Centro de Química e Bioquímica (CQB) has aimed at developing internationally competitive science, particularly at the frontier of chemistry and biochemistry, since its foundation in 2001. The multidisciplinary teams working in the experimental and theoretical labs within CQB involve approximately seventy PhD members and around one hundred collaborators, most of them PhD, Master and undergraduate 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, COST, other exchange and bilateral programs, and projects).

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. We try to make society aware of our research and its benefits through outreach activities and patents. Taking advantage of the consolidated skills of its members, CQB research is organized in two thematic lines, which are aligned with the Societal Challenges defined in Horizon 2020 EU and the priorities for the regional development of the Lisbon area:

Chemistry and Biochemistry for a Clean Environment

Human Health: Molecular Interventions and Regulation Mechanisms

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

Lisbon, May 28, 2017

Maria José Calhorda

Photo: CQB day – June 2016
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 Municipalities and Society
Who are we?

67 Members
- Pos-doc 34%
- University Staff 55%
- Investigador FCT 11%

130 Collaborators
- Students 68%
- PhD collaborators 23%
- Volunteers 9%

Members
- Male: 27
- Female: 40

Collaborators
- Male: 76
- Female: 54
Who we are?

12 Research Groups

Groups network

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
CQB Indicators

In 2016, publications included

- 29% with international collaborations
- 29% with internal collaborations
- 11% in Top 5% journals
- 28% in Top 10% journals
- 68% in Top 25% journals

In 2017

- 56 papers in International peer reviewed journals
- 8 Book Chapters

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521 Papers 2012-2016  
~ 104 / year

- Hundreds of oral & poster presentations in international conferences each year
- Organization of national and international conferences
CQB funding 2014-2016

CQB funding $\approx 5\,600\,K\€$
CQB projects

2016/2017 ongoing

• D3I4AD, A.P. Rauter, 2014-2018, project funding 399 592€, EC

• Multifunctional luminescent spin labile hybrid materials, P.N. Martinho, M.J. CALHORDA, M.D. Carvalho, 2016-2019, project funding 191 879€, FCT

• Novel nanostructured electrodes towards optimal biosensing, A.S. Viana, J. Correia, M.D. Carvalho, O. Monteiro, R. Almeida, 2016-2019, project funding 184 032€, FCT

• Life-impetus: improving current barriers for controlling pharmaceutical compounds in urban wastewater treatment plants, A.P. Carvalho, 2016-2019, project funding, 34 766€, EC

• Sphingolipid organization in the plasma membrane of saccharomyces, R.F.M. de Almeida, A.S. Viana, S. Marinho, H. Soares, 2016-2019, project funding 189 811€, FCT

• CpHMD-L simulations of pHLIP peptides: design of new tumor-targeted drug delivery systems, M. Machuqueiro, M.J. Calhorda, D. Vila-Viçosa, 2016-2019, project funding 185 088€, FCT

• Anion transmembrane transport promoted by drug-like molecules: building a library of anion carriers inspired in ataluren (PTC124), C. Moiteiro, 2016-2019, project funding 99 897€, FCT/COMPETE

• Overcoming environmental problems associated with antifouling agents: synthesis of nature inspired nontoxic biocides and immobilization in polymeric coatings, E. Silva, M. J. Calhorda, 2016-2019, project funding 52 352€, FCT/COMPETE

• Integração de marcas naturais e artificiais para resconstruir migrações de peixes e alterações ortogénicas de nicho, M. Sousa Silva, 2016-2019, project funding 17 400€, FCT
CQB projects

2016/2017 ongoing

- **PCCPRemoval**, O. Monteiro, 2015-2018, project funding 50 000€, iFCT
- **NANOBIOSENSE**, A.S. Viana, 2014-2019, project funding 50 000€, iFCT
- **Synthesis of Nucleotide Mimics as Potential Antitumor Agents Targeting Cyclin-dependent Kinases**, N. Xavier, 2014-2019, project funding 50 000€, iFCT
- **XBONDS4BIOCHEM**, P. Costa, 2015-2018, project funding 50 000€, iFCT
- **Revealing Amyloid fibril formation through the ions of Mass spectrometry**, G. da Costa, 2014-2019, project funding 50 000€
Achievements – Papers 2016

Top 1% SCIMAGO

Layered Double Hydroxide Nanocluster: Aqueous, Concentrated, Stable, and Catalytically-Active Colloids towards Green Chemistry
ACS Nano, 2016, 10, 5550–5559. IF: 12.881, Q1

Top 5% SCIMAGO

Mechanistic Study of the Direct Intramolecular Allylic Amination Reaction Catalyzed by Palladium(II), F.J.S. Duarte, G. Poli, M.J. Calhorda, ACS Catal 2016, 6, 1772–1784. IF: 9.307, Q1 Top 5%


Comment on “Theoretical studies on a carbonaceous molecular bearing: association thermodynamics and dual-mode rolling dynamics”, E.M. Cabaleiro-Lago, J. Rodríguez-Otero, A. Gil Chem Sci, 2016, 7, 2924-2928. IF: 9.144, Q1 Top 5%


pK_a values of titrable amino acids at the water/membrane interface, V.H. Teixeira, D. Vila-Viçosa, P.B.P.S. Reis, M. Machuqueiro, J Chem Theory Comput, 2016, 12, 930-934. IF: 5.301, Q1 Top 5%


TiO_2 anatase intermediary layer acting as template for ZnO pulsed electrodeposition, T. Frade, K. Lobato, J. Carreira, J. Rodrigues, T. Monteiro, A. Gomes, Mat & Design, 2016, 110,18-26. IF: 3.997, Q1, Top 5%

Isololide, a carotenoid metabolite isolated from the brown alga Cystoseira tamariscifolia, is cytotoxic and able to induce apoptosis in hepatocarcinoma cells through caspase-3 activation, decreased Bcl-2 levels, increased p53 expression and PARP cleavage, C. Vizetto-Duarte, L. Custódio, K.N. Gangadhhar, J.H.G. Lago, C. Dias, A.M. Matos, N. Neng, J.M.F. Nogueira, L. Barreira, F. Albericio, A.P. Rauter, J. Varela, Phytomedicine, 2016, 23, 550–557. IF: 2.937, Q1, Top 5%
Achievements – Papers & Prizes

The Prémio Luso - Espanhol de Química, Conferencia Madinaveitia-Lourenço, was awarded by Real Sociedad Española de Química and Sociedade Portuguesa de Química in 2017 to Professor Amélia Pilar Rauter.

The dryVHP project by Fernando Antunes, João Pires da Silva and Fhadil Musa was the winner of the first edition of the Ageas Innovation Award–2016, receiving a monetary prize and a three-month incubation experience at Healthcare City. The team developed a technology that releases hydrogen peroxide very quickly, with little associated water. This technology will improve the sterilization of hospital environments with a faster and cheaper actuation formula for the user.

The InovCarbon project promoted by Ana S. Mestre and Ana P. Carvalho won the 1st prize in the Call for Projects do ScienceIN2Business, organized by FCUL and Tec Labs in the 2016 edition. Besides the monetary prize the researchers will integrate an acceleration program on Tec Labs. The project development will also have the support of Miguel Ferreira e Paulo Sousa Marques from Shark Tank Portugal, from the jury.

Tribute to Portuguese Women Scientists by Ciência Viva to Maria José Calhorda, May 2016.

Key Scientific Articles classified by

Participation in National & International organizations

Participation in editorial boards and special issues 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)
- Editor of Boletin del Grupo Español del Cárbon, nr. 39 (Ana P. Carvalho)
- Editors of Boletin del Grupo Español del Cárbon, nr. 40 (Ana S. Mestre, M. A. Andrade and M. Galhetas)
- Academic Editor of PLOS ONE (M. Machuqueiro)
- 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)
- Member of the Distinguished Board of Reviewers of Journal of Radioanalytical and Nuclear Chemistry, (A.P. Paiva) since 1993
Participation in National & International Organizations

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

- IUPAC Division (VIII) of Chemical Nomenclature and Structure Representation, National Representative (A. P. Rauter)
- IUPAC Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS) Division VIII representative (A. P. Rauter)
- IUPAC Division (III) of Organic and Biomolecular Chemistry, Associate member and Secretary (A. P. Rauter)
- Member of the LisbonLiving+ Consortium (A. P. Rauter)
- Member of the UL network for Health (A. P. Rauter)
- Member of UL Food, Farm and Forestry College (A. P. Rauter)
- Member of COST international Evaluation Panel (A. P. Rauter)
- FCUL Sponsor of the FCT-PhD Program Catalysis and Sustainability (CATSUS) (M. J. Calhorda)
- International Society of Electrochemistry, National Representative (J. Correia)
- International Carbohydrate Organisation National Representative (A. P. Rauter)
- European Carbohydrate Organisation Secretary (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)
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

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, EIT-KIC/IVE/0051/2013

CQB is one of the founders of the consortium LisbonLiving+ built within this project. This consortium involves industry, governmental bodies and academia partners.
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, 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
CMST COST Action CM1406 - Epigenetic Chemical Biology (2015-2019), MC
TD COST Action TD1402 - Multifunctional Nanoparticles for Magnetic Hyperthermia and Indirect Radiation Therapy (RADIOMAG) (2014-2018), MC
CMST COST Action CM1404 - Chemistry of Smart Energy Carriers and Technologies (SMARTCATS) (2014-2018), MC and WG1
TD COST Action TD1305- iPROMEDAI: Improved Protection of Medical Devices Against Infection (2014-2018), WG
ESSEM COST Action ES1407- European network for innovative recovery strategies of rare earth and other critical metals from electric and electronic waste (ReCreew)
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

4F-PBP a Novel NPS identified in seized products at Portugal
Knowledge Transfer

CQB Patents 2013-2016


- Processo de funcionalização de biocidas para imobilização em matrizes poliméricas. PT 108096, 2016


- New C-glycosylpolyphenol 4 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 agentes. US patent application no. 14/384,145, 2016

- 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.

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

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

Participation in “**Ciência Viva**” activities: **European Researchers Night** & **Semana da Ciência e Tecnologia**

**Ser cientista** and **Verão na ULisboa** are programs that aims to provide high school students an approach to the reality of scientific research by the temporary integration into work routines from groups in different scientific areas of science.

Talks, demonstrations and quizzes on **FCUL Open Days** and **Futurália**
Outreach Activities

Innovation week, promoted by ULisboa

Ciência 2016, event promoted by FCT

Workshop to launch the Nutriageing website and Festival da Vida Saudável, co-organized by the Lisbon Municipality, to announce the PERSSILAA project and the Nutriageing website to the general public.

Café da Ciência

Radio/TV broadcasts to comment scientific discoveries

Press Releases: Lusa, Diário de Notícias, Jornal de negócios, RTP, Sapo24, Observador, Diário digital

Social Media: Facebook, CQB website

Short training/updating courses for secondary school teachers

School Visits to CQB and researchers visits to schools

Erasmus +

• Staff mobility for teaching and training activities, Ljubljana University, Ljubljana, Slovenia, April 2016
Thematic Lines

Chemistry and Biochemistry for a Clean Environment
Coordination: Maria José Calhorda

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

Human Health: Molecular Interventions and Regulation Mechanisms
Coordination: Rodrigo F. M. de Almeida
(FCT Principal Investigator)

❌ 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 - 2016


Biodiesel production waste as promising biomass precursor of reusable activated carbons for caffeine removal, Mary K.S. Batista, Ana S. Mestre, Inês Matos, Isabel M. Fonseca, Ana P. Carvalho, RSC Adv., 2016, 6, 45419-45427


European Commission Publications

Chemistry and Biochemistry for a Clean Environment

National Projects, Environment Policy & Governance projects

- Overcoming environmental problems associated with antifouling agents: Synthesis of nature inspired nontoxic biocides and immobilization in polymeric coatings  PTDC/AAGTEC/0739/2014

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

- Multifunctional Luminescent Spin Labile Hybrid Materials
  PTDC/QEQ-QIN/3414/2014
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.
Overview and goals

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
**Human Health: Molecular Interventions and Regulation Mechanisms**

**Key publications 2016 - 2017**

**Scientific Papers**

**Targeting Type 2 Diabetes with C-Glucosyl Dihydrochalcones as Selective Sodium Glucose Co-Transporter 2 (SGLT2) Inhibitors: Synthesis and Biological Evaluation**

**m-cresol affects the lipid bilayer in membrane models and living neurons**
RSC Adv., 2016, 6, 105699-105712

**The role of fibrinogen in ATTR: evidence for chaperone activity loss in disease**
Biochemical J.,2016, 473 (14): 2225,


**Hydrogen peroxide regulates cell adhesion through the redox sensor RPSA**

**European Commission Publications**

The EIP on AHA Nutrition Action Group, Advances in Public Health, 2016, Open access.


Human Health: Molecular Interventions and Regulation Mechanisms

European Projects, National Projects Commitments and QREN

- 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

- 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
GROUPS & HIGHLIGHTS
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 by-products of agricultural or industrial activities or by template methodologies; natural-clay based solids and metal-organic frameworks.

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/
Highlight

Hierarchical zeolites to higher performance catalysts

Hierarchical Zeolites/Zeotypes


Zeolites and zeotypes such as SAPOs 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. The development of intracrystalline or intercrystalline mesoporosity can be achieved through synthesis or post-synthesis methods or even by controlling the experimental conditions such as the use of microwave heating.
Pharmaceuticals were added to a Watch list of Directive 2013/39/EU and Decision 2015/495/EU due to their large consumption, environmental and human treat and recalcitrant behavior in conventional water treatment technologies. Activated carbons materials are one of the best available technologies for their removal and thus to assure water quality and decrease the stress to the aquatic environment. The evaluation of novel precursors (agricultural & industrial residues) for the synthesis of activated carbons for the removal of pharmaceuticals contributes to a more circular economy. Recent studies focused on the regeneration of activated carbons exhausted with caffeine and paracetamol contribute to the deeper understanding of regeneration efficiency of pharmaceuticals’ saturated carbons envisaging several reuse cycles and consequently more sustainable processes.

**Highlight**

Pharmaceuticals’ adsorption by activated carbons: contributions for a sustainable and circular economy


Materials for the Ethane-Ethylene separation by adsorption

Ethane (left) and ethylene (right) adsorbed on adsorption site 1 with slightly negative ESP zone (yellow), site 2 with positive ESP zone (blue), and site 3 with strong negative ESP zone (red) of the IRMOF-8 cluster. The ESP surface shown was calculated without the presence of the adsorbed molecules.

Reverse Selectivity of Zeolites and Metal-organic Frameworks (MOFs) in the Ethane/Ethylene Separation by Adsorption, João Pires, Joana Fernandes, Ana C. Fernandes, Moisés L. Pinto

Understanding Gas Adsorption Selectivity in IRMOF8 Using Molecular Simulation, Renjith S. Pillai, Moisés L. Pinto, João Pires, Miguel Jorge, José R. B. Gomes

Ethane Selective IRMOF-8 and its Significance in Ethane-Ethylene Separation by Adsorption, João Pires, Moisés L. Pinto, Vipin K. Saini
ACS Applied Materials and Interfaces 6 (2014) 12093–12099

The separation of ethylene from ethane is one of the most energy-intensive single distillations practiced. This separation could be alternatively made by an adsorption process if the adsorbent would preferentially adsorb ethane over ethylene. Materials that exhibit this feature are scarce but some, such as IRMOF-8, have been successfully studied in our group.
Based on a sustainable model, starting from sugars or from natural resources towards new drug candidates or functional food ingredients for pharmaceutical and/or 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/
Salvia sclareoides functional ingredients for neurodegenerative disease prevention

- *S. sclareoides* is a non-toxic aromatic herb used in folk medicine to treat memory loss
- Potent inhibitor of acetylcholinesterase
- A new binding site was discovered on AChE for rosmarinic acid
- Both plant extract and its component rosmarinic acid interact with Aβ_{1-42} removing amyloid fibrils to form amorphous aggregates
- Prevents normal Prion protein to convert to Prion infectious isoform


Salvia sclareoides Brot. Is a plant that has been extensively studied by our group and demonstrated a variety of activities relevant to its valorization as functional ingredient. Conventional and supercritical fluid extraction was now studied and the phytochemical profile of the plant infusion also investigated. Its toxicity, and the antioxidant, anti-inflammatory and anticholinesterase activities were evaluated. No remarkable alterations in the composition or in the bioactivities of the infusion were observed after in vitro digestion, supporting the potential of *S. sclareoides* as a source of bioactive ingredients with neuroprotective, anti-inflammatory and antioxidant properties.

In collaboration with:

Funded by:

"Diagnostic and Drug Discovery Initiative for Alzheimer's Disease", Industry-Academia Partnerships and Pathways (IAPP), FP7-People-2013-IAPP, GA 612347
Novel bioactive nucleoside and nucleotide analogs

Synthesis of structurally innovative nucleoside analogs and nucleotide mimetics as bioactive molecules of therapeutic interest. In particular, the development of compounds that may inhibit nucleotide-mediated pathways that are deregulated in cancer is aimed. Some molecules displayed micromolar antiproliferative activities in leukemia (K562) and in breast cancer (MCF-7, BT474) cell lines, similar to that of a standard anticancer agent in the case of MCF-7 cells. Further exploitation of the biological profile of the molecules, namely their antiviral effects and their abilities to inhibit cholinesterases (ChEs), is also focused.


**Project:** Synthesis of Nucleotide Mimics as Potential Antitumor Agents Targeting CDKs (IF/01488/2013/CP1159/CT0006); **PI** Nuno M. Xavier

**Collaborations:** Palacký University & AS CR, Universität Halle-Wittenberg
Highlight

A Quest for the Key Structural Features of Flavonoids for Maximized Activity Against Aβ-Induced Neurotoxicity

Development of a **new synthetic route** towards the flavone core

Significant **reduction of total fibril mass** by catechol-type flavonoids

**Minimization of small amyloid oligomer formation** by flavonoids:
a. Without the 3-OH group
b. Containing the 2-Ph group
c. Containing the C2-C3 double bond

Chrysin Proposed as a Prototype Structure


A set of polyphenols with structure variations for *in vitro* testing over the aggregation of Alzheimer’s disease (AD) amyloid peptide Aβ$_{1-42}$ was assembled. Using thioflavin-T (ThT) monitored kinetics and subsequent mechanistic analysis by curve fitting, it is shown that catechol-type flavonoids reduce Aβ$_{1-42}$ fibril content by 30% at molar ratios over 10. Without affecting secondary nucleation, these compounds accelerate primary nucleation events responsible for early primary oligomer formation, putatively redirecting the latter into off-pathway aggregates. Atomic force microscopy (AFM) imaging of reaction end-points allowed a comprehensive topographical analysis of amyloid aggregate populations formed in the presence of each compound. Formation of Aβ$_{1-42}$ small oligomers, regarded as the most toxic amyloid structures, seems to be limited by flavonoids with a C2 phenyl group, while flavonol 3-OH is not a beneficial structural feature.

**In collaboration with**

**Funded by:**
FP7-PEOPLE-2013-IAPP, GA 612347 (D3i4AD)
SFRH/BD/93170/2013
Antidiabetic dihydrochalcone C-glucosides as potent and selective SGLT2 inhibitors


A recent strategy for treating type 2 diabetes relies on the inhibition of glucose reabsorption in the kidneys by inhibiting sodium glucose co-transporter proteins (SGLTs). The isoform SGLT1 has a high affinity to both glucose and galactose, and is located in the small intestine, heart, trachea, and kidney, while glucose is the only substrate for SGLT2, located only in the kidneys. The SGLTs inhibitors marketed present communal adverse effects such as urinary tract infections, renal-related adverse events, amongst other side effects, most of them related to SGLT1 inhibition, thus encouraging the search for compound diversity aiming at achieving potency and selectivity toward SGLT2. The discovery of a new family of potent and highly selective SGLT2 flavonoid inhibitors (IC50 = 9-23 nM), is here disclosed, whose structure derived from a library of C-glucosyl dihydrochalcons, and their chalcone and dihydrochalcone precursors, generated by employing new, easy to carry out and efficient procedures. These flavonoids also showed no effect on the sodium independent GLUT family of glucose transporters, and were not acutely toxic to cells in culture. Computational modelling provided evidence that the C-glucosyl dihydrochalcons are not pan-assay interference compounds (PAINS), demonstrating that the C-C linked glucosyl group plays an important role in preventing deep membrane insertion, beyond its remarkable role for the achievement of a high selectivity for SGLT2 over SGLT1 and GLUT, by comparison to phlorizin, the O-glucosyl analog, active in the µM range and not selective.
Highlight

Exploring marine halophytes toward functional constituents to improve human health

Limonium algarvense flowers infusions and decoctions

- similar antioxidant properties to those of green tea
- More content of salicilic, gallic and coumaric acids than green tea
- Non toxic
- Higher anti-inflammatory activity than green tea


The halophyte Limonium algarvensis is found in saltmarshes from Algarve in Portugal to Cadiz in Spain. Flower infusions and decoctions were compared to those of Camelia sinensis leaves (green tea). Comparison of the antioxidant and anti-inflammatory potential and toxicity and determination of its phytochemical profile have demonstrated the high-added value of this halophyte as a source of bioactive polyphenols for the prevention of oxidative-stress and inflammation-related diseases.

In collaboration with

Funded by FCT:
PTDC/MAR-EST/4346/2012
CCMAR/Multi/04326/2013
Highlight

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: the nutriageing.fc.ul.pt 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!

Chef Hélio Loureiro

Vegetable gardens growing ingredients, condiments.....

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

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.


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/
Inorganic and Theoretical Chemistry

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 CO₂ 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 inorganic and organometallic reactions, to calculate the properties of molecules and functional materials in order to understand the phenomena underpinning these properties and improve them. We also wish to understand in detail the interactions between bioactive metal complexes 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 relationship 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

- Inorganic molecules and materials for energy and magnetism
- Antifouling molecules and materials for biofouling prevention
- Ionic liquids in biphasic catalysis with molybdenum complexes
- Hybrid Materials for selective catalytic processes
- Mechanisms/properties of transition metal derivatives
- In silico nanobio solutions for medicine and materials
- pH effects on membranes and proteins
- Halogen bonding in (bio)chemical systems

Computational Studies

- The role of hydrophobic interactions in a molecular disease
- Identify new abuse drugs by NMR to prevent health risks
- Inorganic molecules and materials for energy and magnetism
- Halogen bonding in (bio)chemical systems
- pH effects on membranes and proteins
- Ionic liquids in biphasic catalysis with molybdenum complexes
- Hybrid Materials for selective catalytic processes
- Mechanisms/properties of transition metal derivatives
- In silico nanobio solutions for medicine and materials
- The role of hydrophobic interactions in a molecular disease

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After recent report of the first ever cationic iron(III)-oxo species of the Keggin type $[\text{Bi}_6\{\text{FeO}_4\Phi\text{Fe}_{12}\text{O}_{12}(\text{OH})_{10}(\text{H}_2\text{O})_2\}(\mu_2\text{O}_2\text{CCF}_3)_{10}]^{3+}$ (Science 2015, 47, 1359-1362), and the second of its kind after Bino’s homonuclear derivative $[\text{FeO}_4\Phi\text{Fe}_{12}\text{F}_{24}(\mu_2\text{OCH}_3)_{12}]^{5-}$ reported in 2002 (JACS, 2002, 124, 4578-4579), have led us to examine their magnetic properties and compare them with those of the heteronuclear kind where the Fe(III) centres are present as mixed addenda such as the anions $[\text{Fe}_6(\text{OH})_3\text{Ge}_2\text{W}_{18}\text{O}_{68}(\text{OH})_6]^{11-}$ and $[\text{H}_{12}\text{As}_4\text{Fe}_8\text{W}_{30}\text{O}_{120}(\text{H}_2\text{O})_2]^{4-}$. The goal was to search for the commonality between all these iron clusters and correlate the position and stereochemistry of the magnetic iron sites with the overall magnetic properties of these molecular architectures.

The computational analysis shows that the most significant antiferromagnetic spin coupling takes place at the junction between each of the $\{\text{Fe}_3\text{O}_6(\text{OH})_3\}/\{\text{Fe}_3\text{F}_6(\text{OCH}_3)_3\}$ framework motifs (‘$J’$), a possibility that had been previously discarded in the literature on the basis of the Fe–Fe distances. For all the examined iron(III) Keggin structures, it is found that the magnitude of the magnetic couplings within each structural subunit follows the same trend.
The family of Mo(II) and W(II) complexes [M(η-3 allyl)X(CO)₂(L)₂] fragment (X = anion, (L)₂ = two monodentate or one bidentate ligand, allyl = C₃H₅ or substituted allyl) was revisited. A structural search in the CSD afforded 441 molybdenum and 68 tungsten complexes with a pseudo-octahedral geometry. Despite the strong preference for two particular isomers, examples of almost all the others have been found, indicating the structural richness of these species. They undergo a variety of reactions with applications in fields such as catalysis (homogeneous and immobilized in several supports) and bioactivity.
Peptides and proteins protonation equilibrium is strongly influenced by its surrounding media. Remarkably, until now, there have been no quantitative and systematic studies reporting the $pK_a$ shifts in the common titrable amino acids upon lipid membrane insertion. Here, we applied our recently developed CpHMD-L method to calculate the $pK_a$ values of titrable amino acid residues incorporated in Ala-based pentapeptides at the water/membrane interface. We observed that membrane insertion leads to desolvation and a clear stabilization of the neutral forms, and we quantified the increases/decreases of the $pK_a$ values in the anionic/cationic residues along the membrane normal. This work highlights the importance of properly modeling the protonation equilibrium in peptides and proteins interacting with membranes using molecular dynamics simulations.
Antifouling coatings play a vital role in the marine industry for the control of marine biofouling attach and growth on submerged surfaces. This undesired bio-attach has been associated with serious economic and environmental penalties on both stationary and non-stationary marine systems, from shipping, aquaculture (e.g., cages) and other offshore activities. Most conventional antifouling strategies (e.g., controlled depletion polymer coatings (CDPs), self-polishing tin-free copolymer coatings (TF-SPC)) still act by controlled-releasing mechanisms of toxic agents, leading to a relative short antifouling effect and, as a result of the agents loss and due to their intrinsic ecotoxicity and cumulative effects, have been also subjected to severe regulation. In our work, a new antifouling strategy has been developed. It is based on the tethering of antifouling agents in polymeric matrices, such as marine coatings, thus avoiding their release from coatings, acting by contact, and promoting a long-lasting antifouling action. The antifouling efficacy of this strategy has been tested under real static conditions at Estaleiros Navais de Peniche (ENP) dock and dynamic conditions on fishing ENP ships. Auspicious results were found, biocidal silicone-based coatings prototypes tested under static conditions remained clean after 66 months (more than a year), whereas the trial ship test, that has been traveling for about eight months, remained clean for the shipyard satisfaction.
Non-toxic antifouling marine coatings: immobilization of novel nature-inspired sulfated molecules

In the frame of FCT Anti-fouling project, PTDC/AAG-TEC/0739/2014, FCT Sponsor (2016-2019) Partners: Centro Interdisciplinar de Investigação Marinha e Ambiental – CIIMAR/CIMAR (Promotor, Marta Correia da Silva) and Faculdade de Ciências (FFC/FC/UL), Universidade de Lisboa (Elisabete R. Silva, Ana Ferreira and Maria José Calhorda)

Marine biofouling cause serious damages on marine structures, particular in marine transport industry, where ships suffer from premature biocorrosion, devices malfunctions, significant drag friction and subsequent fuel consumption increases. Biofouling prevention on marine structures is crucial for their own and related operations survival. Conventional antifouling strategies, mostly based on the release of toxic agents into the contaminated surfaces, have been associated to serious environmental penalties, as a result of the ecotoxicity and cumulative effect of the applied biocidal agents. Innovative non-toxic antifouling alternative are demanded. In this work, novel synthesized biomimetic sulfated molecules (zosteric acid-inspired), with proved antifouling properties and minimal environmental risk (Nature Scientific Reports, 7, 42424, 2017), are being immobilized in marine coatings by a recent developed immobilization process (WO2016/093719 A1, 2016), in order to provide non-toxic and long-lasting antifouling effects on the generated coatings.

The interest of adding Vitamin A (VitA) to diets, owing to its relevance in several physiological functions, prompted us to design and study delivery systems that would prevent its oxidation. Commercial VitA was immobilized in two different clays (Montmorillonite K-10 and Sepiolite S 15), and in MCM-41 by impregnation. The photo-stability tests showed decreased degradation of VitA in the clays, compared to MCM-41 and the pure VitA. The three materials release Vitamin A under conditions simulating the oral drug administration. The kinetics of the release depended on the support and pH, with Sepiolite originating a classic profile of increasing amount of VitA with time, indicating that no oxidation was taking place. In both Montmorillonite and MCM-41 the amount of released VitA drops after ~2 hours, as it is being oxidized.

Sepiolite could therefore be a good candidate for oral Vitamin A delivery systems.
The future of digital information: from nano/micro to molecular scale


Researchers from Centro de Química e Bioquímica at Faculdade de Ciências, Universidade de Lisboa produced a ground breaking material able to store and disseminate digital information at a molecular level. Under certain conditions, is able to sub-divide, thus propagating the storage ability of digital information. This research was mainly developed by Paulo Nuno Martinho at CQB in collaboration with other researcher from the Universities of Lisboa, Coimbra and Bordeaux. The further development of these materials and their application is now under a national research project funded by Fundação para a Ciência e Tecnologia coordinated by Paulo Nuno Martinho.

The results were published online, on the 17th of March, in Chemical Science, one of the most renowned open access multidisciplinary journals. The article “Dynamic spin interchange in a tridentate Fe(III) Schiff-base compound” by Ana I. Vicente, Abhinav Joseph, Liliana P. Ferreira, Maria de Deus Carvalho, Vítor H. N. Rodrigues, Mathieu Duttine, Hermínio P. Diogo, Manuel E. Minas da Piedade, Maria José Calhorda and Paulo N. Martinho is the combined effort of Universidade de Lisboa, Universidade de Coimbra and the University of Bordeaux.
Biofouling formation on surfaces is one of the most serious problems in a wide range of industrial sectors (e.g. shipping, water purification units). It can promote substrate deterioration, systems clogging, resulting in costly maintenance and retrofitting consequences. Microencapsulation of bioactive agents has emerged as a potential antifouling strategy to provide a controlled release of toxic agents on contaminated surfaces, therefore promoting a longer biocidal protection effect, and protection of the used agents from the surrounding environment (ex: coating matrix). Nonetheless, it has been also allied to environmental issues due to the potential ecotoxicity of the release agents or derivatives and their cumulative effects. Efforts have been done in order to find alternative non-toxic antifouling systems, such as the encapsulation of enzymes. However, biocidal release approaches still are the most efficient and reliable for biofouling control. The present invention provides biocidal polyurethane-polyurea microcapsules (MC’s) characterized by a core-shell morphology, which can offer a controllable biocidal action from a partial/total chemical immobilization of biocides within the microcapsules. Water-in-oil (W/O) microemulsion method combined with interfacial polymerization, and a chemical immobilization strategy of biocides in the MC’s shell [WO2016/093719 A1, 2016] has been used for the purpose.
Among marine organisms, sponges are the richest sources of pharmacologically-active compounds. Stemming from a previous lead discovery program that gathered a comprehensive library of organic extracts of marine sponges from the off-shore region of Portugal, crude extracts of *Erylus cf. deficiens* collected in the Gorringe Bank (Atlantic Ocean) were tested in the innovative high throughput screening (HTS) assay for inhibitors of indoleamine 2,3-dioxygenase (IDO) and showed activity. Bioassay guided fractionation of the dichloromethane extract led to the isolation of four new glycolipids, named erylusamides A–D. The structures of the isolated compounds were established by 1D and 2D nuclear magnetic resonance (NMR) spectroscopy, high-resolution electrospray ionization mass spectrometry (HR-ESI-MS) and chemical derivatization. The metabolites shared a pentasaccharide moiety constituted by unusual highly acetylated D-glucose moieties as well as D-xylose and D-galactose. The aglycones were unprecedented long chain dihydroxyketo amides. Erylusamides A, B and D differ in the length of the hydrocarbon chain, while erylusamide C is a structural isomer of erylusamide B.

**Erylusamines: novel atypical glycolipids from Erylus CF deficiens**  
H. Gaspar, A. Cutignano, L. Grauso, N. Neng, V. Cachatra, A. Fontana, J. Xavier, H. Vieira, S. Santos,  
*Mar Drugs*, 2016, 14, 179.
A theoretical study of methylation and CH/π interactions in DNA intercalation methylated 1,10-phenanthroline in adenine-thymine base pairs, Adrià Gil, Vicenç Branchadell and Maria José Calhorda, RSC Adv. 2016, 6, 85891.

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. Such activity is related to their mode of interaction with DNA and intercalation is a binding mode associated to cytotoxicity towards tumor cells. Methylated phen derivatives also exhibited cytotoxicity, which was found to be deeply connected to the number and position of –CH3 groups. Several works addressing the intercalation of small molecules in DNA have appeared recently in the literature and there is still some debate about the intercalation/deintercalation process and the mechanism that could explain the tuning of cytotoxicity. We try to rationalize the intrinsic forces and substitution patterns ruling the intercalation to get some insight on the relation with cytotoxicity by means of computational techniques. We hope that our work will help to shed light on such important processes of current interest.
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/

Aiming to produce materials with enhanced optical and photocatalytic properties, titanate nanotubes (TNT) modified by cobalt doping (Co-TNT) and by Na⁺ → Co ion-exchange (TNT/Co) were prepared by hydrothermal method. The influence of the doping level and of the cobalt position in the TNT crystalline structure was studied. Although no perceptible influence of the cobalt ion position was observed on the morphology of the prepared titanate nanotubes, the optical behavior of the cobalt modified samples is clearly dependent on either the cobalt ions are substituting the Ti⁴⁺ ions into the TiO₆ octahedra building blocks of the TNT structure (doped samples) or replacing the Na⁺ ions between the TiO₆ interlayers (ion-exchange samples). The catalytic ability of these materials on pollutants photodegradation was investigated. First, the evaluation of hydroxyl radical formation using the terephthalic acid as probe was evaluated. Afterwards, phenol, naphthol yellow S and brilliant green were used as model pollutants. Anticipating real world situations, photocatalytic experiments were performed using solutions combining these pollutants. The results show that the Co modified TNT materials (Co-TNT and TNT/Co) are good catalysts, being the photocatalytic performance dependent on the Co/Ti ratio and on the structural metal location.
A simple and versatile one pot method for the robust attachment of nanocatalytic assemblies on gold surface is developed. To this purpose, carbon disulfide is used to establish a stable linkage between gold surface and magnetite (Fe₃O₄) nanoparticles, functionalized with metalloporphyrins (Co or Fe) containing carboxylic acids as anchor groups. UV–vis spectra prove the functionalization of the nanoparticles by metalloporphyrins and AFM images reveal the density and size of modified nanoparticles attached to gold by CS₂. The efficiency of the immobilization method is demonstrated by the electrochemical performance of the modified electrodes toward oxygen reduction reaction (ORR) in aqueous acidic medium. Koutecky-Levich plots and rotating ring-disk electrode experiments revealed distinct oxygen reduction mechanisms for the nanostructured Co or Fe porphyrin modified electrodes, with the transfer of two or four electrons to form hydrogen peroxide or water, respectively. The chemical nature, composition and size of nanoparticles clearly influence the ORR behavior. The largest magnetite nanoparticles (ca. 40 nm) exhibit the best catalytic response, either modified with iron or cobalt porphyrins. Additionally, electrodes with metalloporphyrin/Fe₃O₄ nanocatalysts exhibit good stability under acidic conditions. Altogether the results highlight the potentialities of this simple and versatile surface modification for the design of electrocatalytic systems.

A novel route to synthesise Bi$_2$S$_3$-sensitised BiOCl nanoparticles from deep eutectic solvent medium at room temperature by a one-pot approach is reported. The influence of the temperature, sulphur source, concentration of reactants and presence of water, on the morphological, structural and microstructural, optical and photocatalytic properties of the synthesised nanoparticles is analysed and discussed. Stable and crystalline BiOCl hybrid structures with shapes from sheet-like to flower-like hierarchical aggregates and (001) and (110) dominant crystallographic orientation were obtained. The sensitisation of BiOCl with Bi$_2$S$_3$ was successfully achieved in situ during synthesis by an ion-exchange process and the relative proportion of the components (BiOCl and Bi$_2$S$_3$) was controlled by the Bi:S ratio in the synthesis medium and by the sulphur precursor. The sensitiser nanomaterial (Bi$_2$S$_3$) extends the BiOCl photoactive region to the visible range. Also it favours charge separation and reducing the electron/hole pair recombination and therefore increasing the photocatalytic performance. The prepared composite materials show high ability to adsorb rhodamine B cationic dye and the complete photocatalytic degradation was achieved within 45 min (75 mg per g of catalyst).
A simple and effective approach to build nanostructured immunosensor platforms is proposed. The one-step strategy relies on i) the in situ formation of dithiocarbamates from the reaction between carbon disulfide and amine groups, present on protein A, ii) their attachment to gold nanoparticles (AuNPs), and iii) the linkage of the modified AuNPs to the electrode surface, which depends on the strong interaction between gold substrates and sulfur moieties. AuNPs and protein A are used to increase the surface coverage of Immunoglobulin G (IgG) and promote the oriented immobilization of the antibodies on the immunosensing interface. The immunosensor performance was assessed in real-time, by surface plasmon resonance and by the highly sensitive total internal reflection imaging ellipsometry, through the specific biorecognition between anti-IgG and the immobilized IgG molecules.

We demonstrate that the presence of AuNPs improves the sensitivity of the anti-IgG specific detection, whereas the presence of co-adsorbed CS$_2$ is responsible for blocking the undesired protein nonspecific adsorption to the gold substrate. Overall, we report a simple and innovative one-step method, to chemically modify gold surfaces with protein A and AuNPs, able to specifically detect antigen/antibody interactions with capability of preventing protein nonspecific adsorption.
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/
Antiparasitic activity of diterpenoids against *Trypanosoma cruzi*

Sergio Alegre-Gómez, Paula Sainz, M. Fátima Simões, Patrícia Rijo, Cristina Moiteiro, Azucena González-Coloma, Rafael A. Martínez-Díaz

*Planta Medica, 83, 2017, 306-311*


Chemical structures of compounds 1-27

Twenty seven diterpenes, including abietanes, labdanes, abeoabietanes, halimanes, and pimaranes, have been evaluated against epimastigote and intracellular amastigote forms of *Trypanosoma cruzi*, and also against LC5 and NCTC cell lines. Royleanones (3, 4 and 5) and a further abietane (12), obtained by purification of *Plectranthus* spp. extracts, were the most active compounds on epimastigotes, showing IC$_{50}$ values similar (1.73 µg/mL, 12) or even lower (0.39, 0.99, and 1.20 µg/mL, 3, 4 and 5 respectively) than the positive control nifurtimox (2.3 µg/mL). On intracellular amastigotes, abietanes 3, 4 and 5 showed a significant activity with IC$_{50}$ values of 0.83< 0.31 and 0.63 µg/mL, but were less potent than the positive control nifurtimox (IC$_{50}$ < 0.16). Compounds 3, 4 and 5 were not cytotoxic to LC5 and NCTC 929 cells at 1 µg/mL.
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/
Polymorphs With $Z' > 1$ are Not Necessarily Less Stable Than Their $Z' = 1$ Analogues

Polymorphism is a common occurrence in molecular organic solids, which consists in the existence of more than one crystal form of the same compound. The phenomenon is difficult to control since the intermolecular forces that determine the supramolecular architecture of a crystal are much weaker than e.g. the covalent bonds responsible for molecular integrity. A number of incidents in the pharmaceutical industry have dramatically evidenced that the lack of control over polymorphism can wreak havoc with the production, patenting, and safe use of medicines. Particularly relevant within this context is, therefore, understanding how an interplay of structural, thermodynamic, and kinetic factors dictate the stability domains of polymorphs, their tendency to interconvert through phase transitions, or their possibility to exist in metastable states. Using 4'-hydroxyacetophenone (HAP) as a model system, and a variety of experimental techniques (e.g. calorimetry, microscopy, X-ray diffraction, spectroscopic measurements in acoustically levitated crystals) we were able to shown that the direct interconversion of polymorphs with very similar thermodynamic stability may be hindered by large kinetic barriers compared to their lattice energies. It was also found that it is possible to selectively and reproducible control the preparation of each HAP polymorph through a solvent mediated phase transition. Finally, it was demonstrated that contrary to a common assumption born from crystallographic arguments alone, polymorphs with more than one molecule in the asymmetric unit ($Z' > 1$) are not necessarily metastable relative to their $Z' = 1$ analogues.
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.

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 (H$_2$O$_2$), a reactive oxygen species (ROS), is a ubiquitous oxidant present in all aerobic organisms. Starting in the 90s the 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 H$_2$O$_2$ in vivo with important implications in health and disease is unquestionable. Several questions remain unanswered regarding our understanding of redox-dependent regulation of gene expression:

- What makes a good H$_2$O$_2$ sensor?
- What are the common chemical and kinetic principles that govern H$_2$O$_2$ signaling?
- Which molecules/pathways are redox regulated?

Cancer is among those diseases where H$_2$O$_2$ can have an important role. To become metastatic, a tumor cell must acquire new adhesion properties that allow migration into the surrounding connective tissue, transmigration across endothelial cells to reach the blood stream and, at the site of metastasis, adhesion to endothelial cells and transmigration to colonize a new tissue. In this work, we identified Ribosomal Protein SA (RPSA) as a target of H$_2$O$_2$ and showed that RPSA in the oxidized state accumulates in clusters that contain specific adhesion molecules. Furthermore, we showed that RPSA oxidation improves cell adhesion efficiency to laminin in vitro and promotes cell extravasation in vivo. Our results unravel a new mechanism for H$_2$O$_2$-dependent modulation of cell adhesion properties and identify RPSA as the H$_2$O$_2$ sensor in this process. This work indicates that high levels of RPSA expression might confer a selective advantage to tumor cells in an oxidative environment.
Separation Science & Technology Group

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 is 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/
Hydrometallurgical recovery of Pd(II) from a spent industrial catalyst of alumina

Highlight

Real leaching solutions composed by HCl+H₂O₂ and the respective salts were applied in liquid-liquid extraction using \( N \)-methyl-\( N \)-cyclohexyloctanthioamide (MCHTA) and \( N,N' \)-dimethyl-\( N,N' \)-dicyclohexylthiodiglycolamide (DMDCHTDGA). Equilibrium Pd(II) extraction isotherms and reutilization experiments show that MCHTA and DMDCHTDGA depict promising loading capacities. The reutilization experiments evidence the recyclability robustness of the solvent to recover Pd(II).
Recently, we have been involved in the development of new generation of microextraction devices, which are much more effective as sample preparation technologies, presenting easy and fast manipulation and are in compliance with the green analytical chemistry principles.

In the analytical point of view they have been tested in monitoring trace and ultra-trace levels of priority and emerging organic compounds, such pharmaceutical and personal care products, drugs of abuse, pesticides, disinfection by-products, flavonoids, phenolic compounds etc., in matrices from areas with impact in society at large.

Highlight

New microextraction technologies for trace analysis of priority compounds


PPCPs
Drugs of abuse
Pesticides
Disinfection by-products
Flavonoids
Phenolic compounds
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. To achieve this goal, different synthesis methodologies have been explored.

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 a variety of methodologies to engineer the oxide structures, morphologies and properties, which is crucial to improve the catalytic activity.

*Energy conversion* – The SSC group are developing new photoanodes that will lead to more efficient and less expensive solar energy conversion devices for dye-sensitised solar cells (DSSC).

*Biomedicine* – One of the biomedical applications of magnetic iron oxide nanoparticles is magnetic hyperthermia, which is based on the heat dissipation by magnetic materials when exposed to alternating magnetic fields. Magnetic hyperthermia is an emergent and promising technique, which has been explored as a therapy for cancer treatment in combination with radiation- and/or chemo-therapy. 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/
The removal of organic pollutants and pharmaceutical drugs from wastewater is currently one of the major concerns in environmental remediation. 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 $\text{Ca}(1-x)\text{Ln}(x)\text{MnO}_3$ ($\text{Ln} = \text{Sm}, \text{Ho}; 0.1 \leq x \leq 0.4$) photocatalysts, B. Barrocas, S. Serio, A. Rovisco, Y. Nunes, M.E.M. Jorge, App Surf Sci, 2016, 360, 798-806.


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Removal of organic pollutants:
For the first time the growth of immobilized $\text{Ca}_{1-x}\text{Ln}_x\text{MnO}_3$ ($\text{Ln} = \text{Sm}, \text{Ho}; 0.1 \leq x \leq 0.4$) by RF magnetron sputtering onto fused silica substrates was carried out. The results showed that some $\text{Ca}_{1-x}\text{HoxMnO}_3$ and $\text{Ca}_{1-x}\text{SmxMnO}_3$ films present higher photocatalytic activity for Rh6G degradation in comparison with TiO2 films and for the same x value the Ho-films exhibited higher photocatalytic activity. For both films series the maximal degradation rate was obtained for $x = 0.2$ and the used photocatalysts evidenced high photochemical stability. Furthermore, it is reported here the importance of these new nanostructured materials in obtaining promising photocatalytic materials with high activity for dye wastewater treatment under visible light irradiation.

Solar photoanodes:
The morphological, structural, optical and photoelectrochemical properties of ZnO thin films deposited on transparent (TCO) substrates by direct current (DC) reactive magnetron sputtering technique depends of deposition conditions. These films will be used as seed layers on the following electrodeposition step, creating conditions to tailor the 1D ZnO films with high surface density.
Our group has been dedicated to the synthesis of ferrite nanoparticles using different methodologies, in order to control their size and morphology, and, by this way, changing their magnetic properties. \( \text{Fe}_3\text{O}_4 \), \( \text{CoFe}_2\text{O}_4 \) and \( \text{MnFe}_2\text{O}_4 \) nanoparticles were obtained using a gelatine–assisted method, which allowed to obtain narrow particle size distribution, and better hyperthermia efficiency than those obtain by other methods. The use of natural templates was also explored, and we demonstrated that the morphologies of the nanoparticles are determined by the threaded templates, the magnetic nanoparticles showing enhanced magnetic anisotropy and associated magnetic coercivities.

This work is closely linked to action COST TD1402 (Multifunctional Nanoparticles for Magnetic Hyperthermia and Indirect Radiation Therapy), in which the group has been strongly involved.
**Structure and Reactivity**

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 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, solubilization/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/
Kinetic studies of Friedel-Crafts acylation reactions over hierarchical zeolites: QSPR studies

Friedel-Crafts reactions are important routes for the synthesis of aromatic ketones that are intermediates in the manufacture of many fine and speciality chemicals, as well as of pharmaceutical compounds. Acylation reactions are generally carried out in batch reactors over conventional Friedel-Crafts catalysts such as AlCl₃ or HF. However, these catalysts cannot be regenerated and imply the use of over-stoichiometric amounts, often leading to expensive downstream processes, with significant toxic and corrosive waste disposal issues. This can be overcome by replacing them by solid acid catalysts such as zeolites which have been widely used as heterogeneous catalysts in industrial processes, such as oil refining and petrochemistry, and also as adsorbents in purification and separation processes. A systematic work involving Friedel-Crafts acylations carried out under mild conditions using well characterized hierarchical zeolites, alongside with a QSPR approach to model both kinetic and adsorption processes, was performed. To our knowledge, QSPR modelling was used for the first time in this type of studies and was shown to be a promising tool to optimize these reactions since it gives important information on the relevant molecular features underlying these processes.
The group revisited its origins by looking again at the kinetics of solvolytic reactions. Since the pioneering work by Hughes and Ingold in 1935, the reactions of tertiary alkyl halides, and in particular of tertiary butyl halides, t-BuX, with hydroxylic solvents have been thoroughly investigated and commonly considered to follow first-order kinetics. However, most of the published studies were limited to the only generally acknowledged meaningful reaction step, viz. the solvolysis reaction, in which t-BuX is consumed to produce the halogen acid, HX. Gonçalves, Martins, and Simões (GMS) have nevertheless shown that the whole kinetic picture was much more complex than this and proposed in the early ‘90s a multistep mechanism involving the putative influence of various subsequent reaction steps beyond the initial solvolysis process. The aim of this work was to quantitatively test, through the use of numerical integration (4th order Runge-Kutta method) associated with nonlinear regression (Levenberg–Marquardt method) the GMS mechanism for the reactions of t-BuX with monoalcohols, and to provide a reliable way to obtain accurate values for all involved rate constants. This was successfully done and confirmed the predicted distinct behaviors of the solvolyses of t-BuX with primary, secondary and tertiary alcohols. The determination of “pure” and accurate rate constants is of paramount importance to compute reliable thermodynamic functions of activation and to establish sound quantitative structure–property relationships.
Comprehension of the hydrophobic/hydrophilic balance effect in aggregation pattern and hydration schemes generating microheterogeneities over limited composition ranges


The sharp transitions observed in some thermodynamic properties during mixing processes reveal changes in molecular aggregation schemes that, in some cases, remain an enigma. A confident characterization of the clusters formed in different composition ranges has been steadily tried using different methodologies, mainly thermodynamic and spectroscopic ones. These studies revealed the existence of microheterogeneities in certain composition domains of aqueous amphiphilic systems. From a thermodynamic point of view, microheterogeneity may be envisaged as nano-sized entities where segregation of one or two components takes place, without yielding a macroscopic phase separation. The Kirkwood–Buff integrals applied to partial molar volumes, isothermal compressibility and water activity and resulting preferential solvation parameters, and other experimental techniques namely surface tension, electrospray mass spectroscopy, solution calorimetry and molecular spectroscopy, probing specific/non-specific solute-solvent molecular interactions, allowed the confirmation and identification of precise aggregation patterns. Our goal is to clarify aqueous-amphiphilic binary systems self-assembly, and several model systems are currently under study, since they may model complex mixtures with biophysical and industrial interest. Now, we are focused in aqueous alkoxyamines mixtures due to their importance, industrially in the controlled production of polymers, and also pharmacologically, as they have been considered a new family of prodrugs against cancer, due to spontaneous free radicals’ production which can be used as therapeutic agents.

The surface tension is linearly related to the reciprocal of components’ molar surface areas and there is no simple mixing rule linking the ideal/real surface tension to pure-component surface tensions. Supported on our previous work on surface phase thermodynamics, where theoretical expressions for ideal surface tensions and limiting slopes for the surface tension dependence on composition were obtained, and on the analysis of the fitting quality of numerous empirical relationships used in the literature, a new semi-empirical equation to the fit experimental data was perceived. This equation has an hyperbolic term, typical of all “best equations”, and constrains two parameters assigning physical significance to two fitting parameters, supported on the ideal model, and dependent on pure components surface tension and surface molar area. A comparative analysis of 4 aqueous-organic mixtures, encompassing polar/non polar and protic/aprotic co-solvents with 5 often used empirical equations revealed the new equation performed best. The major limitation of this equation is requiring knowledge of pure components critical volumes, data which may not be available in the literature. Nonetheless, its purely empirical version (unconstrained parameters) is also superior to all literature equations examined. Efforts in the surface phase description, aiming the calculation of molar areas and partial molar areas, targeting a molecular picture of surface phase changes with composition are ongoing. Further potential applications of the proposed equation to other L/V interfaces have since then been disclosed in studies by other authors, involving molten salt mixtures of rare earth and alkali halides, and concluded the global model was consistent, and provided the best surface phase description.
Isoniazid (INH) is still one of the two most effective antitubercular drugs and is part of all multitherapeutic regimens recommended by WHO. Due to the increasing resistance of *Mycobacterium tuberculosis* (*Mtb*) to INH, new INH-based compounds have been proposed to try to circumvent this problem. Among the most promising compounds, a new, QSAR-based designed, INH derivative with an alkyl chain in C\textsubscript{10} (INH-C\textsubscript{10}), showed a six-fold increase in activity against a katG S315T mutated strain of *Mtb*. In collaboration with Prof. P. Loewen in Canada, we carried out kinetic assays to assess the amount of free radicals produced in the first step of the reaction of INH-C\textsubscript{10}, and the results showed that in the S315T mutant, INH-C\textsubscript{10} produced radicals faster that in the native form. We also observed that radical formation in INH acylated derivatives was deactivated by comparison with INH, independently of the alkyl chain size. Some water-membrane interface MD simulations were also carried out. Preliminary results suggest that, despite its smaller reactivity, the hydrophobic nature of INH-C\textsubscript{10} may promote a better trafficking through the *Mtb* membrane, leading to higher concentrations in the vicinity of KatG, thus resulting in lower MIC values. These findings encourage us to keep searching for new INH-based antituberculars with promising activity against resistant (mutated) *Mtb* strains.
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Equipment

FTICR-MS

Stopped-Flow with absorption and fluorescence detection

Imaging Ellipsometer

Multimode Atomic Force Microscope
Equipment

Steady-state & time-resolved spectrofluorimeter with polarization modes and double grating monochromators

Scanning Electrochemical Microscopy

NMR spectrometer*

*DQB equipment

Surface area and pore size analyzer
Equipment

Probe Beam Deflection

Conventional Ellipsometer

Electrochemical Quartz Crystal Microbalance

Surface Plasmon Resonance

Photocurrent Spectroscopy

Contact Angle Goniometer
Equipment

- $^{57}$Fe Mössbauer spectroscopy (transmission and conversion electron modes)
- Abbe Refractometer
- Anaerobic Chamber
- Capillary electrophoresis with diode array detector (CE-DAD)
- Differential Scanning Calorimeter (DSC)
- Electrochemical Workstations
- Four Probe Conductivity Measurement Setup
- FTICR Mass Spectrometer (FCUL Equipment - Rede Nacional de Espectrometria de Massa)
- FTIR Spectrometer
- Gas chromatography hyphenated to mass spectrometer (GC-MS)
- Gas chromatography with flame ionization detector (GC-FID)
- High performance liquid chromatography with diode array detector (HPLC-DAD)
- Imaging Ellipsometer
- Multimode Atomic Force Microscope
- NMR spectrometer (DQB equipment)
- Photocurrent Spectroscopy Workstation
- Plasma Chamber
- Precision Solution Calorimeter
- Probe Beam Deflection Workstation
- Scanning Electrochemical Microscope
- Single Wavelength Ellipsometer
- Steady-state & time-resolved spectrofluorimeter with polarization modes and double grating monochromators
- Stopped-Flow with absorption and fluorescence detection
- Surface area and pore size analyzer
- Surface Plasmon Resonance Workstation
- Thermogravimetry (TGA) Instrument
- UV-Vis spectrophotometer with integrating sphere
- X-Ray Diffractometer (DQB equipment)
Booklet data collection & organization

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We thank Fundação para a Ciência e Tecnologia for funding UID/MULTI/00612