Emel’yanenko, F. Agapito, A.A. Pimerzin, M.A. Varfolomeev, S.P. Verevkin  
J. Chem. Thermodyn., 2015, 91, 186-193. IF: 2.679, Q1

**Assessment and comparison of the properties of biodiesel synthesized from three different wet microalgae biomass**  
J. Appl. Physiol. (in press). IF: 2.559, Q1

**Molecular details of INH-C10 binding to wt KatG and to its S315T mutant**  
V. H. Teixeira, C. Ventura, R. Leitão, C. Ráfols, E. Bosch, F. Martins, and M. Machuqueiro  
Mol. Pharm., 2015, 12, 898–909. IF: 4.384, Q1

**Constant-pH molecular dynamics study of kyotorphin in an explicit bilayer**  
P. R. Magalhães, M. Machuqueiro, A. M. Baptista  

**Constant-pH MD simulations of an oleic acid bilayer**  
D. Vila-Viçosa, V. H. Teixeira, A. M. Baptista, M. Machuqueiro  

**Raising awareness of new psychoactive substances: chemical analysis and in vitro toxicity screening of “legal high” packages containing synthetic cathinones**  
A. M. Araújo, M. J. Valente, M. Carvalho, D. D. Silva, H. Gaspar, F. Carvalho, M. L. Bastos, P. G. Pinho  
Arch. Toxicol., 2015, 89, 757–771. IF: 5.980, Q1

**Determination of mitragynine in urine matrices by bar adsorptive microextraction and HPLC analysis**  
N. R. Neng, S. M. Ahmad, H. Gaspar, J. M. F. Nogueira  
Talanta, 2015, 144, 105–109., IF: 3.545, Q1

**The antimicrobial activity of heterotrophic bacteria isolated from the marine sponge Erylus deficiens (Astrophorida, Geodiidae)**  
Front Microbiol., 2015, 6, article 389, 1–14. IF: 3.989, Q1

**4F-PPB (‘4-fluoro-α-pyrrolidinobutylphenehol), a new substance of abuse: structural characterization and purity NMR profiling**  

**Pore size matters! Helical heterogeneous catalysts in olefin oxidation**  

**Molybdenum(II) catalyst precursors in olefin oxidation reactions**  
C.D. Nunes, M. J. Calhorda  
This article belongs to a special issue: Advances in Transition Metal Catalysis, Edited by Maurizio Peruzzini and Maria Caporali

**Vanadyl cationic complexes as catalysts in olefin oxidation**  
Dalton Trans. 2015, 44, 5152–5158. IF: 4.197 Q1

**How the Intercalation of Phenanthroline Affects the Structure, Energetics and Bond Properties of DNA Base Pairs. Theoretical Study Applied to Adenine-Thymine and Guanine-Cytosine Tetramers**  
A.Gil, V. Branchadell, M.J. Calhorda  

**Fe(III) SalEen derived Schiff base complexes as potential contrast agents**  
B. P. Cardoso, A. I. Vicente, J. B. J Ward, P. J. Sebastião, F. V. Chávez, S. Barroso, A. Carvalho, S. J. Keely, P. N. Martinho, M. J. Calhorda  

**Asymmetric Binuclear Ni(II) and Cu(II) Schiff Base Metallopolymers**  
S. Realista, A. S. Viana, B. P. Cardoso, A. M. Botelho do Rego, P. D. Vaz, A. I. Melato, P. N. Martinho, M. J. Calhorda  
RSC Adv., 2015, 5, 39495–39504. IF: 3.840, Q1

**Catalytic activity of Mo(II) complexes in homogeneous and heterogeneous conditions**  
M. V. Dias, M. S. Saraiva, P. Ferreira, and M. J. Calhorda  
Organometallics, 2015, 34, 1465–1478. IF: 4.126, Q1
Comparing spectroscopic and electrochemical properties of complexes of type \( [\text{Cp}^*\text{Mn}(\text{3-CHS})(\text{CO})_2] \) \( \text{Cp}^* = \text{Cp}, \text{Ind}, \text{Flu}; \text{M} = \text{Mo}, W \): a complementary experimental and DFT study
J. Organomet. Chem., 2015, 792, 154-166. IF: 2.173, Q1

Luminescent Di- and Trinuclear Boron Complexes Based on Aromatic Iminopyrrolyl Spacer Ligands: Synthesis, Characterization and Application in OLEDs

Synthesis and Reactivity of Taddol-Based Chiral Fe(ii) PNp Pincer Complexes - Solution Equilibria between \( x_2 \text{P,N}^\text{and x3} \text{P,N,P} \)-Bond PNp Pincer Ligands
C. Holzracker, B. Stöger, M. D. Carvalho, L. P. Ferreira, E.Pittenauer, G. Allmaier, L. F. Veirós, S. Realista, A. Gil, M. J. Calhorda, D. Müller, K. Kirchner
Dalton Trans., 2015, 44, 13071–13086. IF: 4.197 Q1

Preference for sulfoxide S- or O-bonding to 3d transition metals – DFT insights
B.P. Cardoso, B. Royo, M. J. Calhorda
J. Organomet. Chem., 2015, 792, 167-176. IF: 2.173, Q1

Highly selective and recyclable MoO₃ nanoparticles in epoxidation catalysis
C. I. Fernandes, P. D. Vaz, C. D. Nunes
Appl. Catal. A: Gen., 2015, in press. IF: 3.942, Q1

MoO₃ nanoparticles as highly efficient olefin epoxidation catalysts
A.Bento, A. Sanches, E. Medina, C. D. Nunes, P. D. Vaz

L-Histidine Based Organoclays for the Storage and Release of Therapeutic Nitric Oxide
A. C. Fernandes, M. L. Pinto, F.Antunes, J. Pires

Understanding Gas Adsorption Selectivity in IRMOF-8 Using Molecular Simulation
R.S. Pillai, M. L. Pinto, J. Pires, M. Jorge, J. R. B. Gomes
ACS Appl. Mater. Interfaces, 2015, 7, 624-637. IF: 6.723, Q1

Simple Analysis of Historical Lime Mortars
J. Pires

Adsorption of a Textile Dye on Commercial Activated Carbon: A Simple Experiment to Explore the Role of the Surface Chemistry and Ionic Strength
A. Martins, N. Nunes

Sustainable activated Carbons prepared from a Sucrose derived Hydrochar: Remarkable Adsorbents for Pharmaceutical Compounds
A.S. Mestre, E. Tyszko, M.A. Andrade, M. Galheta, C. Freire, A.P. Carvalho
RSC Adv., 2015, 5, 19696-19707. IF: 3.84, Q1

New antitumor 6-chloropurine nucleosides inducing apoptosis and G2/M cell cycle arrest
S. Schwarz, B. Siewert, R. Csuk, A. P. Rauter,

Self-organizing Behaviour of Glycosteroidal Bolaphiles: Insights into Lipidic Microsegregation
R. Xu, F. A. Ii-Rachedi, N. M. Xavier, S. Chambert, F. Ferkous, Y. Queeneau, S. J. Cowling, E. J. Davis, J. W. Goodby,

Improved potentiometric and optic sensitivity of polyaniline film to dissolved oxygen by incorporating iron-porphyrin

Biotecnologically obtained nanocomposites: A practical application for Photodegradation of Safranin-T under UV-Vis and solar light
J.P. Costa, A.V. Girão, O.C. Monteiro, T. Trindade, M.C. Costa

M. Santos, S. Carvalho, I. Marques, C. Moiteiro, V. Félix
Org. Biomol. Chem., 2015, 13, 3070-3085. IF: 3.562, Q1

Superoxide dismutase enzymesomes: carrier capacity optimization, in vivo behaviour and therapeutic activity

Electrochemical behaviour of a Cobalt-Chromium-Molybdenum dental alloy in artificial saliva: Influence of phosphate ions and mucin components
A.Gomes, S.R. de Aguiar, M. Nicolai, M. Almeida

Non-destructive analysis of Portuguese "dinheiros" using XRF overcoming patina constraints
S. Pessanha, M.Costa, M.I.Oliveira, M. E. M. Jorge, M.L. Carvalho
Appl Phys A-Mater, 119, 1173-1178. IF: 1.704, Q2

Use of quantitative structure–property relationships to study the solvation process of 18-crown-6
Thermochim Acta, 2015, 604, 140-144. IF: 2.184, Q2

Novel insights for permeant lead structures through in vitro skin diffusion assays of Prunus lusitanica L., the Portugal Laurel
M.C. Costa, P. Duarte, N.R. Neng, J.M.F. Nogueira, F. Costa, C. Rosado
Thermodynamic Study of Aqueous 2-(Isopropylamino)ethanol. A Sterically Hindered New Amine Absorbent for CO2 capture

Activity Coefficients in the Surface Phase of Liquid Mixtures

Trends in the Hydrogen Activation and Storage by Adsorbed 3D Transition Metal Atoms onto Graphene and Nanotube Surfaces: A DFT Study and Molecular Orbital Analysis

Nematotoxic and phytotoxic activity of Satureja Montana and Ruta graveolens essential oils on Pinus pinaster shoot cultures an P. pinaster with Bursaphelenchus xylophilus in vitro co-cultures.

larvicidal Activity Against Aedes aegypti of Foeniculum vulgare Essential Oils from Portugal and Cape Verde

Transthyretin Amyloidosis: Chaperone Concentration Changes and Increased Proteolysis in the Pathway to Disease

Re(I) and Tc(I) Complexes for Targeting Nitric Oxide Synthase: Influence of the Chelator in the Affinity for the Enzyme

Reversible lysine modification on proteins by using functionalized boronic acids
P.M. Cal, R.F.Frade, C. Cordeiro, P.M. Gois Chemistry, 2015 May 26;21(22):8182-7. IF:5.731 Q1

Effect of the irradiation wavelength on the performance of nanoporous carbon as an additive of TiO2

The influence of the textural properties of activated carbons on acetaminophen adsorption at different temperatures

Design, synthesis and bioevaluation of tacrine hybrids with cinnamate and cinnamylidene acetate derivatives as potential anti-Alzheimer drugs.

Electrochemical oxidation of paraquat in neutral medium

Spin transition in arrays of gold nanoparticles and spin crossover molecules

Formation and properties of membrane ordered domains by phytoceramide: role of sphingoid base hydroxylation

The extracellular matrix modulates H2O2 degradation and redox signaling in endothelial cells.

Energetic characterization of the system (water + 1-propoxypropan-2-ol) at T = 298.15 K

Alkaline hydrolysis of tertiary N-([2-pyridy])carbamates. Contradictory evidence between nucleophilic and general base catalysis
D. Silva, F. Norberto, S. Santos, P. Hervés React Kinet Mech Cat 2015, 115, 421–430. IF: 1.17 Q3

Hyperthermia studies of ferrite nanoparticles synthesized in the presence of cotton

Validation of the Steinrath Index Predictions for the Degree of Soil Aggressiveness Toward Copper Corrosion in Soils Contaminated with Chlorides

Development of tertiary thioamide derivatives to recover palladium(II) from simulated complex chloride solutions
O. Ortet, A.P. Paiva Hydrometallurgy, 2015, 151, 33–51. IF: 1.933, Q1

New Strategy to prevent adhesion of Biofouling to Coatings

Friction reduction on recent non-releasing biocidal coatings by a newly designed friction test rig

Publications
Publications

Stir-bar Sorptive Extraction: 15 years making sample preparation more environment-friendly
J.M.F. Nogueira

Unravelling the antioxidant potential and the phenolic composition of different anatomical organs of the marine halophyte Limonium algarvense

Application of Bar Adsorptive Microextraction-Large-Volume Injection-Gas Chromatography-Mass Spectrometric Method for the Determination of Trace Levels of Agrochemicals in Real Matrices
J.R. Bernarda, S.M. Ahmad, C. Almeida, N.R. Neng, J.M.F. Nogueira

Biological Activities and Chemical Composition of Methanolic Extracts of Selected Autochthonous Microalgae Strains from the Red Sea
Mar Drugs, 2015, 13(6), 3531-3549. IF: 2.853 Q2

Determination of mitragynine in urine matrices by bar adsorptive microextraction
N.R. Neng, S.M. Ahmad, H. Gaspar, J.M.F. Nogueira
Talanta, 2015, 144, 105-109. IF: 3.545 Q1

Determination of Steroid Sex Hormones in Real Matrices by Bar Adsorptive Microextraction (BAμE)
C. Almeida, J.M.F. Nogueira
Talanta, 2015, 136, 145-154. IF: 3.545 Q1

Synthesis of titanate nanofibers co-sensitized with ZnS and Bi253 nanocrystallities and their application on pollutants removal

Recovery of palladium(II) from a spent automobile catalyst leaching solution

Biomembrane Organization and Function: The Decisive Role of Ordered Lipid Domains
J.T. Marqués, C. A. C. Antunes, F. C. Santos, R. F. M. de Almeida

Glycal Transformation into 2-Deoxy Glycosides
C. Dias, A. Martins, M. S. Santos, A. P. Rauter, M. Malik

Hierarchical Zeolites: Preparation, Properties and Catalytic Applications
A. P. Carvalho, N. Nunes, A. Martins

Potential of Mentha pulegium for mosquito control
D. Rocha, M. Novo, O. Matos, A. C. Figueiredo, M. Delgado, M. D. Cabral, M. Liberato, C. Moiteiro
Revista de Ciências Agrárias, 2015, 38, 157-167

Zeólitos hierárquicos: de curiosidade laboratorial à próxima geração de catalisadores industriais
A. Martins, N. Nunes, A.P. Carvalho
Ingenium, 2015, Maio/Junho, 90-93

Liquid-Liquid Extraction of Palladium(II) from Chloride Media by N,N’-Dimethyl-N,N’-Dicyclohexylthiodiglycolamide
O. Ortet, A.P. Paiva
Separation and Purification Technology, October 2015 (accepted)

Environmental application of Ti/TiO2 anodes prepared by DC-magnetron sputtering: degradation of acid orange 7
S. Sério, L.C. Silva, M. E. Melo Jorge, S. Ferreira, L.Cirilaco, M. J. Pacheco, A.Lopes
Environmental Engineering and Management Journal (accepted)

Anchoring of gold nanoparticles on graphene oxide and noncovalent interactions with porphyrinoids
S. M. Andrade, C. J. Bueno-Alejo, V. V. Serra, J. M.M. Rodrigues, M. G.P.M.S. Neves, A. S. Viana, S. M.B. Costa,
ChemNanoMat, (accepted)

Complex internal rearrangement processes triggered by electron transfer to acetic acid
Journal of Physics: Conference Series (accepted)
Equipment

FTICR-MS

Stopped-Flow with absorption and fluorescence detection

Imaging Ellipsometer

Multimode Atomic Force Microscope
Steady-state and time-resolved spectrofluorimeter with polarization modes and double grating monochromators

Scanning Electrochemical Microscopy

NMR spectrometer*

*DQB equipment

FTIR
Equipment

Probe Beam Deflection

Conventional Ellipsometer

Electrochemical Quartz Crystal Microbalance

Surface Plasmon Resonance

Photocurrent Spectroscopy

Contact Angle Goniometer
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