



**Universidade do Minho**

**Escola de Ciências**

**Relatório de Actividades**

**Centro de Química/UM**

**Ano 2013**

**Dezembro 2013**

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## PARTE I

### 1. Descrição da subunidade e reflexão sobre o grau de adequação da sua organização e funcionamento

The Chemistry Research Centre of the University of Minho (CQ/UM) is a research unit that functions within the School of Sciences of the University of Minho promoting research in the domain of Chemistry. A rating of “excellent” was awarded to the unit in the most recent evaluation process (2008). The CQ/UM is now financed by the Foundation for Science and Technology (FCT) FEDER-COMPETE through the project FCOMP-01-0124-FEDER-037302 (ref<sup>a</sup> FCT PEst-C/QUI/UI0686/2013) entitled “Projecto Estratégico-UI 686- 2013-2014”. FCT gives also financial support through the Portuguese Nuclear Magnetic Resonance network.

The CQ members are either full-time equivalent researchers (FTEs - with a PhD degree), PhD students or collaborators (MSc students and young graduate researchers supported by financed projects). The CQ/UM had 39 FTEs, 32 PhD students and 39 collaborators. The CQ/UM team will be updated soon with respect to December 2013.

The members of the Centre are distributed between 4 research groups according to their scientific interests and affinities and the PhD students are sometimes supervised by members of two research groups:

- Synthesis and Applications of Amino Acids (AA) with 5.5 FTEs, 4.5 PhD students and 9 collaborators;
- Biological Chemistry (BC) with 5 FTEs and 3.5 PhD students and 3 collaborators.
- Electrochemistry and Environment (EE) with 16 FTEs, 10 PhD students and 15 collaborators;
- Synthesis and Applications of Heterocycles (HC) with 16.5 FTEs, 14 PhD students and 12 collaborators;

The FCT finances also the contract of a “Bolsista de Gestão de Ciência e Tecnologia” to accomplish the correct management of the research unit and of all the research projects.

The internal regulations of the CQ/UM determine the organization and management procedures of the research unit. These are based on a coordinating committee and on a scientific council that includes all FTEs, both presided by the Coordinator of the research unit. The coordinating committee is composed by the four principal investigators of the research groups and by one delegate from each research group. This committee coordinates the research policy, plans the activities of the unit and prepares the annual and pluriannual plans, reports and budgets for approval by the scientific council. The Coordinator of the unit officially represents the unit, convenes the committees meetings and implements the decisions of these bodies.

An advisory committee was created and accompanies and advises future research activities of the Centre, in accordance with FCT regulations.

Reflexions:

More administrative support from the UM is committee was created in accordance with FCT regulations to accompany and advise on the research activities and management of the unit.necessary for the management and to respond to calls from European projects to attract more funds and to contribute to an increased internationalization of the research undertaken in the CQ/UM. An advisory management performed by an expert at the level of the School of Sciences would be very helpful for all the research centers of the School in terms of dialogue with the FCT in order to avoid some problems with the acceptance of the expenses.

## **2. Principais objetivos**

Three scientific domains have been identified as the basis for research within the CQ/UM: Medicinal Chemistry, the Environment and new Advanced Nanomaterials.

The main objective of the AA group continues to be the development of new methods and intermediates for peptide synthesis and their application in the production of peptides, peptide analogues, peptidomimetics and heterocyclic peptide derivatives with possible biological activity and potential application in the fields of drug discovery and new materials. In 2013 this work has been developed on new synthetic methods for the preparation of new N-alkyldehydroamino acids, fluorescent beta-beta diarylalanines, the synthesis and application of alpha,alpha-dialkylglycines and new bis-amino acids; unnatural amino acids for chemosensory applications; synthesis of new cyclic RGD-peptides; photocleavable protecting groups and phototriggers; synthesis and molecular modeling of antimicrobial peptaibols, development of new dehydropeptidichydrogelatorsand synthesis and biological applications of NIR probes.

One of the objectives within the BC group continues to be the design, synthesis, characterization and in vitro and in vivo evaluation of novel metal complexes and nanostructures potentially useful for medical imaging (PET, SPECT, MRI, Fluorescence) and therapy. The development of metal chelate constructs and nanostructures functionalised with metal chelates endowed with imaging and terapy capabilities, teragnostics, is also sought. Development of aqueous two-phase systems (ATPS) for purification of plasmid for molecular therapies continues to be another goal of the BC group. The use of new ATPS with ionic liquids and the utilization of continuous systems are being explored. Other interests include the application of molecular modelling for drug design peptidomimetics and the simulation of DNA in room temperature ionic liquids (RTILs).

During 2013 the interests of the EE group have evolved and are now centred on the preparation or characterization of materials and the development of methods. These include novel materials that may find application in domains of catalysis, environmental protection or drug encapsulation. The design and

preparation of metal complexes with non-linear optical activity has continued. Various polymer formulations are being prepared and evaluated for use in biomedical applications, surface-protecting layers or in optical lens production. Various group members apply electrochemical methods to develop clean synthetic processes, to evaluate anti-oxidant capacity or to effect preliminary screening of anti-cancer drugs. Electrochemical processes are being applied in energy recovery from wastewaters and electrochemical methods are being used for the evaluation of components for improved electrochemical generators.

The HC group holds key synthetic chemistry competencies that include expertise in the design, preparation and characterization of a broad range of heterocyclic compounds, carba- and aza-sugar derivatives and macrocyclic complexes. The use of metal-catalysed reactions (namely Suzuki-Miyaura, Sonogashira, Buchwald-Hartwig and Cu(I)-azide-alkyne cycloaddition) and/or the development of new synthetic methods, including asymmetric synthesis allow the preparation of a wide range of novel molecules. Most of these compounds are tailored to meet the societal needs in terms of new drug candidates or materials.

The biological activity of the new compounds is tested through national and international collaborations, in particular as antioxidant, antipsychotic, anticancer, antiangiogenic, antitubercular, antifungal and antibacterial agents. These studies include the encapsulation of new anticancer compounds in nanoliposomes for drug delivery purposes.

Synthetic chemistry has an important role in the preparation of advanced materials and new heterocycles will be designed and prepared for nonlinear optical, photochromic, OLEDs, DSSCs, catalytic and sensor applications. The chemical functionalization of carbon nanotubes for composite applications or as precursors of functionalized graphene nanoribbons is also a growing research area within the research group.

### **3. Resultados alcançados durante o ano de 2013**

The AA group developed new strategies for the preparation of cyclic RGD peptides to conjugate with mono and bifunctional metal chelators. The synthesis of non-proteinogenic AAs and heterocycles for application as UV and NIR fluorescent imaging probes, chemosensors and bioactive compounds was continued. The synthesis and characterization of new peptidichydrogelators was continued. Conformational (NMR and FT-IR) and membrane activity studies of antimicrobial peptaibols started with the solution and solid phase synthesis of model peptaibols and analogues, aided by molecular dynamic simulations. The synthesis of  $\alpha,\alpha$ -dialkylglycines by solid phase Ugi reaction continued together with the synthesis of N-alkylamino acids. The design and synthesis of novel heterocyclic photocleavable protecting groups by one- and two-photon excitation for the caging of amino acids (including neurotransmitters), biogenic amines and its

biosynthetic precursors was continued. The study of the electrochemical behaviour of new AA derivatives was also pursued.

In the BC group novel chelating agents triaza and tetraaza type were developed and characterized. The relaxivity of the respective complexes of Mn (II) and Gd (III) was determined. In vivo studies of conjugated cyclic RGD peptide labeled with  $^{68}\text{Ga}$  (III) as potential radiopharmaceutical agents diagnosis were performed.

An adequate aqueous two-phase system with an ionic liquid was selected and studied for the purification of plasmid DNA. Molecular simulations of non-natural amino acids have demonstrated their potential use in the design of peptidomimetics and also the molecular recognition process of hair keratin/peptide complexes.

The results obtained by EE group members reflect new interests and refocussing of group attention on novel materials and new analytical and synthetic methods within the domain of "Sustainable Chemistry".

Environmentally-friendly heterogeneous catalysts have been developed using nanostructured materials. Drug delivery systems using zeolites to encapsulate anti-cancer drugs, have been prepared and tested. In collaboration with other members of the Centre, metal coordination complexes, have been prepared and characterized to prepare materials for application in non-linear optical devices.

Polymer formulations have been optimized to demonstrate additive effectiveness in resisting degradation. Biodegradable and synthetic polymers have been prepared and evaluated for potential use in biomedical applications.

Novel polymer electrolyte formulations and separator membranes have been prepared for applications in advanced displays and high-energy batteries. Hybrid gels, with appropriate formulations and properties, have been prepared for various applications including optical lens production and surface coating materials.

Low-impact electro-synthetic methods have been developed to modify organic substrates and cyclize of unsaturated organic compounds. A microbial fuel cell was developed to treat wastewater and carbon nanotube electrocatalysts were also used to remove recalcitrant pollutants from wastewater.

Electroanalytical methods were used to screen anticancer drug candidates and a new electrochemical method was developed to characterize the antioxidant capacity of specific compounds.

In the HC group, metal-catalyzed couplings and nucleophilic aromatic substitutions were used to prepare scaffolds and functionalized thienopyridines/pyrimidines as antitumorals or antiangiogenics. The latter were selected by rational design as inhibitors of VEGFR-2 tyrosine kinase membrane receptor. The compounds were tested in enzymatic assays at cellular and biomolecular level through collaborations. The encapsulation of the antitumorals in nanoliposomes was studied by fluorescence for drug delivery purposes. Psoralen analogues and cyanopyrazole derivatives were synthesized and tested as anti-tumor agents or xanthine oxidase inhibitors.

Different chromene, imidazole, pyrimidine and purine derivatives, from in silico screening or inspired by bioactive natural compounds were designed and prepared by new synthetic methods. Their biological activity as anticancer, antimicrobial (including Mtb) and antipsychotic agents was evaluated through collaborative work. A number of promising drug candidates was identified and inspired further work in this area.

New enantioselective Diels-Alder reactions involving erythrose dienes or 2,4-pentadienol and azadienophiles led to cycloadducts used as precursors of aza-sugar type compounds. Click chemistry was used for the synthesis of new glycoconjugates containing a 1,2,3-triazole unit bearing amino acids, esters and coumarins.

A wide range of novel heterocyclic systems were prepared through several synthetic methodologies. The linear and nonlinear optical, thermal, catalytic and sensor properties of these heterocycles were evaluated in solution and in solid matrices (PMMA polymer and nanofibers) for photochromic and NLO applications, through national and international collaborations.

The non-covalent functionalization of CNTs with perylene bisimides resulted in the efficient dispersion of the tubes in aqueous solution, a promising approach for the formation of polymer composites.

#### **4. Atividades para valorização do conhecimento desenvolvidas durante o ano de 2013**

In the context of the research carried out by the members of this Centre, knowledge transfer may involve the formal registration of methods, products or applications as national or international patents or the optimization of synthetic or analytical processes that are requested by industrial partners. While these activities are not considered to be principal objectives of the members of the Centre they have been undertaken in the past and are welcomed by the members of the Centre as contracted tasks that provide additional financial income.

Currently members of the EE group collaborate with industrial partners in solving specific problems related to the characterization of chemical substances. These are short-term projects that are paid for as analytical services.

A substantial part of the research carried out by members of this group involves collaboration across scientific boundaries, with research colleagues from other Sciences or Engineering domains. These joint projects are expected to continue as scientifically productive collaborations. Some examples of collaborative interactions include projects in which members of the HC group synthesize ligands that are incorporated into organometallic complexes for NLO and catalysis, characterized by members of the EE group and from the Centre of Physics (CFUM). Other new materials prepared by HC and AA groups are evaluated through theoretical and experimental studies concerning their optical (linear, nonlinear) and sensor properties by researchers from Polytechnic Valencia Univ. Spain, Bordeaux Univ. France and from

UC, UTAD and UNLisboa. Glycosidase inhibitory studies were carried out on 1-azafagomine and 5-epi-1-azafagomine carboxamide derivatives in collaboration with School of Health and Life Sciences at UM (SHLS). New simple compounds are been up-graded for testing as inhibitors of the entrance of lactose in the cell at SHLS.

Testing the new compounds involves national and international collaborators (ICVS and TAACF-USA for antituberculosis activity, the USC-Spain for antipsychotic activity,, Universidade Fernando Pessoa- Porto, Fac. Pharmacy-UPorto, Fac-Medicine-UPorto, IPATIMUP, the Leiden University Medical Center – Netherlands, the Biology and Biological Engineering Dept.-UM and CBMA-UM for antifungal, antimicrobial and antitumor activities. Studies of encapsulation of new fluorescent antitumor compounds in nanoliposomes for drug delivery are done in collaboration with CFUM. Tyrosine kinase inhibition assays and docking studies using the crystallographic structure of the receptors and the compounds prepared at the CQ/UM are performed at the Inst. Politécnico de Bragança.

Detailed one- and two-photon excitation studies of fluorescent caged biomolecules involved members of the AA group in collaboration with researchers from Strathclyde University, Glasgow, UK. The new hydrogels prepared by the AA group were characterized in collaboration with the Brandeis University, Waltham, Massachusetts, USA and with the Department of Chemistry of the University of Reading, UK. The rheological properties of hydrogels have been studied in collaboration with Dr. Loic Hilliou of the Polymer Engineering Centre of the University of Minho. The enantioselective synthesis of new fluorescent alanine derivatives from dehydroalanines was initiated in collaboration with Prof. Christopher Frost from the University of Bath, UK.

Evaluation of the antitumor activity of psoralen derivatives was carried out in collaboration with IBB-UM (Instituto de Biotecnologia e Bioengenharia-UM). The new hydrogels prepared by the AA group were characterized in collaboration with the Brandeis University, Waltham, Massachusetts, USA. The imaging agents synthesized by the BC, HC and the AA groups are also evaluated within national (UC) and international collaborations (École Polytechnique Fédéral de Lausanne, Switzerland; Centre de Biophysique Moléculaire CNRS, France). Department of Chemistry, University of Bath, UK. Studies using microfluids devices with aqueous two-phase systems were started with the Algoritmi research centre of the School of Engineering.

The synthesis of carbon-based nanomaterials and the functionalization of CNTs involves researchers from the HC and EE groups in collaboration with members of the Polymer Engineering Department, for the preparation and characterization of new materials and composites.

## **5. Atividades de interação com a sociedade implementadas durante 2013**

- "Olimpíadas de Química Júnior" - em colaboração com a Sociedade Portuguesa de Química, a 9ª edição desta atividade decorreu nos laboratórios do Departamento de Química e no anfiteatro da Escola de



Ciências da Universidade do Minho, no dia 13 de Abril de 2013. Nesta edição das OQJ participaram 30 escolas com 30 equipas, o que se traduziu num número de participantes (90 alunos e 30 professores acompanhantes). Foi organizado por Maria Manuela Silva, Maria José Medeiros, Gabriela Botelho, Susana Costa, Manuela Raposo e Sílvia Lima.

- "Estágios Ciência Viva no Laboratório" - "Ocupação Científica de Jovens nas Férias – Edição 2013 (Ciência Viva)", de 9 a 20 de Julho de 2013, evento organizado por Alice Dias e Maria José Medeiros e contou com a participação de Maria Alice Carvalho (2 estágios: "Síntese de N-óxidos heterocíclicos com potencial atividade anticancerígena", 1 a 5 julho; Síntese de pirimidopirimidinas com potencial atividade antituberculose" 1 a 5 Julho.

- Integrados na iniciativa Festa da Ciência 2013 da Escola de Ciências da Universidade do Minho, (Universidade do Minho - Campus de Gualtar, 13 a 16 de Maio) o Departamento de Química realizou as seguintes atividades:

- "Nós e a Química", sessão experimental, evento organizado por Alice Dias, João Paulo André, Maria José Medeiros, Iwona Kuzniarska-Biernacka e contou com a colaboração dos alunos da Licenciatura em Química na demonstração da experiências.

- "Galeria de Prémios Nobel da Química", exposição itinerante;

- "Água - Estado Líquido (II)", exposição fotográfica;

- Concurso "Faz e traz uma Tabela Periódica" organizado por Carlos Jorge Silva e que contou com a participação de alunos dos 9º e 10º ano de escolaridade.

Química para Jovens Cientistas: sessões experimentais, 13 e 14 de maio de 2013, evento organizado por Alice Dias, João Paulo André, Iwona Kuzniarska-Biernacka e Maria José Medeiros. Contou com a colaboração de alunos da Lic. Química na demonstração das experiências. (135 alunos, 7 sessões de 1 hora, Colégio João Paulo II, Externato Carvalho Araújo, EB2,3 de Gualtar, ES de Vila Verde, 7º -11º anos de escolaridade.)

Química para Jovens Cientistas: sessões experimentais, 16 de maio de 2013, evento organizado por Alice Dias, João Paulo André, Iwona Kuzniarska-Biernacka e Maria José Medeiros. Contou com a colaboração de alunos da Lic. Química na demonstração das experiências. (24 alunos, 1 sessão de 1 hora, Colégio João Paulo II 3º anos de escolaridade.)

Exposição "10 passos na química...", 13 a 16 de maio de 2013, exposição, da autoria do Núcleo Académico de Química em colaboração com o Departamento de Química da Universidade do Minho.

- "QSI:Uminho, Química sob investigação" sessões experimentais, elaboração de uma apresentação oral, projeção de vídeos sobre a Química no dia-a-dia e palestras realizados ao longo de uma semana 22 a 26 de julho, 23 participantes. Esta iniciativa foi organizada por Maria Alice Carvalho com colaboração de António Gil Fortes, Luís Monteiro, Paula Ferreira, António Maurício Fonseca, José Alberto Martins, Sameiro Gonçalves, João Carlos Marcos e Michael John Smith.

- Integrados na iniciativa Noite Europeia dos Investigadores 2013 da Escola de Ciências, Universidade do Minho, 27 de setembro de 2013, o Departamento de Química realizou duas atividades hands on em Ciência e Tecnologia:

- Integrados na iniciativa De Portas Abertas à Ciência e Tecnologia 2013 da Escola de Ciências da Universidade do Minho, (Universidade do Minho - Campus de Gualtar, 20 a 22 de novembro) o Departamento de Química realizou as seguintes atividades:

- “Química para Pequenos Cientistas”, 20 dezembro de 2013, sessão experimental dirigida aos alunos do ensino pré-escolar e 1º ciclo do ensino básico e contou com a participação de Alice Dias, António Gil Fortes e Maria Alice Carvalho. (3 sessões de 1 hora, 66 alunos).

- “Química do dia-a-dia”, sessão experimental dirigida aos alunos do 3º ciclo do ensino básico e contou com a participação de Sílvia Pereira-Lima, Ana Paula Bettencourt Estevão, Maria do Sameiro Gonçalves, Luís Monteiro e M. Manuela Raposo.

Integradas na atividade Tertúlia FNACiências

- FNAC (Braga) - Tertúlia “FNAC Ciência” – “Diálogo entre a Química e a Arqueologia: O uso de consumo na época Romana”, César Oliveira e Rui Manuel Morais (Dep. História, ICS-UMinho) 21 de março.

- FNAC (Braga) - Tertúlia “FNAC Ciência” – “Celebrando efemérides Bioquímicas em 2013 - dos enzimas ao DNA”, João Carlos Marcos e Miguel Castanho (FMULisboa), 17 de outubro.

3. Integradas na atividade Noite Europeia dos Investigadores-2013, realizada no Museu D. Diogo de Sousa, Braga, em 27 Setembro, 2013.

- João Paulo André, palestra “Ópera, Veneno e outros químicos”, Escola de Ciências da Universidade do Minho (“A Minha Escola de Ciências”), 1 de Outubro de 2013.

## **6. Coordenação e participação em projetos de investigação com financiamento externo**

- **PTDC/QUI-BIQ/118389/2010** “Structure based design, biological activity and model membrane permeation studies of antimicrobial peptides bearing unnatural amino acids” total financial support 99.330,00 Euros. UM proponent S.P. Costa (AA), total financial support UM 99.330 Euros 2012- 2015, 27.076,84 Euros for 2013.

- **PTDC/QUI-QUI/111060/2009** “New antitumoral and antiangiogenic heterocyclic compounds: synthesis, molecular modelling, screening of enzymatic inhibition and studies in tumor and endothelial cell lines with tyrosine kinase membrane receptors as targets.” total financial support 134.000 Euros. UM proponent M.J.R.P. Queiroz (HC), total financial support UM 30.744 Euros dec. 2010- June 2014, 4.867,22 Euros for 2013.

- **PTDC/CTM/105597/2008** Nonlinear spectroscopy of push-pull organic molecules (PI/CFUM, team members HC, AA total 165000€) – from 01/11/09 ongoing till december 2013,
- **PTDC/CTM-NAN/119184/2010** (PI: Univ. Aveiro, Team members from Biocant and HC, from 01-03-2012 total funding 131140€) ongoing - Modulation of induced pluripotent stem cells differentiation by carbon nanotube templates – StemCelCan. UM funding 23634,00
- **PTDC/QEQ-MED/1671/2012** “Concise and Highly Stereoselective Strategy in the Synthesis of Azasugars. Theoretical Studies and Biological Evaluation of Products (PI/HC CQUM total funding 197.479,00€ início e fim previsto do projeto 03-06-2013 a 02-06-2015, funding 29.621,85€ 2013.
- **PTDC/CTM/099124/2008** “Electrochromic thin film transistors for smart windows applications - ELECTRA”, (PI-UNL, team member from EE, total 180.000€) jan. 2009- July 2013, funding UM 28.000,00€, 12087, 27€ 2013.
- **PTDC/CTM-NAN/119979/2010** Synthesis of solar-activated materials for the controlled release of volatile compounds (PI: CFUM team member from EE total funding 151.140,00€) 01-03-2012- 28-02-2015, 1000€ 2013.
- **PTDC/EPH-ARQ/5204/2012** “Dialogue among sciences - Multidisciplinary analysis of navegability and anchoring during the Roman period (Esposende), (PI: UP, team members from EE, total funding 85.621,00 euros), funding UM 7500,00€, 2013-2000€.
- **O Novo Norte – Programa Operacional Regional do Norte, “Programas Integrados de IC&DT - SAESCTN-PIIC&DT/1/2011”**, Projeto aprovado: n-SteP – Nanostructured systems for Tailored Performance, WP1, WP2 - Preparation and characterization of the catalysts (PI:IPC-UM, team members from BC, EE and HC ) (Total funding -2013/2014: 47000 euros, 2013, 10.000 euros.
- **Ação Integrada Luso-Espanhola Refª E 136/12**, Desenvolvimento de sensores para a deteção de biotoxinas em bivalves, 4000 euros para a UMinho (team members from EE) (2013: 1500 euros)

## 7. Financiamento

Incluir os detalhes de financiamento, separando a execução em 2013 e os montantes obtidos nesse ano, nas rúbricas em que tal for aplicável.

	<b>Financiamento atribuído em 2013</b>	<b>Financiamento recebido em 2013</b>	<b>Financiamento executado em 2013</b>	<b>Nº de Projetos em curso</b>
<b>Projeto Estratégico FCT</b>	75.011,00€	24.068,85€	70.636,73€*	1
<b>Projectos FCT</b>	131.266,22€	95.576,87€	96.585,58€*	4
<b>Proj. Nacionais</b>	1.500,00€	1.500,00€	1.500,00€	1

<b>(bilaterais,...)</b>				
<b>Proj. Internacionais (FP7, ...)</b>				
<b>Rede Nacional de RMN-UM</b>	21.500,00€	21.500,00€	20.687,56	1
<b>Proj. Industria internacional</b>				
<b>Proj. Industria nacional</b>				
<b>Total</b>	229.277,22€	141.645,72€	189.409,87€	7

\* O financiamento executado é superior ao recebido devido a adiantamento de verbas por parte da Universidade.

## 8. Indicadores genéricos

Nesta secção deve ser dada informação relativa aos investigadores e ao número de teses de Mestrado e de Doutoramento concluídas e em curso, durante 2013.

### 8.1. Equipa de Investigação

<b>Investigação</b>	<b>2013</b>
<b>Classificação</b>	Excellent
<b>Investigadores</b>	
Docentes/Investigadores Ens. Superior	26
Compromisso com a Ciência	4
Colaboradores	39
Post-Docs	9
Doutorandos	32
Mestrandos	67

### 8.2. N.º de teses de Mestrado e de Doutoramento concluídas e em curso, durante 2013.

<b>N.º de teses de Mestrado</b>	<b>Concluídas</b>	36
	<b>Em curso</b>	31
<b>N.º de teses de Doutoramento</b>	<b>Concluídas</b>	5
	<b>Em curso</b>	28

## 9. Investigação

### 9.1. Grupos de Investigação

<b>Designação do grupo de investigação</b>	Synthesis and Application of Amino Acids (AA)
<b>Coordenador</b>	Paula Margarida Ferreira
<b>Área de investigação</b>	Amino acid and Peptide Chemistry
<b>Instituição de Acolhimento</b>	CQ/UM School of Sciences
<b>Membros do grupo</b>	<p><b>FTERS:</b></p> <p>Permanent staff</p> <p>Lúis S. Monteiro, Paula M.T. Ferreira, , Susana P. G. Costa, Maria Sameiro Gonçalves, Sílvia P. Lima.</p> <p><b>Post-Doc researchers</b></p> <p>Rosa Batista SFRH/BPD/79333/2011 (HC/AA)</p> <p><b>PhD researchers</b></p> <p>Ana Piloto Cerqueira SFRH/BD/61459/2009(AA) – concluded in december 2013</p> <p>André Fontes SFRH/BD/63676/2009 (AA/BC)</p> <p>Arsénio Sá SFRH/BD/63639/2009 (AA/BC)</p> <p>Ana Soares SFRH/BD/80813/2011 (AA)</p> <p>Cátia Esteves SFRH/BD/68360/2010 (AA/HC)</p> <p>Maria Helena Vilaça SFRH/BD/72651/2010 (AA/BC)</p> <p>Rosa Cristina Ferreira SFRH/BD/86408/2012 (AA/HC)</p>

<b>Designação do grupo de investigação</b>	Biological Chemistry (BC)
<b>Coordenador</b>	João Carlos Marcos
<b>Área de investigação</b>	Biological Chemistry
<b>Instituição de Acolhimento</b>	CQ/UM School of Sciences
<b>Membros do grupo</b>	<p><b>FTERS:</b></p> <p>Permanent staff</p> <p>João Carlos Marcos, João Paulo André, José Alberto Martins</p> <p><b>Researchers hired under the Programme</b></p> <p><b>“Compromisso com a Ciência”</b></p> <p>Nuno Micaêlo e Issam Oueslati (the 5 years contract finished)</p>

	<p>on April 2013)</p> <p><b>PhD students</b></p> <p>Maria Helena Vilaça SFRH/BD/72651/2010 (BC/AA)</p> <p>André Fontes SFRH/BD/63676/2009 (BC/AA)</p> <p>Arsénio Sá SFRH/BD/63639/2009 (BC/AA)</p> <p>Miguel Ferreira SFRH/BD/63994/2009 (BC)</p> <p>Tarsila Castro SFRH/BD/79195/2011 (BC)</p>
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<b>Designação do grupo de investigação</b>	Electrochemistry and the Environment (EE)
<b>Coordenador</b>	Michael John Smith
<b>Área de investigação</b>	Electrochemical, Catalysis, Analytical Chemistry, Materials Chemistry, Physical Chemistry
<b>Instituição de Acolhimento</b>	CQ/UM School of Sciences
<b>Membros do grupo</b>	<p><b>FTEs:</b></p> <p>Permanent staff- Michael J Smith, Maria José Medeiros, Carlos Jorge Silva, António Maurício Fonseca, Pier Parpot, Maria de Fátima Bento, Maria Dulce Geraldo, Ana Paula Bettencourt, Maria Isabel Correia Neves, Maria Manuela Silva, Maria Gabriela Botelho.</p> <p><b>Researchers hired under the Programme</b></p> <p><b>“Compromisso com a Ciência”-</b> César Oliveira, Iwona Kuzniarska-Biernacka (this five year contract finished in august 2013)</p> <p><b>Research hired in the scope of a research project</b></p> <p>- Iwona Kuzniarska-Biernacka for a period of two years since sept. 2013</p> <p><b>Post-doctoral researchers:</b></p> <p>Sandra Barros SFRH/BPD/85399/2012 (EE)</p> <p>Rui Pereira SFRH/BPD/87759/2012 (EE)</p> <p>Rui Gusmão SFRH / BPD / 86690 / 2012 (EE/HC)</p> <p><b>PhD students:</b></p> <p>Ana Catarina Teixeira catro Lopes SFRH/BD/62507/2009- concluded Sept 2013</p> <p>Daniela Correia SFRH/BD/82411/2011 (EE)</p>

	<p>Juliana Dias SFRH/BD/90215/2012 (EE)</p> <p>Maria Cidália Rodrigues Castro SFRH/BD/78037/2011 (EE/HC)</p> <p>Raquel Miriam dos Santos SFRH/BDE/15657/2007-concluded Sept 2013</p> <p>Raquel Santos Oliveira SFRH/BD/64189/2009 (EE)</p> <p>Renato Gonçalves SFRH/BD/88397/2012 (EE)</p> <p>Rita Daniela Barros Leones SFRH/BD/90366/2012 (EE)</p> <p>Rita Maria Burguete Bacelar Marreiros SFRH/BD/62601/2009 (EE)</p> <p>Sara Sofia Marques Fernandes SFRH/BD/87786/2012 (EE/HC)</p> <p>Sandra Daniela Freitas da Costa Moreira SFRH/BD/46618/2008-concluded in 2013 (EE)</p>
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<b>Designação do grupo de investigação</b>	Synthesis and Application of Heterocycles (HC)
<b>Coordenador</b>	Maria Fernanda Proença
<b>Área de investigação</b>	Heterocyclic Chemistry
<b>Instituição de Acolhimento</b>	CQ/UM School of Sciences
<b>Membros do grupo</b>	<p><b>FTEs:</b></p> <p>Permanent staff - Maria Fernanda de Jesus Rego Paiva Proença, Ana Maria Ferreira de Oliveira-Campos, Maria João Ribeiro Peixoto de Queiroz, Maria José da Chão Alves, Maria Manuela Marques Raposo, Ana Paula da Assunção Esteves, Alice Maria Dias, Maria Alice Carvalho, António Belmiro Gil Fortes</p> <p><b>Post-Doc grant researchers:</b></p> <p>Agathe Begouin SFRH/BPD/36753/2007 from Nov07 (HC)</p> <p>Ricardo Calhelha SFRH/BPD/68344/2010 from Jan 11, also affiliated to CIMO/Escola Superior Agrária/IPBragança (HC)</p> <p>Marta Costa SFRH/BPD/79609/2011 (HC)</p> <p>Rosa Batista SFRH/BPD/79333/2011 (HC/AA)</p> <p>Rui Filipe Araújo SFRH/BPD/88920/2012 (HC)</p> <p>Rui Gusmão SFRH / BPD / 86690 / 2012 (HC/ EE)</p>

	<p>Maria del Carmen de la Fuente Seijo (under the scope of a research Project)</p> <p><b>PhD students:</b></p> <p>Ashly Rocha SFRH/BD/79565/2011 (HC)</p> <p>Cátia Esteves SFRH/BD/68360/2010 (HC/AA)</p> <p>Carla Santana Francisco SFRH/BD/48636/2008 (HC)- concluded in december 2013.</p> <p>Cristina Elisabete A. De Sousa SFRH/BD/87292/2012 (HC)</p> <p>Cristina Rafaela Guimarães SFRH/BD/78307/2011 (HC)</p> <p>Elina Marinho SFRH/BD/73659/2010 (HC)</p> <p>Juliana Andrade grant of “Programa Ciência sem fronteiras” 246713/2012-7 (HC)</p> <p>Maria Cidália Rodrigues Castro SFRH/BD/78037/2011 (HC/EE)</p> <p>Maria Solange Dantas de Carvalho SFRH/BD/47052/2008 (HC) - concluded in july 2013.</p> <p>Nádia Senhorães SFRH/BD/73721/2010 (HC)</p> <p>Rosa Cristina Ferreira SFRH/BD/86408/2012 (HC/AA)</p> <p>Sara Sofia Marques Fernandes SFRH/BD/87786/2012 (HC/EE)</p> <p>Sandrina Heleno SFRH/BD/70304/2010 (HC)</p> <p>Tatiana Dias SFRH/BD/88245/2012 (HC)</p> <p>Vera Alexandra P. Machado SFRH/BD/77373/2011 (HC)</p> <p>Vera Cristiana Moreira Duarte SFRH/BD/61290/2009 (HC)</p>
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## 9.2. Produtividade Científica

### 1. Artigos em revistas internacionais (referenciadas no ISI)

**AA** (10AA+2AA/HC+2AA/BC=14)

**AA1** - Piloto, A. M.; Hungerford, G.; Costa, S. P. G.; Gonçalves, M. S. T., “Acridinyl methyl esters as photoactive precursors in the release of neurotransmitter amino acids”, *Photochem. Photobiol. Sci.* 2013, 12:339-347. <http://dx.doi.org/10.1039/C2PP25261A> (IF12=2.923)

**AA2** - Raju, B. R.; Firmino, A. D. G.; Costa, A. L. S.; Coutinho, P. J. G.; Gonçalves, M. S. T., “Synthesis and photophysical properties of side-chain chlorinated benzo[a]phenoxazinium chlorides”, *Tetrahedron* 2013, 69:2451-2461. <http://dx.doi.org/10.1016/j.tet.2013.01.035> (IF12=2.803).



- AA3** - Firmino, A. D. G.; Raju, B. R.; Gonçalves, M. S. T., "Microwave synthesis of novel water-soluble 2-, 5- and 9-substituted benzo[a]phenoxazinium chlorides in comparison with conventional heating" *Eur. J. Org. Chem.* 2013, 1506-1514. <http://dx.doi.org/10.1002/ejoc.201201354> (IF12=3.344).
- AA4** - Fernandes, M. J. G.; Costa, S. P. G.; Gonçalves, M. S. T., "Synthesis and light triggered release of catecholamines from pyrenylmethylcarbamate cages" *New J. Chem.*, 2013,37:2369-2376. <http://dx.doi.org/10.1039/C3NJ00247K> (IF12=2.966).
- AA5** - Raju, B. R.; Naik, S.; Coutinho, P.J. G.; Gonçalves, M. S. T., "Novel Nile Blue derivatives as fluorescent probes for DNA", *Dyes Pigm.*2013, 99:220-227. <http://dx.doi.org/10.1016/j.dyepig.2013.05.007> (IF12=3.532).
- AA6** - Piloto, A. M.; Hungerford, G.; Costa, S. P. G.; Gonçalves, M. S. T., "Photoinduced release of neurotransmitter amino acids from novel coumarin fused julolidine ester cages", *Eur. J. Org. Chem.*2013, 34:7715-7723. <http://dx.doi.org/10.1002/ejoc.201300730> (IF12=3.344).
- AA7** - Aguiar, N. R.; Castro, V. I.; Ribeiro, A. I.; Fernandes, R. D. V.; Carvalho, C. M.; Costa, S. P. G.; Pereira-Lima, S. M. M. A., "alpha,alpha-Dialkylglycines obtained by solid phase Ugi reaction performed over isocyanide functionalized resins", *Tetrahedron*, 2013, 69: 9161-9165. <http://dx.doi.org/10.1016/j.tet.2013.08.002> (IF12=2.803).
- AA8** - Ferreira, P. M. T.; Monteiro, L. S.; Pereira, G.; Castanheira, E. M. S.; Frost, C. G., "Synthesis of Fluorescent Alanines by a Rhodium-Catalysed Conjugate Addition of Arylboronic Acids to Dehydroalanine Derivatives", *Eur. J. Org. Chem.*, 2013, 3, 550-556. <http://dx.doi.org/10.1002/ejoc.201201198> (IF12=3.344).
- AA9** - Pereira, G.; Vilaca, H.; Ferreira, P. M. T., "Synthesis of new beta-amidodehydroaminobutyric acid derivatives and of new tyrosine derivatives using copper catalyzed C-N and C-O coupling reactions", *Amino Acids*, 2013, 2, 335-344. <http://dx.doi.org/10.1007/s00726-012-1337-4> (IF12=3.914).
- AA10** - Pereira, G.; Castanheira, E. M. S.; Schellenberg, P.; Belsley, M.; Ferreira, P. M. T.; Monteiro, L. S., "Synthesis and photophysical studies of new pyrenyl amino acids", *Tetrahedron*, 2013, 69, 10254-10261. <http://dx.doi.org/10.1016/j.tet.2013.10.035> (IF12=2.803).
- AA11/HC23** - Batista, R. M. F.; Costa, S. P. G.; Raposo, M. M. M. "Naphthyl-imidazo-anthraquinones as novel colorimetric and fluorimetric chemosensors for ion sensing" *J. Photochem. Photobiol. Chem. A* 2013, 259:33-40.

<http://dx.doi.org/10.1016/j.jphotochem.2013.03.001>

(IF12=2.416)

**AA12/HC24** - Pina, J.; Seixas de Melo J. S.; Batista, R. M. F.; Costa, S. P. G.; Raposo, M. M. M., "Triphenylamine-benzimidazole derivatives: synthesis, excited-state characterization and DFT studies" *J. Org. Chem.* 2013, 78:11389-11395. <http://dx.doi.org/10.1021/jo401803u> (IF12=4.564).

**AA13/BC9** - Ferreira, M. F.; Martins, A. F.; Martins, C. I. O.; Ferreira, P. M.; Toth, E.; Rodrigues, T. B.; Calle, D.; Cerdan, S.; Lopez-Larrubia, P.; Martins, J. A.; Geraldes, C. F. G. C. "Amide conjugates of the DO3A-N-(alpha-amino)propionate ligand: leads for stable, high relaxivity contrast agents for MRI?", *Contrast Media & Molecular Imaging*, 2013, 8, 40-49. <http://dx.doi.org/10.1002/cmimi.1492> (IF12=2.872).

**AA14/BC8** - de Sá, A.; Bonnet, C. S.; Geraldes, C. F. G. C.; Toth, E.; Ferreira, P. M. T.; Andre, J. P., "Thermodynamic stability and relaxation studies of small, triaza-macrocyclic Mn(II) chelates", *Dalton Trans.*, 2013, 42, 4522-4532. <http://dx.doi.org/10.1039/c2dt32496b> (IF12=3.806).

**BC** (7BC + 2BC/AA + 1BC/HC = 10)

**BC1** - Barros, S. C.; Louro, R. O.; Micaelo, N. M.; Martins, J. A.; Marcos, J. C.; Cavaco-Paulo, A. NMR and molecular modelling studies on elastase inhibitor-peptides for wound management. *Reactive & Functional Polymers* 2013, 73(10) 1357-1365 <http://dx.doi.org/10.1016/j.reactfunctpolym.2013.02.011> (IF: 2.505).

**BC2** - Gonçalves, C.; Lalatonne, Y.; Melro, L.; Badino, G.; Ferreira, M. F. M.; L. David, C. F. G. C. Geraldes, L. Motte, Martins, J. A.; Gama, F. M. New dextrin nanomagnetogels as contrast agents for magnetic resonance imaging, *J. Mater. Chem. B*, 2013, 1(42): 5853-5864. <http://dx.doi.org/10.1039/c3tb21063d>

**BC3** - Martins, J.A. and Micaelo, N.M. "Short-range order in polyethylene melts: Identification and characterization" *Macromolecules*, 2013, 46(19):7977-7988, <http://dx.doi.org/10.1021/ma4009934> (IF: 5.521)

**BC4** - Cruz, A. and Micaelo, N. and Félix, V. and Song, J.-Y. and Kitamura, S.-I. and Suzuki, S. and Mendo, S. "SugE: A gene involved in tributyltin (TBT) resistance of *Aeromonas molluscorum* Av27" *Journal of General and Applied Microbiology*, 2013, 59(1):39-47 <http://dx.doi.org/10.2323/jgam.59.47> (IF: 1.12)

**BC5** - Caramelo-Nunes, C., Almeida, P., Marcos, J.C., Tomaz, C.T., "Specific recognition of supercoiled plasmid DNA by affinity chromatography using the intercalator DAPP as ligand" *Journal of Chromatography B* 2013, 928:121-124 <http://dx.doi.org/10.1016/j.jchromb.2013.04.001> (IF=2.487)

**BC6** - Caramelo-Nunes, C., Bicho, D., Almeida, P., Marcos, J.C., Tomaz, C.T., "Dynamic binding capacity and specificity of 3,8-diamino-6-phenylphenanthridine-Sepharose support for purification of supercoiled plasmid deoxyribonucleic acid" *Journal of Chromatography A* 2013, 1307:91-98. <http://dx.doi.org/10.1016/j.chroma.2013.07.078> (IF = 4.612)

**BC7** - André, J. P. Opera and Poison: A Secret and Enjoyable Approach to Teaching and Learning Chemistry, *Journal of Chemical Education*, 2013, 90:352-357. <http://dx.doi.org/10.1021/ed300445b> (IF:0.817)

**BC8/AA14** - de Sá, A.; Bonnet, C. S.; Geraldés, C. F. G. C.; Tóth, É.; Ferreira, P. M.T; André, J. P. Thermodynamic stability and relaxation studies of small, triaza-macrocylic Mn(II) chelates, *Dalton Transactions*, 2013, 42:4522-4532. <http://dx.doi.org/10.1039/c2dt32496b> (IF12=3.806).

**BC9/AA13** - Ferreira, M. F.; Martins, A. F.; Martins, C. I. O.; Ferreira, P. M.; Toth, E.; Rodrigues, T. B.; Calle, D.; Cerdan, S.; Lopez-Larrubia, P.; Martins, J. A.; Geraldés, C F. G. C. Amide conjugates of the DO3A-N-(alpha-amino)propionate ligand: leads for stable, high relaxivity contrast agents for MRI?. *Contrast Med. Mol. Imaging* 2013, 8:40-49. <http://dx.doi.org/10.1002/cmml.1492> (IF12=2.872).

**BC10/HC29** - Duarte, V.C.M. and Faustino, H. and Alves, M.J. and Gil Fortes, A. and Micaelo, N. "Asymmetric Diels-Alder cycloadditions of d-erythrose 1,3-butadienes to achiral t-butyl 2H-azirine 3-carboxylate" *Tetrahedron Asymmetry*, 2013, 24(18):1063-1068. <http://dx.doi.org/10.1016/j.tetasy.2013.05.015>  
IF: 2.143

**EE** (41EE+4EE/HC=45)

**EE1** - Kuźniarska-Biernacka, I; Fonseca, A. M; Neves, I.C; "Manganese complexes with triazenido ligands encapsulated in NaY zeolite as heterogeneous catalysts", *Inorganica Chimica Acta* 2013, 394:591-597. DOI: 10.1016/j.ica.2012.09.027 (IF2012 = 1.687)

**EE2** - Machado, A.V; Amorim, S; Botelho, G; Neves, I.; M. Fonseca, A.M.; "Nanocomposites of poly( $\epsilon$ -caprolactone) doped with titanium species", *J. Mater. Sci.* 2013, 48:3578-3585. DOI: 10.1007/s10853-013-7154-7 (IF2012 = 2.133)

**EE3** - Kuźniarska-Biernacka, I; Rodrigues, O; Carvalho, M. A.; Parpot, P; Biernacki, K.; Magalhães, A.L; Fonseca, A.M.; Neves, I C; "Electrochemical and catalytic studies of manganese(III) complex with tetradentate Schiff base encapsulated in NaY zeolite" *Eur. J. Inorg. Chem.* 2013, 2768-2776. DOI: 10.1002/ejic.201201517 (IF2012 = 3.120)

**EE4** - Ferreira, M; Pinto, M; Soares, F.O.S.G.P; Pereira, M. F. R; Órfão, J. J. M; Figueiredo, J. L; Neves, I. C; Fonseca, A. M; Parpot, P; "The electrochemical mineralization of oxalic and oxamic acids using modified electrodes based on carbon nanotubes", *Chem. Eng. J.* 2013, 228:374–380. (IF2012 = 3.473)

- EE5** - Fonseca, A. M., Neves, I. C; "Study of silver species stabilized in different microporous zeolites Microporous & Mesoporous Materials", *Micropor. Mesopor. Mat.* 2013, 181:83-87. DOI: 10.1016/j.micromeso.2013.07.018 (IF2012 = 3.365)
- EE6** - Vilaca, N; Amorim, R; Machado, A. F; Parpot, P; Pereira, M. F.R; Sardo, M; Rocha, J; Fonseca, A. M; Neves, I. C; Baltazar, F; "Potentiation of 5-fluorouracil encapsulated in zeolites as drug delivery systems for in vitro models of colorectal carcinoma", *Colloid. Surfaces B* 2013, 112:237-244. Doi:10.1016/j.colsurfb.2013.07.042 (IF2012 = 3.554)
- EE7** - Lopes, A.C; Costa, C.M; Serra, R.S; Neves, I.C; Gomez-Ribelles, J.L; Lanceros-Méndez, S; Dielectric Relaxation, ac Conductivity and Electric Modulus in Poly(vinylidene fluoride) - NaY Zeolite Composites, *Solid State Ionics* 2013, 253:42-50. DOI: 10.1016/j.ssi.2013.01.013 (IF12 = 2.046)
- EE8** - Gonçalves, R.; Lopes, A.C.; Botelho, G.; Neves, I.C.; Lanceros-Méndez, S.; Influence of solvent properties on the electrical response of poly(vinylidene fluoride)/NaY composites, *J. Polym. Res.* 2013, 20:143. DOI: 10.1007/s10965-013-0143-3 (IF12 =2.019)
- EE9** - Duñach, E; Medeiros, M. J; Olivero, S; "Electrochemical Catalytic Cyclization Reactions using Environmentally Friendly Methodologies", *J. Electrochem. Soc.*, 2013, 160, G3112-G3116, doi: 10.1149/2.016307jes (IF = 2.588)
- EE10** – Santos, R. M; Pimenta, A; Botelho, G; Machado, A.V; "Influence of the testing conditions on the efficiency and durability of stabilizers against ABS photo-oxidation" *Polymer Testing* 2013, 32: 78–85 (IF12=1.646)
- EE11** – Gonçalves, R; Martins, P. M; Caparrós, C; Martins, P; Benelmekki, M; Botelho, G; Lanceros-Mendez, S; Gutierrez, J; Barandiaran, J. M; "Nucleation of the electroactive  $\beta$ -phase, dielectric and magnetic response of poly(vinylidene fluoride) composites with Fe<sub>2</sub>O<sub>3</sub> nanoparticles" *Journal of Non-Crystalline Solids* 2013, 361: 93 (IF12=1.597)
- EE12** – Martins, P; Costa, C. M; Benelmekki, M; Botelho G; Lanceros-Mendez, S; "Interface characterization and thermal degradation of ferrite/poly(vinylidene fluoride) multiferroic nanocomposites" *Journal of Materials Science* 2013, 48: 2681-2689. (IF12=2.163)
- EE13** – Lopes, A. C; Carabineiro, S; Pereira, M. F. R; Botelho, G; Lanceros-Mendez, S; "Nanoparticle Size and Concentration Dependence of the Electroactive Phase Content, Electrical and Optical Properties of Ag/poly(vinylidene Fluoride) Composites" *The Journal of Physical Chemistry* 2013, 14: 1926-1933 (IF12=4.814)
- EE14** - Delgado-Lima, A; Botelho, G; Silva, M.M; Machado, A.V; "Durability of PCL nanocomposites under different environments" *Journal of Polymers and Environment* 2013, 21: 710–717 (IF12=1.495)
- EE15** – Santos, R; Botelho, G; Cramez, C; Machado, A. V; "Outdoor and Accelerated Weathering Of Acrylonitrilebutadiene-Styrene: A Correlation Study" *Polymer Degradation and Stability* 2013, 98: 2111-2115. (IF12=2.770)

- EE16** - Muiuane, V. P; Ferreira, M; Bignet, P; Bettencourt, A. P; Parpot, P; "Production of formic acid from biomass-based compounds using a filter press type electrolyzer", *J. Environ. Chem. Eng.* 2013, 1: 1237–1244. <http://dx.doi.org/10.1016/j.jece.2013.09.014>. (IF12=new journal, not defined)
- EE17** - Pio, C; Mirante, F; Oliveira, C; Matos, M; Caseiro, A; Oliveira, C; Querol, X; Alves, C; Martins, N; Cerqueira, M; Camões, F; Silva, H; Plana, F; "Size-segregated chemical composition of aerosol emissions in an urban road tunnel in Portugal" *Atmospheric Environment* 2013, 71, 15-25. <http://dx.doi.org/10.1016/j.atmosenv.2013.01.037> (IF12=3.110)
- EE18** – Oliveira, R; Pereira, N; Geraldo D; Bento F; "Reactivity of hydroxy-containing aromatic compounds towards electrogenerated hydroxyl radicals", *Electrochimica Acta* 2013, 105: 371 – 377. <http://dx.doi.org/10.1016/j.electacta.2013.04.124> (IF12=3,777)
- EE19** – Oliveira, R; Bento, F; Stella, C; Thoin, L; Amatore, C; "Direct Electroanalytical Method for Alternative Assessment of Global Antioxidant Capacity Using Microchannel Electrodes", *Analytical Chemistry* 2013, 85: 9057 - 9063. <http://pubs.acs.org/doi/abs/10.1021/ac401566w> (IF12=5,695)
- EE20** – Leones R; Costa C; Machado A; Esperança J; Silva M; Lanceros-Méndez S; "Development of solid polymer electrolytes based on poly(vinylidene fluoride-trifluoroethylene) and the [N1 1 1 2(OH)]NTf2 ionic liquid for energy storage applications", *Solid State Ionics* 2013, 253: 143-150. <http://dx.doi.org/10.1016/j.ssi.2013.09.042> (FI12=2.046)
- EE21** - Leones R; Rodrigues L; Fernandes M; Ferreira R; Cesarino I; A. Pawlicka A; Carlos L; de Zea Bermudez V; Silva M; "Electro-optical properties of the DNA-Eu<sup>3+</sup> bio-membranes", *Journal of Electroanalytical Chemistry* 2013, 708C: 116-123. <http://dx.doi.org/10.1016/j.jelechem.2013.08.031> (FI12 = 2.672)
- EE22** - Nunes-Pereira J; Costa C; Leones R; Silva M; Lanceros-Méndez S; "Li-ion battery membranes separators based on poly(vinylidene fluoride-trifluoroethylene)/carbon nanotube composites", *Solid State Ionics* 2013, 249-250: 63-71. <http://dx.doi.org/10.1016/j.ssi.2013.07.021> (FI12 = 2.046)
- EE23** - Alves R; Silva M; "The influence of glycerol and formaldehyde in gelatin-based polymer electrolytes", *Molecular Crystals & Liquid Crystals*, 2013, 00: 1-10. <http://dx.doi.org/10.1080/15421406.2013.822739> (FI11 = 0.580)
- EE24** - Peixoto L; Rodrigues A; Martins G; Nicolau A; Brito A; Silva M; Parpot P; Nogueira R; "A flat microbial fuel cell for decentralized wastewater valorisation: process performance and optimization potential", *Environmental Technology*, 2013, 34 (13-14): 1947-1956. <http://dx.doi.org/10.1080/09593330.2013.827223> (FI12 = 1.606)
- EE25** - Gonçalves C; Rodrigues L; Silva M; Ferreira R; Carlos L; Hümmel J., de Zea Bermudez V; "Di-urethanesil hybrid electrolytes doped with Mg(CF<sub>3</sub>SO<sub>3</sub>)<sub>2</sub>", *Ionics*, 2013. <http://dx.doi.org/10.1007/s11581-013-0959-1> (FI12 = 1.674)

- EE26** - Costa C; Nunes-Pereira J; Sencadas V; Silva M; Lanceros-Méndez S; “Effect of fiber orientation in gelled poly(vinylidene fluoride) electrospun membranes for Li-ion battery applications”, *Journal of Materials Science*, 2013, 48 (Issue 19): 6833-6840. <http://dx.doi.org/10.1007/s10853-013-7489-0> (FI12 = 2.163)
- EE27** - Ferreira B; Fernandes M; Rodrigues L; Silva M; Smith M; de Zea Bermudez V; “Vibrational analysis of d-PCL(530) / siloxane-based hybrid electrolytes doped with two lithium salts” *Ionics* 2013, 19:1803-1809. <http://dx.doi.org/10.1007/s11581-013-0917-y> (FI12 = 1.674)
- EE28** – Costa C; Silva M; Lanceros-Méndez S; “Battery separators based on vinylidene fluoride (VDF) polymers and copolymers for lithium ion battery applications”, *RSC Advances*, 2013, 3(29): 11404-11417. <http://dx.doi.org/10.1039/C3RA40732B> (FI12 = 2.562)
- EE29** - Delgado-Lima A; G. Botelho G; Silva M; Machado V; “Durability of PCL nanocomposites under different environments” *Journal of Polymers and the Environment*, 2013, 21: 710-717. <http://dx.doi.org/10.1007/s10924-013-0585-z> (FI12 = 1.495)
- EE30** – Alves R; Rodrigues L; Andrade J; Fernandes M; Pinto J., Pereira L; Paulicka A; Martins R; Fortunato E; V. de Zea Bermudez V; Silva M; “Gelatin/Zn(CF<sub>3</sub>SO<sub>3</sub>)<sub>2</sub> polymer electrolytes for electrochromic devices”, *Electroanalysis*, 2013, 25 (Issue 6): 1483-1490. <http://dx.doi.org/10.1002/elan.201300038> (FI12 = 2.817)
- EE31** - Rodrigues L; Silva M; Smith M; Gonçalves A; Fortunato E; “Preparation and characterization of hybrid oxyethylene/siloxane electrolyte systems”, *Electroanalysis*, 2013, 25(Issue 2): 515-522. <http://dx.doi.org/10.1002/elan.201200508> (FI12 = 2.817)
- EE32** - Nunes-Pereira J; Lopes C; Costa C; Silva M; Lanceros-Méndez S; “Microporous membranes of MaY zeolite/poly(vinylidene fluoride-trifluoroethylene) for Li-ion battery separators”, *Journal of Electroanalytical Chemistry*, 2013, 689: 223-232. <http://dx.doi.org/10.1016/j.jelechem.2012.10.030> (FI12 = 2.672)
- EE33** – Costa C; Sencadas V; Rocha J., Silva M; Lanceros-Méndez S; “Evaluation of the main processing parameters influencing the performance of poly(vinylidene fluoride - trifluoroethylene) lithium ion battery separators”, *Journal of Solid State Electrochemistry*, 2013, 17: 861-870 <http://dx.doi.org/10.1007/s10008-012-1928-8> (FI11 = 2.279)
- EE34** – Costa, C; Nunes-Pereira, J; Rodrigues, L; Silva, M; Gomez Ribelles, J., Lanceros-Méndez, S; “Novel poly(vinylidene fluoride-trifluoroethylene)/poly (ethylene oxide) blends for battery separators in lithium-ion applications”, *Electrochimica Acta*, 88 (2013) 473-476. <http://dx.doi.org/10.1016/j.electacta.2012.10.098> (FI12 = 3.777)
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**HC** (22HC+ 4HC/EE+2HC/AA+1HC/BC=29)

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**HC8** - Heleno, S.A.; Martins, A.; Ferreira, I.C.F.R.; Sokovic´, M.; Esteves, A.P.; C´iric´, A.; Glamoc´lija, J.; Queiroz, M.-J.R.P. “Antimicrobial and demelanizing activity of Ganoderma lucidum extract, p-



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**HC25/EE42** - Araújo, Rui Filipe; Silva, Carlos Jorge; Paiva, Maria Conceição; Melle Franco, Manuel; Proença, Maria Fernanda; "Efficient Dispersion of Multi-walled Carbon Nanotubes in Aqueous Solution by Non-covalent Interaction with Perylene Bisimides", *RSC Adv.*, 2013, 3, 24535. <http://dx.doi.org/10.1039/c3ra42422g> . IF(2012) 2.562

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**HC27/EE44** - Kuzniarska-Biernacka, I.; Carvalho, M.A.; Rasmussen; S.B; Bañares, M.A.; Biernacki, K.; Magalhães, A.L.; Rolo, A.; Fonseca, A.M.; Neves, I.C. "Copper(II)imida-salen complexes encapsulated into NaY zeolite for oxidation reactions", *Eur. J. Inorg Chem.*, 2013, 5408-5417. <http://dx.doi.org/10.1002/ejic.201300656> IF2012 =3.12

**HC28/EE45** - Kuźniarska-Biernacka, I; Rodrigues, O; Carvalho, M.A.; Parpot, P.; Biernacki, K. ; Magalhães, A. L.; Fonseca, A. M.; Neves, I. C. "Electrochemical and catalytic studies of manganese(III) complex with tetradentate Schiff base encapsulated in NaY zeolite", *Eur. J. Inorg. Chem.*, 2013, 2768-2776. <http://dx.doi.org/10.1002/ejic.201201517> . IF2012=3.12

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**AA** - Raju, B. R.; Sampaio, D. M. F.; Silva, M. M.; Coutinho, P. J. G.; Gonçalves, M. S. T., "Ultrasound promoted synthesis of Nile Blue derivatives", *Ultrason. Sonochem.* 2014, 21:360-366. <http://dx.doi.org/10.1016/j.ultsonch.2013.05.010> (IF12=3.516).

**AA/HC** - Batista, R. M. F.; Costa, S. P. G.; Raposo, M. M. M., "Selective colorimetric and fluorimetric detection of cyanide in aqueous solution using novel heterocyclic imidazo-anthraquinones", *Sensors Actuators B: Chem.*, 2014, 191:791-799. <http://dx.doi.org/10.1016/j.snb.2013.10.030> (IF12=3.535).

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**AA/HC** - Batista, R. M. F.; Costa, S. P. G.; Raposo, M. M. M., “Cyanide and fluoride colorimetric sensing by novel imidazo-anthraquinones functionalized with indole and carbazole”, Supramol. Chem. 2014, 26:71-80. [\(IF12=1.546\)](http://dx.doi.org/10.1080/10610278.2013.824082)

**AA/BC** - Ferreira M. F.; Pereira G.; Martins, A. F.; Martins, C. I. O.; Prata, M. I. M.; Petoud, S.; Toth, E.; Ferreira, P. M. T.; Martins, J. A.; Geraldes, C. F. G. C., “Ln[DO3A-N- $\alpha$ -(pyrenebutanamido)propionate] complexes: optimized relaxivity and NIR optical properties”, Dalton Trans., accepted in Nov. 2013.

[\(IF12=3.806\)](http://dx.doi.org/10.1039/C3DT52958D)

**BC** - Latif, M.A.M. and Tejo, B.A. and Abedikargiban, R. and Abdul Rahman, M.B. and Micaêlo, N.M. "Modeling stability and flexibility of  $\alpha$ -Chymotrypsin in room temperature ionic liquids" Journal of Biomolecular Structure and Dynamics accepted june, published on line july 2013, [\(IF: 4.986\)](http://dx.doi.org/10.1080/07391102.2013.813411)

## 2. Artigos em revistas nacionais

### 3. Actas de Congressos internacionais

**AA** (6AA+4AA/HC=10)

**AA1** - Piloto, A. M.; Costa, S. P. G.; Gonçalves, M. S. T., “Azaheterocycles as caging groups: synthesis and photolysis studies with a model carboxylic acid”. In Proceedings of the 16th International Electronic Conference on Synthetic Organic Chemistry, a016, 1-30 November, 2012: Sciforum Electronic Conferences Series, Seijas, J. A.; Tato, M. P. V. and Lin, S.-K. (Eds), MDPI, Basel, Switzerland, 2013. (ISBN: 3-906980-26-X). <http://www.sciforum.net/conference/ecsoc-16/paper/1141/paper>

**AA2** - Piloto, A. M.; Fonseca, A. S. C.; Costa, S. P. G.; Gonçalves, M. S. T., “Selective photorelease of model amino acids from coumarin ester conjugates”. In Proceedings of the 16th International Electronic Conference on Synthetic Organic Chemistry, a034, 1-30 November, 2012: Sciforum Electronic Conferences Series, 2012. Seijas, J. A.; Tato, M. P. V. and Lin, S.-K. (Eds), MDPI, Basel, Switzerland, 2013. (ISBN: 3-906980-26-X). [http://www.usc.es/congresos/ecsoc/16/hall\\_a\\_GOS/a034/index.pdf](http://www.usc.es/congresos/ecsoc/16/hall_a_GOS/a034/index.pdf)

**AA3** - Soares, A. M. S.; Costa, S. P. G.; Gonçalves, M. S. T., “Photoresponsive prodrugs of butyric acid based on amino naphthopyranones”. In Proceedings of the 16th International Electronic Conference on Synthetic Organic Chemistry, a017, 1-30 November, 2012: Sciforum Electronic Conferences Series, Seijas, J. A.; Tato, M. P. V. and Lin, S.-K. (Eds), MDPI, Basel, Switzerland, 2013. (ISBN: 3-906980-26-X). [http://www.usc.es/congresos/ecsoc/16/hall\\_a\\_GOS/a017/index.pdf](http://www.usc.es/congresos/ecsoc/16/hall_a_GOS/a017/index.pdf)

**AA4** - Raju, B. R.; Sampaio, D. M. F.; Coutinho, P. J. G.; Gonçalves, M. S. T., "Ultrasonic mediated synthesis of new benzo[a]phenoxazinium chlorides and their photophysical studies". In Proceedings of the 16th International Electronic Conference on Synthetic Organic Chemistry, 1-30 November, 2012: SciforumElectronicConferences Series, Seijas, J. A.; Tato, M. P. V. and Lin, S.-K. (Eds), MDPI, Basel, Switzerland, 2013.(ISBN: 3-906980-26-X).

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**AA5** - Raju, B. R.; Gonçalves, M. S. T.; Coutinho, P. J. G., "Studies of DNA interactions with functionalized benzo[a]phenoxazinium chlorides". In Proceedings of the 16th International Electronic Conference on Synthetic Organic Chemistry, 1-30 November, 2012: SciforumElectronicConferences Series, Seijas, J. A.; Tato, M. P. V. and Lin, S.-K. (Eds), MDPI, Basel, Switzerland, 2013.(ISBN: 3-906980-26-X).

<http://www.sciforum.net/conference/ecsoc-16/paper/1116>

**AA6** - Raju, B. R.; Dias, A. I. F.; Coutinho, P. J. G.; Gonçalves, M. S. T., "Synthesis and photophysical behaviour in AOT/cyclohexane w/o microemulsions of a new benzo[a]phenoxazinium chloride with 3-((3-chloropropyl)disulfanyl)propyl)amino group". In Proceedings of the 16th International Electronic Conference on Synthetic Organic Chemistry, 1-30 November, 2012: SciforumElectronicConferences Series, Seijas, J. A.; Tato, M. P. V. and Lin, S.-K. (Eds), MDPI, Basel, Switzerland, 2013.(ISBN: 3-906980-26-X). <http://www.sciforum.net/conference/ecsoc-16/paper/1117>

**AA7/HC5** - Lima, N. E. M.; Batista, R. M. F.; Costa, S. P. G.; Raposo, M. M. M., "Iodine-catalysed synthesis of a novel meso-substituted dipyrromethane and its evaluation as a cation chemosensor", Proceedings of the 17th Int. Electron. Conf. Synth. Org. Chem., 1-30 November 2013; Sciforum Electronic Conference Series, 2013, 17, a002, <http://dx.doi.org/10.3390/ecsoc-17-a002> .

**AA8/HC6** - Ferreira, R. C. M.; Batista, R. M. F.; Costa, S. P. G.; Raposo, M. M. M., "Synthesis and photophysical characterization of novel tri-(hetero)arylimidazoles", Proceedings of the 17th Int. Electron. Conf. Synth. Org. Chem., 1-30 November 2013; Sciforum Electronic Conference Series, 2013, 17, a042, <http://dx.doi.org/10.3390/ecsoc-17-a042> .

**AA9/HC7** - Batista, R. M. F.; Costa, S. P. G.; Raposo, M. M. M., "Synthesis and evaluation of an imidazo-benzocrown ether functionalised amino acid as a new fluorimetric chemosensor for metal ion detection", Proceedings of the 17th Int. Electron. Conf. Synth. Org. Chem., 1-30 November 2013; Sciforum Electronic Conference Series, 2013, 17, b004, <http://dx.doi.org/10.3390/ecsoc-17-b004> .

**AA10/HC8** - Esteves, C. I. C.; Raposo, M. M. M.; Costa, S. P. G., "Amino acids based on 2,4,5-triarylimidazoles: synthesis and evaluation as new chemosensors for ion recognition", Proceedings of the 17th Int. Electron. Conf. Synth. Org. Chem., 1-30 November 2013; Sciforum Electronic Conference Series, 2013, 17, b015, <http://dx.doi.org/10.3390/ecsoc-17-b015>

- EE1** – Neto M; Leones R; Sentanin F; Esperança J; Medeiros M; Pawlicka A; Silva M; “Electrochemical applications of electrolytes based on ionic liquids”, ECS Transactions, 2013, 45(29): 235-244. <http://dx.doi/10.1149/04529.0235ecst>
- EE2** - Ribeiro, J. F; Sousa, R; Silva, M. F; Gonçalves, L. M; Silva, M. M; Correia, J. H; “Thin-film materials for solid-state rechargeable lithium batteries”, ECS Transactions, 2013, 45(29): 139-142. <http://dx.doi/10.1149/04529.0139ecst>
- EE3** - Duñach, E; Medeiros, M. J; Olivero, S; “Indirect Electrochemical Cyclisation of Bromoalkoxylated Derivatives using Environmentally Friendly Methodologies”, ECS Transactions, 2013, 45 (30), 9-13, doi: 10.1149/04530.0009ecst.
- EE4** - J. F. Ribeiro, R. Sousa, J. A. Sousa, L. M. Gonçalves, M.M. Silva, L. Dupont, J. H. Correia, “Flexible Thin-Film Rechargeable Lithium Battery”, Transducers 2013, 45(29): 235-244. <http://dx.doi/10.1109/Transducers.2013.6627248>
- EE5** - Madalena Lira, Carlos Alves, Gabriela Botelho “Influence of the thermo-oxidative degradation on the chemical structure of contact lenses” Proceedings of the 8th Iberoamerican Optics Meeting and 11th Latin American Meeting on Optics, Lasers, and Applications, edited by Manuel Filipe P. C. Martins Costa, 8785 (2013) <http://dx.doi/10.1117/12.2028261>
- EE6** - Rita B. Figueira, E. V. Pereira, C. J. R. Silva, M. Salta, Organic-inorganic hybrid coatings for corrosion protection of steel, Proceedings from International Conference Durable Structures 2012 - From construction to rehabilitation, LNEC, Lisbon, Portugal, May 30th – 1st June, 2013, (Electronic file number E6).
- EE7** - Rita B. Figueira, C. J. R. Silva, E. V. Pereira, R. Fontinha, M. Salta, Deposition of hybrid sol-gel films on hot dip galvanized reinforcing steel, Eurocorr 2013 – European Corrosion Congress Extended Abstracts., Estoril, Portugal, September 1-5, 2013. ISBN 978-989-8601-31-5 (Electronic file number 1566).
- EE8** - Rita B. Figueira, Carlos J. R. Silva, Elsa V. Pereira, M. Manuela Salta, Hybrid Sol-gel Coatings to Prevent Corrosion on Hot-dip Galvanized Steel in contact with cementitious media” Proceedings from 21st Annual International Conference on Composites/Nano Engineering (ICCE – 21), Tenerife, Spain, July 21-27, 2013 (Electronic file number 245)
- EE9** - Maria Luísa Costa, C. J. Silva, Desenvolvimento e uso do jogo didático “Corrida da Química” e sua implementação no ensino da Química no 8º ano de escolaridade, in Bento D. Silva, Leandro S. Almeida, Alfonso Barca, Manuel Peralbo, Amanda Franco & Ricardo Monginho; Atas do XII Congresso Internacional Galego-Português de Psicopedagogia, CIEd – Centro de Investigação em Educação, Instituto de Educação, Universidade do Minho, Braga (Portugal), ISBN 978-989-8525-22-2, pg 2695 – 2975. <http://webs.ie.uminho.pt/xiigp/#>

**EE10** - L. F. Oliveira, J. Marques, Coutinho, P. J. G. Coutinho, P. Parpot, Tavares, C. J. Tavares, "Photocatalytic thin films coupled with polymeric microcapsules for the controlled-release of volatile agents upon solar activation", Journal of Physics. Conference series [1742-6588] 439 (2013) 012018

**EE11** - César Oliveira, Alfredo Araújo, Iwona Kuźniarska-Biernacka, Rui Morais, Pier Parpot, Isabel C. Neves e António M. Fonseca "análise de fragmentos cerâmicos de potes melieiros e colmeias por cromatografia gasosa acoplada à espectroscopia de massa", II Congresso Internacional da SECAH-EX OFFICINA HISPANA, Museu de arqueologia D. Diogo de Sousa, Braga (Portugal), 2013

#### **HC** (2HC+4HC/AA=6)

**HC1** - Castro, M. C. R.; Coelho, P.; Raposo, M. M. M., "Synthesis and characterization of the photochromic properties of new dyes bearing benzothiazole or benzothiazolium acceptor groups", Proceedings of the 17th Int. Electron. Conf. Synth. Org. Chem., 1-30 November 2013; Sciforum Electronic Conference Series, 2013, 17, a029, <http://dx.doi.org/10.3390/ecsoc-17-a029>.

**HC2** - Fernandes, S. S. M.; Raposo, M. M. M., "Synthesis and characterization of formyl-thienylpyridazines as versatile precursors for several optical applications", Proceedings of the 17th Int. Electron. Conf. Synth. Org. Chem., 1-30 November 2013; Sciforum Electronic Conference Series, 2013, 17, a038, <http://dx.doi.org/10.3390/ecsoc-17-a038>.

**HC3** - Castro, M. C. R.; Coelho, C.; Raposo, M. M. M., "Synthesis and characterization of the photochromic properties of new dyes bearing benzothiazole or benzothiazolium acceptor groups", a029, 17th International Electronic Conference on Synthetic Organic Chemistry, 1-30 November 2013; Sciforum Electronic Conferences Series, <http://www.sciforum.net/conference/ecsoc-17>.

**HC4** - Fernandes, S. S. M.; Raposo, M. M. M., "Synthesis and characterization of formyl-thienylpyridazines as versatile precursors for several optical applications", a038, 17th International Electronic Conference on Synthetic Organic Chemistry, 1-30 November 2013; Sciforum Electronic Conferences Series, <http://www.sciforum.net/conference/ecsoc-17>.

**HC5/AA7** - Lima, N. E. M.; Batista, R. M. F.; Costa, S. P. G.; Raposo, M. M. M., "Iodine-catalysed synthesis of a novel meso-substituted dipyrromethane and its evaluation as a cation chemosensor", Proceedings of the 17th Int. Electron. Conf. Synth. Org. Chem., 1-30 November 2013; Sciforum Electronic Conference Series, 2013, 17, a002, <http://dx.doi.org/10.3390/ecsoc-17-a002>.

**HC6/AA8** - Ferreira, R. C. M.; Batista, R. M. F.; Costa, S. P. G.; Raposo, M. M. M., "Synthesis and photophysical characterization of novel tri-(hetero)arylimidazoles", Proceedings of the 17th Int. Electron. Conf. Synth. Org. Chem., 1-30 November 2013; Sciforum Electronic Conference Series, 2013, 17, a042, <http://dx.doi.org/10.3390/ecsoc-17-a042>.

**HC7/AA9** - Batista, R. M. F.; Costa, S. P. G.; Raposo, M. M. M., "Synthesis and evaluation of an imidazo-benzocrown ether functionalised amino acid as a new fluorimetric chemosensor for metal ion detection",

Proceedings of the 17th Int. Electron. Conf. Synth. Org. Chem., 1-30 November 2013; Sciforum Electronic Conference Series, 2013, 17, b004, <http://dx.doi.org/10.3390/ecsoc-17-b004> .

**HC8/AA10** - Esteves, C. I. C.; Raposo, M. M. M.; Costa, S. P. G., "Amino acids based on 2,4,5-triarylimidazoles: synthesis and evaluation as new chemosensors for ion recognition", Proceedings of the 17th Int. Electron. Conf. Synth. Org. Chem., 1-30 November 2013; Sciforum Electronic Conference Series, 2013, 17, b015, <http://dx.doi.org/10.3390/ecsoc-17-b015>

#### **4. Actas de Congressos nacionais**

#### **5. Comunicações em congressos internacionais**

##### **2AA**

**AA1** - Lopes, M.; Alves, C. T.; Raju, B. R.; Gonçalves, M. S. T.; Coutinho, P. J. G.; Henriques, M.; Belo, I., "Antifungal Photodynamic Efficacy of Benzo[a]phenoxazinium Chlorides Against *Candida albicans* Biofilms", poster communication, 2nd Fungal Biofilms Meeting, May 20th & 21st, 2013, University of the West of Scotland, Glasgow, Scotland, UK.

**AA2** - Hungerford, G.; Piloto, A. M.; Costa, S. P.G.; Gonçalves, M. S. T., "Monitoring the photoinduced release of neurotransmitter amino acids from coumarin fused julolidine ester cages via fluorescence", poster communication (PO363), International Photochemistry Conference ICP2013, Leuven, Belgium, 21-26 July 2013.

##### **3BC**

**BC1** - César Bernardo, Michael Belsley, Paulo Coutinho, Isabel Moura, Mikhail Vasilevskiy, José A.Martins, Peter Schellenberg, 2013, "Energy transfer in quantum nanodot superstructures of fractal dimensions", 13th Conference on Methods and Applications of Fluorescence: Spectroscopy, Imaging and Probes (MAF-13) - Genoa, Italy, September 8-11.

**BC2** - César Bernardo, Michael Belsley, Paulo Coutinho, Mikhail Vasilevskiy, José A.Martins, Peter Schellenberg, 2013, "Fluorescence probing of energy transfer in quantum nanodot superstructures", 8th Workshop on Advanced Multiphoton and Fluorescence Lifetime Imaging Techniques - Saarland University, Saarbrücken, Germany, July 1-2.

**BC3** - César Bernardo, Michael Belsley, Paulo Coutinho, Mikhail Vasilevskiy, José A.Martins, Peter Schellenberg, 2013, "Self-assembled quantum dots based polycrystalline superstructures with energy transfer properties" , Advanced school on modern trends of biophotonics for diagnosis and treatment of cancer and Microbial Control - University of Sao Paulo, Brazil, April 11-19.

**EE** (28EE+1EE/HC=29)



**EE1** - Amorim, R.; Vilaça, N.; Fonseca, A.M.; Neves, I.C.; Baltazar, F. “Zeolites as suitable Drug Delivery Systems for anticancer drugs in in vitro models of colorectal carcinoma”, SPSAS Advances in molecular oncology: Translating molecular biology into cancer treatment, 3-8 February 2013, São Paulo, Brazil.

**EE2** - Oliveira, C.; Araújo, A.; Kuźniarska-Biernacka, I.; Morais, R.; Parpot, P.; Neves, I.C.; Fonseca, A.M. “Análise de fragmentos cerâmicos de potes meleiros e colmeias por cromatografia gasosa acoplada à espectroscopia de massa”, II Congresso Internacional de la Secah – Ex oficina Hispana, Museu de arqueologia D. Diogo de Sousa, Braga, 3 a 6 de abril de 2013.

**EE3** - Machado, A.; Amorim, R.; Morais-Santos, F.; Parpot, P.; Fonseca, A.M.; Neves, I.C.; Baltazar, F. "Potentiation of 5-fluorouracil entrapped in zeolites as drug delivery systems for in vitro models of colorectal and breast carcinomas", Book of abstracts of Translational Research in Cancer – Bringing basic Science and pathology to clinical oncology – XXII Porto Cancer Meeting, Ipatimup, Porto, P25, pp.59, 11-12 de abril 2013.

**EE4** - Neves, I.C.; Fonseca, A.M.; Oliveira, C.; Parpot, P.; Kuźniarska-Biernacka, I.; Morais, R. “Characterization of ceramic fragments from Esposende´s Bético Augustano shipwreck by XRD and SEM-EDS”, Simpósio: O irado mar Atlântico, o naufrágio Bético Augustano de Esposende (Norte de Portugal), Museu de Arqueologia D. Diogo de Sousa, Braga, 1 de Março de 2013.

**EE5** - Oliveira, C.; Kuźniarska-Biernacka, I.; Parpot, P.; Neves, I.C.; Fonseca, A.M.; Morais, R. “Chemical analysis of organic residues in amphorae from the Baetica shipwreck of Esposende”, Simpósio: O irado mar Atlântico, o naufrágio Bético Augustano de Esposende (Norte de Portugal), Museu de Arqueologia D. Diogo de Sousa, Braga, 1 de Março de 2013.

**EE6** – Barros, Sandra; Cesarino, Ivana; Pawlicka, Agnieszka; Silva, Manuela. “Synthesis of thermo-responsive chitosan-cellulose (HPMC) hydrogels using the freeze-thaw strategy”, Materials Today Virtual Conference: Biomaterials, 19 a 21 de novembro de 2013.

**EE7** – Leones, Rita; Fernandes, Mariana; Ferreira, Rute; Pawlicka, Agnieszka; Carlos, Luís; de Zea Bermudez, Verónica; Silva, Manuela. “DNA and lanthanide salts based on conducting bio-membranes”, Materials Today Virtual Conference: Biomaterials, 19 a 21 de novembro de 2013.

**EE8** – Pereira, Rui; Silva, Manuela; de Zea Bermudez, Verónica. “Using silk fibroin to design multifunctional materials”, Materials Today Virtual Conference: Biomaterials, 19 a 21 de novembro de 2013.

**EE9** – Ribeiro, João; Sousa, Rui; Sousa, J.; Goncalves, Luís; Silva, Manuela; Dupont, L.; Correia, J. “Thin-Film Lithium Batteries Materials”, Vacuum2013, Paris, França, 09 a 13 de setembro de 2013.

**EE10** – Ribeiro, João; Sousa, Rui; Sousa, J.; Goncalves, Luís; Silva, Manuela; Dupont, L.; Correia, J. "Flexible thin-film rechargeable lithium batteries", Transducers 2013, Barcelona, Espanha, 16 a 20 de junho de 2013.

**EE11** - Neto, M.J.; Leones, R.; Sentanin; F.; Esperança, J.M. S. S.; Medeiros, M.J.; Pawlicka, A.; Silva M.M. "Indirect Electroreductive Cyclisation of unsaturated halides in Ionic Liquid Medium", 5th International Congress on Ionic Liquids (COIL-5), Vilamoura, Algarve, Portugal, April 21-25, 2013.

**EE12** – Leones, Rita; Fernandes, Mariana; Esperança, José; Pawlicka, Agnieszka; de Zea Bermudez, Verónica; Silva, Manuela. "Polymer electrolyte based on DNA and N,N,N-trimethyl-N-(2-hydroxyethyl)ammonium bis(trifluoromethylsulfonyl)imide, [N1 1 1 2(OH)]NTf2", 5th International Congress on Ionic Liquids (COIL-5), Vilamoura, Algarve, Portugal, 21 a 25 de abril de 2013.

**EE13** - Neto, M.J.; Leones, R.; Sentanin; F.; Esperança, J.M. S. S.; Medeiros, M.J.; Pawlicka, A.; Silva M.M., Novel polymer electrolyte based on gellan and ionic liquids, 5th International Congress on Ionic Liquids (COIL-5), Vilamoura, Algarve, Portugal, April 21-25, 2013.

**EE14** – Cardoso, Marita; Fernandes, Mariana; Rodrigues, Luísa; Silva, Manuela; de Zea Bermudez, Verónica. "Protic ionic liquid-based anhydrous proton conducting di-ureasil hybrid electrolytes" , 5th International Congress on Ionic Liquids (COIL-5), Vilamoura, Algarve, Portugal, 21 a 25 de abril de 2013.

**EE15** – Alves, C.; Lira, M.; Botelho, G. "Influence of the thermal-oxidative degradation on the contact lens parameters" Congresso Internacional de Optometria e Ciências da Visão (CIOC2013), Universidade do Minho, Braga, 13 e 14 de Abril de 2013.

**EE16** - Correia, D.M.; Ribeiro, C.; Coelho, J.C.; Botelho, G.; Gomez Ribelles, J.L.; LancerosMéndez, S.; Sencadas, V. "Influence of electrospinning parameters on poly(hydroxybutyrate) electrospun membranes fiber size for tissue engineering applications" second Materials Today – Frontiers of Microscopy Virtual Conference, 24th-26th April 2013.

**EE17** - Lira, M.; Alves, C.; Botelho, G. "Influence of the thermo-oxidative degradation on the chemical structure of contact lenses" VIII Iberoamerican Conference on Optics, XI Latinamerican meeting on Optics, Lasers and Applications FCUP, Porto, Portugal, July 22-26, 2013.

**EE18** – Barra, G.M.O.; Palmeira, S.; Botelho, M.G.C.S.L.; Neves, I.C. "Obtenção e caracterização de Compósitos de Polianilina/zeólitos" 12º Congresso Brasileiro de Polímeros, Florianópolis, Brasil, 22 a 26 de setembro de 2013. Comunicação em painel

**EE19** - Moreira, S. D.F.C.; Silva, J. P.; Silva, Carlos J.; Capan, I.; Gomes, M. J. M.; Costa, Manuel F. M. "Gold nanoparticles embedded in organic/inorganic hybrid matrix. Electrical and electrochemical behavior", SPIE microtechnologies, Grenoble (France), 24-26 April, 2013.

**EE20** - Campos, A.L.C.; Moreira, S.D.; Silva, C.J.R.; Gomes, M.J.M. "Efeito de Tyndall em soluções coloidais de ouro", 2do Simposio Iberoamericano de Divulgación y Formación en Nanotecnología, NANODYF '2013, Medellin (Colombia), 15-19, Julho, 2013

**EE21** - Fontinha, I.R.; Salta, M.M.; Zheludkevich, M. L.; Ferreira, M.G.S.; Figueira, R.B.; Pereira, E. V.; Silva, C.J.R. "Influence of the pH on the corrosion protection of epoxysilica-zirconia sol-gel coatings

applied on EN AW-6063 aluminium alloy”, 224th ECS Meeting, San Francisco, USA, October 27th – November 1st, 2013.

**EE22** - Figueira, Rita B.; Silva, Carlos J. R.; Pereira, Elsa V.; Salta, M. Manuela. “Hybrid Sol-gel Coatings to Prevent Corrosion on Hot-dip Galvanized Steel in contact with cementitious media”, 21st Annual International Conference on Composites or Nano Engineering, ICCE-21, Tenerife, Canary Islands (Spain) 21-27 July, 2013.

**EE23** - Figueira, Rita B.; Silva, C. J. R.; Pereira, E. V.; Fontinha, R.; Salta, M. “Deposition of hybrid sol-gel films on hot dip galvanized reinforcing steel”, Eurocorr 2013, European Corrosion Congress, Estoril (Portugal), 1-5 September, 2013.

**EE24** - Costa, Maria Luísa; Silva, C.J. “Desenvolvimento e uso do jogo didático “Corrida da Química” e sua implementação no ensino da Química no 8º ano de escolaridade. XIIGIPS -XII Congresso Internacional Galego-Português de Psicopedagogia, Braga (Portugal), 11-13, Setembro, 2013.

**EE25** - Figueira, R.B.; Silva, C.J.R.; Pereira E.V.; Salta, M.M. “Electrochemical evaluation of hot-dip galvanized steel (HDGS) coated with organic-inorganic hybrid sol-gel in cementitious materials”, 224th ECS Meeting, San Francisco, USA, October 27th – November 1st, 2013.

**EE26** - Gonçalves, Luis F. F. F.; Silva, Carlos J. R.; Gomes, M.Jesus M. “Optical properties of organic-inorganic hybrid nanocomposites doped with CdS nanoparticles”, Cost Action MP0901 NANOTP “Workshop on characterization of semiconductor nanostructures; the role of defects, Zagreb (Croácia), 2–4 December 2013.

**EE27** - Morais, Rui; Oliveira, César; Araújo, Alfredo. “As ânforas lusitanas na época de Augusto”, International Congress “International Congress - Lusitanian amphorae: production and diffusion”, Tróia, Portugal, 2013.

**EE28** - Amaral L., Coelho P., Santana F.1, Brito A.G., Peixoto L., Ribeiro D., Martins G., Parpot P, “Restaurative Water Technologies: From an Old Tradition to a New Paradigm”, 44th World Chemistry Congress (IUPAC), Istanbul, Symposium I, Turkey, 11 - 16 August, 2013 (Keynote lecture).

**EE29/HC20** - Araújo, R.F.; Proença, M. Fernanda; Silva, Carlos J.R.; Paiva, M. Conceição. “Efficient Dispersion of Multi-walled Carbon Nanotubes in Aqueous Solution by Non-covalent Interaction with Perylene Bisimides”, Nano Portugal-2013- Nanoscience and Nanotechnology International Conference, Porto (Portugal), 13-15 February, 2013.

#### **HC** (19 HC+1HC/EE=20)

**HC1** - Senhorães, Nádia; Dias, Alice M.; Proença, M. Fernanda “A novel and efficient approach to the synthesis of 2,6-diaminopurines”, poster presented in the “18th European Symposium on Organic Chemistry”, 17-12 July, 2013, Marseille, France. <http://hdl.handle.net/1822/26976>

**HC2** - Senhorães, Nádia; Dias, Alice M.; Proença, M. Fernanda, "A new simple and efficient synthesis of benzimidazoles", poster presented in the "18th European Symposium on Organic Chemistry", 17-12 July, 2013, Marseille, France. <http://hdl.handle.net/1822/26975>

**HC3** - Elina Marinho, M. Fernanda Proença, "A novel approach for the synthesis of 4-phenylaminoquinazolines", ESOC 2013, Marseille, France, 7-12 July 2013.

**HC4** - Elina Marinho, M. Fernanda Proença, "Aromatic amidines incorporating the piperazine nucleus", ESOC 2013, Marseille, France, 7-12 July 2013.

**HC5** - Tatiana A Dias, M Fernanda Proença, "2-Hydroxychalcones and carbon acid derivatives: reactivity studies in acid media", ESOC 2013, Marseille, France, 7-12 July 2013.

**HC6** - Tatiana A. Dias, Cecília L. Duarte, Cristovao F. Lima, M. Fernanda Proença, Cristina Pereira-Wilson, "Superior anticancer activity of halogenated chalcones and flavonols over the natural flavonol quercetin", ESOC 2013, Marseille, France, 7-12 July 2013.

**HC7** - Alves, A. C., Sousa, R., Carvalho, M. A., Cardoso, E., Figueiredo, J., Pereira, R., Fernandes, S. (2013). Engaging Engineering freshman students in Mathematics, Sciences and Programming courses. Proceedings of the ASME 2013 International Mechanical Engineering Congress & Exposition (IMECE2013), November 15-21, 2013, S. Diego, California, USA. Abstract & Technical presentation.

**HC8** - Begouin, A.; Peixoto, D.; Queiroz, Maria-João R.P. "Synthesis of 3-halo-2-(hetero)arylthienopyridine derivatives as key precursors of potential antitumorals", 49th International Conference on Medicinal Chemistry (RICT 2013), 3-5 July 2013, Nice-France.

**HC9** - Queiroz, Maria-João R.P.; Begouin, A.; Campos, J.F.; Peixoto, D.; Froufe, H.J.C. Calhelha, R.C.; Abreu, R.M.V.; Ferreira, I.C.F.R. "Synthesis of new N-[3-(thieno[3,2-b]pyridine-7-ylthio)phenyl]benzamides as potential inhibitors of VEGFR2 using rational design", 49th International Conference on Medicinal Chemistry (RICT 2013), 3-5 July 2013, Nice-France.

**HC10** - Machado, V.; Costa, Raquel; Peixoto, D.; Abreu, R.M.V.; Calhelha, R.C.; Ferreira, I.C.F.R.; Soares, R.; Queiroz, Maria-João R.P. "New di(hetero)arylthioethers 1,3-diaryllureas in the thieno[3,2-b]pyridine series as VEGFR2 tyrosine kinase inhibitors: docking, synthesis, enzymatic and cellular assays" 49th International Conference on Medicinal Chemistry (RICT 2013), 3-5 July 2013, Nice-France.

**HC11** - Heleno, S.; Dejan Stojković, A.; Barros, L.; Glamočlija, J.; Soković, M.; Martins, A.; Queiroz, M. J.R.P.; Ferreira, I.C.F.R. "Chemical composition and bioactivity of wild samples of *Morchella esculenta* from Portugal and Serbia" The 7th International Workshop on Edible Mycorrhizal Mushrooms. Guatemala, July 30th - August 3rd, 2013; 62-63p.

**HC12** - Guimarães, R.; Barros, L.; Dueñas, M.; Carvalho, A.M.; Queiroz, M.J.R.P.; Santos-Buelga, C.; Ferreira, I.C.F.R. Phenolic profile of *Arbutus unedo* L. and *Prunus spinosa* L. wild fruits. International Symposium on Profiling. 2nd - 4th September 2013, Caparica – Portugal. S17, 45p.

**HC13** - Sandrina A. Heleno, Isabel C.F.R. Ferreira, Anabela Martins, Ana P. Esteves, Maria-João R.P. Queiroz. Synthesis of acetylated glucuronide derivatives of p-hydroxybenzoic and cinnamic acids, two compounds commonly found in wild mushrooms. International Symposium on Profiling. 2nd - 4th September 2013, Caparica – Portugal. S20, 48p.

**HC14** - Heleno, S. A.; Ferreira, I.C.F.R.; Calhela, R.C.; Martins, A.; Queiroz, Maria João R.P. Inhibitory activity of *Coprinopsis atramentaria* extract, organic acids and their possible methylated synthesized metabolites on growth of human tumor cell lines. XIX Encontro Galego-Português de Química, 13 de novembro de 2013, Vigo, Espanha. SAU-03, 73p.

**HC15** - Calhela, R.C.; Begouin, A.; Campos, J.F.; Ferreira, I.C.F.R.; Queiroz, M.-J.R.P.; Abreu, R.M.V. Virtual screening of thieno[3,2-b]pyridine arylthioether (hetero)aryltriazole derivatives as potential tyrosine kinase VEGFR2 inhibitors. XIX Encontro Galego-Português de Química, 13 de novembro de 2013, Vigo, Espanha. SAU-06, 76p.

**HC16** - Guimarães, R.; Barros, L.; Reis, F.; Dueñas, M.; Carvalho, A.M.; Santos-Buelga, C.; Queiroz, M.J.R.P.; Ferreira, I.C.F.R. Phenolic profile of wild fruits of *Rosa canina* sl. from Northeast Portugal. The Second North and East European Congress on Food. NEEFood – 2013. 26-29 May 2013, Kyiv, Ukraine; 196p.

**HC17** - Heleno, S.A.; Stojković, D.; Barros, L.; Reis, F.S.; Glamočlija, J.; Soković, M. Martins, A.; Queiroz, M.J.R.P.; Ferreira, I.C.F.R. A comparative study of chemical composition of *Morchella esculenta* (L.) Pers. from Portugal and Serbia. The Second North and East European Congress on Food. NEEFood – 2013. 26-29 May 2013, Kyiv, Ukraine; 197p.

**HC18** - Calhela, R.C.; Peixoto, D.; Soares, P.; Ferreira, I.C.F.R.; Abreu, R.M.V.; Queiroz, M. J.R.P. Epidermal growth factor receptor inhibitory activity of new potential antitumor di(hetero)arylethers and di(hetero)arylamines in the thieno[3,2-b]pyridine series. International Symposium on Profiling. 2nd - 4th September 2013, Caparica – Portugal. P12, 129p.

**HC19** - Guimarães, R.; Barros, L.; Dueñas, M.; Carvalho, A.M.; Queiroz, M.J.R.P.; Santos-Buelga, C.; Ferreira, I.C.F.R. Composition in anthocyanins of wild fruits from Northeastern Portugal. 7th International Workshop on Anthocyanins. 9th-11th September, 2013, Porto, Portugal P46, 104p.

**HC20/EE29** - Araújo, R.F.; Proença, M. Fernanda; Silva, Carlos J.R.; Paiva, M. Conceição. “Efficient Dispersion of Multi-walled Carbon Nanotubes in Aqueous Solution by Non-covalent Interaction with Perylene Bisimides”, Nano Portugal-2013- Nanoscience and Nanotechnology International Conference, Porto (Portugal), 13-15 February, 2013.

## 6. Comunicações em congressos nacionais

**AA** (11AA+4AA/HC+1AA/BC+2AA/BC/HC =18)

**AA1** - Piloto, A. M.; Costa, S. P. G.; Gonçalves, M. T., "Photoactivation and controlled release of butyric acid heterocyclic cages", poster communication (PC65), 1st Symposium on Medicinal Chemistry of University of Minho, 17th May 2013, Braga, Portugal.

**AA2** - Leitão, M. I.; Raju, B. R.; Cruz, M. G.; Sousa, M. J.; Gonçalves, M. S. T., "Synthesis and study of antiproliferative activity of novel derivatives of benzo[a]phenoxazine", poster communication (PC46), 1st Symposium on Medicinal Chemistry of University of Minho, 17th May 2013, Braga, Portugal.

**AA3** - Castro, V.I.B.; Carvalho, C.M.; Fernandes, R.D.V.; Aguiam, N.R.;Costa, S.P.G.; Pereira-Lima, S.M.M.A., "Optimizations studies on the microwave assisted synthesis of antimicrobial Peptaibols",poster communication (P21), 1st Symposium on Medicinal Chemistry, 17th May 2013, Braga, Portugal.

**AA4** - Pereira, S.; Machado, N.; Monteiro, L. S.; Pereira-Lima, S., "Synthesis of dipeptides containing combinations of N-alkyl, dehydro and Ca, $\alpha$ -dimethyl amino acid residues", poster communication, 1st Symposium on Medicinal Chemistry, 17th May 2013, Braga, Portugal.

**AA5** - Machado, N.; Pereira, S.; Monteiro, L. S.; Pereira-Lima, S., "Efficient N-Alkylation of Ca, $\alpha$ -dimethylglycine derivatives", poster communication, 1st Symposium on Medicinal Chemistry, 17th May 2013, Braga, Portugal.

**AA6** - Domingues, B. B.; Felgueiras, C. F. F.; Ferreira, M. A. L. ; Pereira, A. S. R.; Gonçalves, M. S. T.; Costa, S. P. G.; Fonseca, A. S. C., "Synthesis and photorelease studies from model quinolone conjugates", poster communication (P1.24), 23rd National Meeting of Portuguese Society of Chemistry, 12-14 July 2013, Aveiro, Portugal.

**AA7** - Soares, A. M. S.; Costa, S. P. G.; Gonçalves, M. S. T., "Light-activated cages for the release of a model carboxylic acid", poster communication (P1.64), 23rd National Meeting of Portuguese Society of Chemistry, 12-14 July 2013, Aveiro, Portugal.

**AA8** - Carvalho, M. M. T.; Raju, B. R.; Coutinho, P. J. G.; Gonçalves, M. S. T., "Benzo[a]phenoxazinium chlorides possessing chlorinated terminals: synthesis, photophysics and photostability studies", poster communication (PC52), 10th National Meeting of Organic Chemistry, 1st Portuguese-Brazilian Organic Chemistry Symposium, 4-6th September 2013, Lisbon, Portugal.

**AA9** - Soares, A. M. S.; Costa, S. P. G.; Gonçalves, M. S. T., "Synthesis and photolysis studies of 5-aminolevulinic acid conjugates based on 2-oxo-naphtho[1,2-b]pyran", poster communication (PC130), 10th National Meeting of Organic Chemistry, 1st Portuguese-Brazilian Organic Chemistry Symposium, 4-6th September 2013, Lisbon, Portugal.

**AA10** - Carvalho, C. M.; Castro, V. I. B.;Costa, S. P. G.; Pereira-Lima, S. M. M. A., "NMR and IR conformational studies of the influence of bulky C-tetrasubstituted amino acids on Peptaibolinmimetics", poster communication (PC139), 10th National Meeting of Organic Chemistry, 1st Portuguese-Brazilian Organic Chemistry Symposium, 4-6th September 2013, Lisbon, Portugal.

**AA11** - Castro, V. I. B.;Carvalho, C. M.; Fernandes, R. D. V.; Costa, S. P. G.; Pereira-Lima, S. M. M. A., "Solid phase microwave assisted synthesis of Peptaibolinmimetics bearing  $\alpha,\alpha$ -dialkylglycines", poster communication (PC82), 10th National Meeting of Organic Chemistry, 1st Portuguese-Brazilian Organic Chemistry Symposium, 4-6th September 2013,Lisbon, Portugal.

**AA12/BC6** - Ferreira, P.M.T.; Vilaça, H.; Pereira, G.; Castro, T.; Faria, T.; Brito, R.;Micaelo, N.; Xu, B.; Martins, J.A., "New hydrogelsbasedonsmalldehydropeptidesforbiomedicalapplications" (comunicação oral convidada Paula M.T. Ferreira) at the XXIII Encontro Nacional da SPQ,12-14 of June, 2013, Aveiro, Portugal.

**AA13/HC54/EE28** - Pasquier, A.;Gellé, F.;Kuzniarska-Biernacka, I.;Batista, R. M. F.;Costa, S. P. G.;Raposo, M. M. M.;Fonseca, A. M.;Neves, I. C., "Encapsulated Cu(II) complex as heterogeneous catalyst for limonene oxidation", poster communication (P41), 9th National Meeting of the Catalysis and Porous Materials Division, 6-7th May 2013, Porto, Portugal.

**AA14/HC55/EE29** - Gellé, F.; Pasquier, A.; Kuzniarska-Biernacka, I.; Batista, R. M. F.; Costa, S. P. G.;Raposo, M. M. M.; Fonseca, A. M.; Neves, I. C., "Phenol oxidation catalysed by copper(II) complex encapsulated on ZMS-5 zeolite", poster communication (P19), 9th National Meeting of the Catalysis and Porous Materials Division, 6-7th May 2013, Porto, Portugal.

**AA15/HC42** - Esteves, C. I. C.;Raposo, M. M. M.;Costa, S. P. G., "Unnatural amino acids based on 2,4,5-triarylimidazoles as fluorescent labels for peptides", poster communication (P32), 1st Symposium on Medicinal Chemistry, 17 May 2013, Braga, Portugal.

**AA16/HC43** - Esteves, C. I. C.; Raposo, M. M. M.; Costa, S. P. G., "Amino acid based hydrazones: synthesis and evaluation as new chemosensors for ion recognition", poster communication (PC25), 10th National Meeting of Organic Chemistry, 1st Portuguese-Brazilian Organic Chemistry Symposium, 4-6th September 2013, Lisbon, Portugal.

**AA17/HC45** - Batista, R. M. F.;Pina, J.;Seixas de Melo, J.;Costa, S. P. G.;Raposo, M. M. M., "Synthesis and photophysical characterization of novel triphenylamine-benzimidazole derivatives", poster communication(PC69), 10th National Meeting of Organic Chemistry, 1st Portuguese-Brazilian Organic Chemistry Symposium, 4-6th September 2013, Lisbon, Portugal.

**AA18/HC44** - Ferreira, R. C. M.;Dias, C. P. R.;Costa, S. P. G.;Belsley, M.;Raposo, M. M. M., "Synthesis and characterization of novel thiazolo[5,4-d]thiazoles as two photon absorbers (TPA)", poster communication (PC30), 10th National Meeting of Organic Chemistry, 1st Portuguese-Brazilian Organic Chemistry Symposium, 4-6th September 2013, Lisbon, Portugal.

**BC** (4BC+2BC/HC+1BC/AA=7)

**BC1** - César Bernardo, Michael Belsley, Paulo Coutinho, Mikhail Vasilevskiy, José A. Martins, Peter Schellenberg, 2013, "Self-assembled quantum dots based polycrystalline superstructures with energy transfer properties" , NanoPT, Porto , Portugal, February 13-15.

**BC2** - A. de Sá, D.S. Ferreira, R.L. Reis, P.M.T. Ferreira, J.P. André, N3O3-type bifunctional chelators for Ga<sup>3+</sup>, 1st Symposium on Medicinal Chemistry of University of Minho, Braga, 17 de Maio 2013

**BC3** - A. Fontes, P. M. Ferreira, C. F. G. C. Geraldes, J. P. André, 1H NMR studies of DO3A-aAHAPEG750 lanthanide complexes, 1st Symposium on Medicinal Chemistry of University of Minho, Braga, 17 Maio 2013

**BC4** - João Paulo André, Química - Uma Ciência na Ficção Queirosiana, XXIII ENSPQ Aveiro, 14 de Junho 2013

**BC5/HC46** - C.R. Barroso, J.P. André, A.P. Esteves, Synthesis of glycoconjugates as precursors of targeted Mn(II)-based MRI contrast agentes, ENQO, Lisboa, Portugal, 4-6 de Setembro 2013

**BC6/AA12** - Ferreira, P.M.T.; Vilaça, H.; Pereira, G.; Castro, T.; Faria, T.; Brito, R.; Micaelo, N.; Xu, B.; Martins, J.A., "New hydrogels based on small dehydropeptides for biomedical applications" (comunicação oral convidada Paula M.T. Ferreira) at the XXIII Encontro Nacional da SPQ, 12-14 of June, 2013, Aveiro, Portugal.

**BC7/HC47** - Barroso, C.R.; André, J.P.; Esteves, A.P. "Synthesis of macrocyclic ligands as precursors of targeted Mn(II)-based MRI contrast agents", 1st Symposium on Medicinal Chemistry, 2013, Braga – Portugal

**EE** (21EE+4EE/HC+2EE/HC/AA=27)

**EE1** - Silva, Carlos J.R.; Moreira, Sandra D.F.C.; Silva, J.P.B.; Costa, Manuel F.M.; Gomes, M.J.M. "Electrochemical properties of a gold nanoparticles doped organic/inorganic hybrid matrix gel", 3rd Forum on Electrochemical and Innovation - Electrochemistry and Materials, Vila Real (Portugal) 16, 17 setembro, 2013.

**EE2** - Figueira, R.B.; Pereira, E.V.; Silva, C. J.R.; Salta, M.M. "Organic-Inorganic Hybrid Sol-Gel Coatings to prevent Corrosion of Galvanized Reinforced Steel", 3rd Forum on Electrochemical and Innovation - Electrochemistry and Materials, Vila Real (Portugal) 16, 17 setembro, 2013.

**EE3** - Figueira, Rita M.; Pereira, Elsa V.; Silva, Carlos J. R.; Salta, Maria Manuela. "Electrochemical system for assessing hybrid coatings for corrosion protection of hot dip galvanized steel in concrete", XVIII Meeting of the Portuguese Electrochemical Society, Porto (Portugal), 25-27 March, 2013.

**EE4** – Oliveira, R.; Bento, F.; Geraldo, D. "Evaluation of radical scavenging activity of antioxidants by means of electrogenerated HO radical", Jornadas de Eletroquímica e Inovação 2013, Vila Real, September, 2013.



**EE5** – Bento, F.; Oliveira, R.; Vilas Boas, A.; Geraldo, D. “Degradation of alizarin red promoted by electrogenerated HO radicals: A kinetic study”, Jornadas de Eletroquímica e Inovação 2013, Vila Real, September, 2013.

**EE6** – Geraldo, D.; Bento, F.; Oliveira, R.; Gonzalez-Costas J.; Gonzalez-Romero E. “A new approach to domoic acid detection”, Jornadas de Eletroquímica e Inovação 2013, Vila Real, September, 2013.

**EE7** – Pereira, Nelson; Oliveira, Raquel; Geraldo, Dulce; Bento, Fátima; “Reactivity of hydroxybenzoic acid derivatives towards electrogenerated HO radicals”, XVIII Meeting of the Portuguese Electrochemical Society, Porto, March, 2013.

**EE8** – Santos, Carlos; Oliveira, Raquel; Geraldo, Dulce; Marcos, João; Rodrigues, João; Bento, Fátima. “Protein oxidation by electrogenerated hydroxyl radicals”, XVIII Meeting of the Portuguese Electrochemical Society, Porto, March, 2013.

**EE9** –L. Peixoto, D. Cruz, G. Martins, O. S.G.P. Soares, M F.R. Pereira, J. L. Figueiredo, R. Nogueira, A. G. Brito, P. Parpot, “Optimization of bioelectricity generation by *Geobacter sulfurreducens* in microbial fuel cell”, XVIII Meeting of the Portuguese Electrochemical Society, Porto, Portugal, 25-27 March 2013.

**EE10** –J. Marques, P. J. Coutinho, P. Parpot, J. R. Góis, J.F. Coelho, F. D. Magalhães, C. J. Tavares, “Encapsulation and Characterization of Polymeric Capsules Coated with TiO<sub>2</sub> Particles”, 9º Encontro Nacional de Catálise e Materiais Porosos, Porto, Portugal, 6- 7 May 2013.

**EE11** – V. P. Muiuane, M. Ferreira, P. Bignet, A. P. Bettencourt, P. Parpot, “Biomass valorization: production of formic acid from glucose using electrochemical methods”, XVIII Meeting of the Portuguese Electrochemical Society, Porto, Portugal, 25-27 March 2013.

**EE12** - Pinto, M.F.; Ferreira, M.; Neves, I.C.; Fonseca, A.M.; Peixoto, L.; Brito, A.G.; Nogueira, R.; Soares, O.S.G.P.; Órfão, J.J.M.; Pereira, M.F.R.; Figueiredo, J.L.; Parpot, P. “Electrocatalysts based on carbon nanotubes: application to wastewater treatments”, 3rd Forum on Electrochemistry and Innovation, Electrochemistry and Nanomaterials, UTD, Vila Real, 16-17 de Setembro de 2013.

**EE13** - Pinto, M.F.; Ferreira, M.; Neves, I.C.; Fonseca, A.M.; Soares, O.S.G.P.; Órfão, J.J.M.; Pereira, M.F.R.; Figueiredo, J.L.; Parpot, P. " Electrochemical mineralization of aniline and azo dyes at metallic catalysts based on carbon nanotubes ", 18th Meeting of the Portuguese Electrochemical Society, Porto – Portugal, 25th-27th March 2013.

**EE14** - Crépin, L.; Neves, I.C.; Fonseca, A.M.; Pereira, M.F.R.; Parpot, P. “Oxidation Electrocatalytic of Emergent Pollutants by Carbon Toray and Carbon Nanotubes”, Livro de Resumos das Comunicações do 9º Encontro Nacional de Catálise e Materiais Porosos, P13, pp. 53, Porto, Portugal. 6-7 de maio de 2013.

**EE15** - Machado, A.F.; Santos, J.D.; Neto, P.; Amorim, R.; Morais-Santos, F.; Parpot, P.; Pereira, M.F.R.; Fonseca, A.M.; Baltazar, F.; Neves, I.C., “Drug delivery systems based on zeolites”, 9º Encontro Nacional de Catálise e Materiais Porosos, P28, pp. 68, Porto, Portugal. 6-7 de maio de 2013.

**EE16** - Pilet, M.; Araújo, A.; Oliveira, C.; Kuźniarska-Biernacka, I.; Parpot, P.; Fonseca, A.M.; Neves, I.C.; Morais, R. "Structural and Chemical Characterisation of Ancient ceramic Fragments", 9º Encontro Nacional de Catálise e Materiais Porosos, P43, pp. 83, Porto, Portugal, 6-7 de maio de 2013.

**EE17** - Machado, A.F.; Amorim, R.; Morais-Santos, F.; Parpot, P.; Pereira, M.F.R.; Fonseca, A.M.; Baltazar, F.; Neves, I.C. "An experimental study of 5-fluorouracil encapsulated in nanoporosity of zeolite structures as carriers for drug delivery", 1st Symposium on Medicinal Chemistry, Universidad of Minho, Braga, , PC48, pp.65,17 maio 2013.

**EE18** - Gonçalves, B.; Botelho, G.; Medeiros, M.J.; Silva, C.J.R.; "Análise de componentes voláteis na gasolina", XXIII Encontro Nacional da Sociedade Portuguesa de Química, Aveiro, 12-14 Junho, 2013.

**EE19** - Lima, A.C.; Salazar, H.; Lopes, A.C.; Ribeiro, C.; Botelho, G.; Lanceros-Mendez S. "Tailoring P(VDF-TrFE)/zeolite membranes for drug release applications" 9º Encontro nacional de Catálise e materiais Porosos, Faculdade de Farmácia- Universidade do Porto, 6 e 7 de Maio de 2013

**EE20** - Fernandes, J.; Correia, D.; Sencadas, V.; Botelho, G.; Lanceros-Mendez S. "Poly(hydroxybutyrate)-Poly(ethylene oxide) electrospun fibers containing chloexidine for controlled drug delivery applications" XXIII Encontro Nacional da Sociedade Portuguesa de Química, Universidade de Aveiro, 12 a 14 de Junho de 2013.

**EE21** - Muiuane, V.P. Ferreira, M.; Bignet, P.; Bettencourt, A.P.; Parpot, P. "Biomass valorization: production of formic acid from glucose using electrochemical methods", 18th Meeting of the Portuguese Electrochemical Society, Porto, Portugal, 25 a 27 de março de 2013.

**EE22/HC49** – Leite, A.C.; Lobo, F.; Correia, C.; Carvalho, M.A.; Proença, M.F.; Bettencourt, A.P. "Evaluation of the antioxidant activity of new phenolic imidazole derivatives by cyclic voltammetry", 18th Meeting of the Portuguese Electrochemical Society, Porto, Portugal, 25 a 27 de março de 2013.

**EE23/HC50** – Bettencourt, A.P.; Lobo, F.; Leite, A.C.; Correia, C.; Carvalho, M.A.; Proença, M.F. "New phenolic imidazole derivatives: evaluation of antioxidant activity", E-INOV 2013, Jornadas de Eletroquímica e Inovação, Vila Real, Portugal, 16 a 17 de Novembro de 2013.

**EE24/HC51** – Gusmão, R.; Fortes M.; Oliveira, R.; Bento, F.; Geraldo, D.; Proença, F., Paiva, C. "Screen Printed Electrodes Modified with Carboxylated Multiwall Carbon Nanotubes for the Analysis of Hydroquinone and Ascorbic Acid", Jornadas de Eletroquímica e Inovação 2013, Vila Real, September, 2013.

**EE25/HC48** - Rui F. Araújo, Carlos J. Silva, M. Conceição Paiva, M. Fernanda Proença, Efficient dispersion of multiwalled carbon nanotubes in aqueous solution by non-covalent interaction with perylene bisimides, NanoPortugal 2013, 13-15 February, Porto, Portugal

**EE26/AA13/HC52** - Pasquier, A.;Gellé, F.;Kuźniarska-Biernacka, I.;Batista, R. M. F.;Costa, S. P. G.;Raposo, M. M. M.;Fonseca, A. M.;Neves, I. C., "Encapsulated Cu(II) complex as heterogeneous catalyst

for limonene oxidation”, poster communication (P41), 9th National Meeting of the Catalysis and Porous Materials Division, 6-7th May 2013, Porto, Portugal.

**EE27/AA14/HC53** - Gellé, F.; Pasquier, A.; Kuźniarska-Biernacka, I.; Batista, R. M. F.; Costa, S. P. G.; Raposo, M. M. M.; Fonseca, A. M.; Neves, I. C., “Phenol oxidation catalysed by copper(II) complex encapsulated on ZMS-5 zeolite”, poster communication (P19), 9th National Meeting of the Catalysis and Porous Materials Division, 6-7th May 2013, Porto, Portugal.

**HC** (2 orais+41HC+4HC/AA+2HC/BC+4HC/EE+2HC/EE/AA=55

### **Comunicações orais**

**HC1** - T.A Dias, M. Costa, M.F. Proença, “The acid catalyzed reaction of 2-hydroxychalcones and carbon acids”, oral communication, 10º Encontro Nacional de Química Orgânica, Lisboa, 4-6 September 2013.

**HC2** - Queiroz, M.-J.R.P.; Begouin, A.; Peixoto, D. "New strategies for the synthesis of 2-(hetero)arylthieno[2,3-b] or [3,2-b]pyridine scaffolds from 2,3-dihalopyridine", selected for oral communication (OC1), 10º Encontro Nacional de Química Orgânica-1º Simpósio Luso-Brasileiro de Química Orgânica (10ENQO-1SLB), Fac. Farmácia, Univ. de Lisboa, 4-6 Sept. 2013 Lisboa, Portugal

### **Comunicações em poster**

**HC1** - Ribeiro, Ana I.; Dias, Alice M.; Proença, M. Fernanda; Gabriel, Carla. Vieira, Magna; Cerqueira, Fátima “Synthesis and Antimicrobial Activity of 5-Aminoimidazoles Incorporating N-phenylhydrazonoyl Moiety”, poster presented in the “1st Symposium on Medicinal Chemistry”, 17 maio 2013, Braga, Portugal. <http://hdl.handle.net/1822/27022>

**HC2** - Sampaio, Diogo; Martins, Andrea; Dias, Alice M.; Proença, M. Fernanda “Synthesis of 6-(N-methyl)carboxamidino-2-oxopurines as Potential Antimycobacterial Agents”, poster presented in the “1st Symposium on Medicinal Chemistry”, Braga, Portugal. <http://hdl.handle.net/1822/27030>

**HC3** - Senhorães, Nádia; Sousa, Raquel; Dias, Alice M.; Proença, M. Fernanda; Lima, Cristovão F.; Pereira-Wilson, Cristina “Synthesis and Anticancer Activity of 6-Aryl Adenines”, poster presented in the “1st Symposium on Medicinal Chemistry”, 17 maio 2013, Braga, Portugal. <http://hdl.handle.net/1822/27028>

**HC4** - Ferreira, M. La Salete; Dias, Alice M. “Separação de carotenoides, clorofilas e flavonoides em folhas de plantas: uma abordagem simples e ecológica”, poster presented in the “XXIII Encontro Nacional da Sociedade Portuguesa de Química”, 12-14 June 2013, Aveiro, Portugal. <http://hdl.handle.net/1822/27029>

**HC5** - Senhorães, Nádia; Dias, Alice M.; Proença, Maria Fernanda “A Novel and Facile Synthetic Approach to N9-Substituted Guanines”, poster presented in the “10º Encontro Nacional de Química Orgânica”, 4-6 september 2013, Lisboa, Portugal. <http://hdl.handle.net/1822/27031>

**HC6** - Senhorães, Nádia; Dias, Alice M.; Proença, M. Fernanda “The Synthesis of 2-Aryl-hypoxanthines: A Novel and Efficient Synthetic Approach”, poster presented in the “10º Encontro Nacional de Química Orgânica”, 4-6 september 2013, Lisboa, Portugal. <http://hdl.handle.net/1822/27034>

**HC7** - Ribeiro, Ana I.; Gabriel, Carla; Dias, Alice M.; Proença, M. Fernanda; Cerqueira, Fátima “Synthesis and Antimicrobial Activity of 5-Aminoimidazoles Incorporating a Substituted N-phenyl Amidrazonoyl Moiety”, poster presented in the “10º Encontro Nacional de Química Orgânica”, 4-6 september 2013, Lisboa, Portugal. <http://hdl.handle.net/1822/27033>

**HC8** - Sampaio, Diogo; Dias, Alice M.; Proença, Maria Fernanda “Regiospecific Synthesis of N-Substituted 2-Oxopurine-6-Carboxamidines”, poster presented in the “10º Encontro Nacional de Química Orgânica”, 4-6 september 2013, Lisboa, Portugal. <http://hdl.handle.net/1822/27032>

**HC9** - Brito A, Costa M, Proença F, “Pyrido[2,3-b]indolizines: a one-pot synthesis in green media”, 10º Encontro Nacional de Química Orgânica, Lisboa, 4-6 September 2013.

**HC10** - Proença F, Costa M, Areias F, Castro M, Brea J, Loza M, “Synthesis of new chromene derivatives and pharmacological evaluation for adenosine receptors” 10º Encontro Nacional de Química Orgânica, Lisboa, 4-6 September 2013.

**HC11** - Costa M, Proença F, Pereira O, Lima C, Pereira-Wilson C, “Chromeno-imidazo[1,2-a]pyridines: synthesis and anticancer activity”, 10º Encontro Nacional de Química Orgânica, Lisboa, 4-6 September 2013.

**HC12** - Rodrigues A, Costa M, Proença F, “3-aminocoumarins: synthesis and reaction with active carbonyl compounds”, 10º Encontro Nacional de Química Orgânica, Lisboa, 4-6 September 2013.

**HC13** - Elina Marinho, M. Fernanda Proença, “A cascade condensation-cyclization reaction leading to novel triazachrysenes derivative” 10º Encontro Nacional de Química Orgânica, Lisboa, 4-6 September 2013.

**HC14** - A.Brito, M. Costa, M. F. Proença, “Pyrido[2,3-b]indolizines: a one-pot synthesis in green media” 10º Encontro Nacional de Química Orgânica, Lisboa, 4-6 September 2013.

**HC15** - Tatiana A. Dias, Marta Costa, M. Fernanda Proença, «Some reactions of active methylene compounds with 2-hydroxychalcones», 10º Encontro Nacional de Química Orgânica, Lisboa, 4-6 September 2013.

**HC16** - Fernandes,F.; Rocha, A.; Lima, C.F.; Proença, M. F.; Carvalho, M.A.; Pereira-Wilson, C. “Anticarcinogenic effect of pyrimido[5,4-d]pyrimidines in human colon cancer”, 1st Symposium on Medicinal Chemistry, Minho University, 17 May, 2013.

**HC17** - Cruz, M. ; Proença, M.F.; Carvalho, M.A.; Sousa, M.J. "SAR studies of 9-arylpurine derivatives on *Saccharomyces cerevisiae*", 1st Symposium on Medicinal Chemistry, Minho University, 17 May, 2013.

**HC18** - Leite, A.C.; Lobo, F.; Correia, C.; Carvalho, M.A.; Proença, M.F.; Bettencour, A.P. "Evaluation of the antioxidant activity of new phenolic imidazole derivatives by cyclic voltammetry", XVIII Meeting of the Portuguese Electrochemical Society, Porto, 25-27 March, 2013.

**HC19** - Eunice Cunha, M. Conceição Paiva, M. Fernanda Proença, Rui F. Araújo, Florinda Costa, António J. Fernandes, Manuel Melle-Franco, Marta A. Ferro, Functionalized graphene nanoribbons by unzipping of carbon nanotubes, NanoPortugal 2013, 13-15 February, Porto, Portugal.

**HC20** - Conceição, R., Cruz, M., Leite, C., Carvalho, M.A, "Antioxidant activity of non-phenolic nitrogen heterocycles using the 2-deoxy-D-ribose degradation method", 1st Symposium on Medicinal Chemistry, Minho University, 17 May, 2013.

**HC21** - Cunha S., Esteves A, "Sugar-based precursors of new potential inhibitors of xanthine oxidase: synthesis and characterization", 10º Encontro Nacional de Química Orgânica, 2013, Lisbon - Portugal

**HC22** - Cunha, S.D.; Oliveira-Campos, A.M.; Esteves, A.P. "Precursors of new potential inhibitors of xanthine oxidase: synthesis and characterization", 1st Symposium on Medicinal Chemistry, 2013, Braga - Portugal

**HC23** - Heleno, S.A.; Ferreira, I.C.F.R.; Esteves, A.P.; Ciric, A.; Glamoclija, J.; Martins, A.; Sokovic, M.; Queiroz, M.J.R.P. "Antimicrobial activity of *Ganoderma lucidum* extract, p-hydroxybenzoic and cinnamic acids and their synthetic acetylated glucuronide methyl esters", 1st Symposium on Medicinal Chemistry, 2013, Braga – Portugal.

**HC24** - Heleno, S.A.; Ferreira, I.C.F.R.; Calhelha, R.C.; Martins, A.; Esteves, A.P.; Queiroz, M.-J.R.P. "Growth inhibitory activity of *Coprinopsis atramentaria* extract, phenolic acids, cinnamic acid and protected acetylated glucuronides on human tumor and non-tumor cell lines ", XXIII Encontro Nacional da Sociedade Portuguesa de Química, Aveiro (Portugal), 12-14 June 2013.

**HC25** - Campos, J.F.; Begouin, A.; Peixoto, D.; Froufe, H.J.C.; Abreu, R.M.V.; Ferreira, I.C.F.R.; Queiroz, M.-J. R.P. "Synthesis of new N-[3-(thieno[3,2-b]pyridine-7-ylthio)phenyl]benzamides as potential inhibitors the tyrosine kinase domain of VEGFR2", 1st Symposium on Medicinal Chemistry of University of Minho, 17 May 2013, Braga, Portugal.

**HC26** - Calhelha, R.C.; Campos, J.F.; Peixoto, D.; Abreu, R.M.V.; Ferreira, I.C.F.R., Queiroz, M.-J.R.P. "Synthesis and evaluation of the antitumor potential of new aminated or methoxylated di(hetero)arylthioethers in the thieno[3,2-b]pyridine series", 1st Symposium on Medicinal Chemistry of University of Minho, 17 May 2013, Braga, Portugal.

**HC27** - Maria Inês Leitão, Agathe Begouin, Maria-João R. P. Queiroz, " Synthesis of a brominated 7-di(hetero)arylthioether in the thieno[3,2-b]pyridine series and preparation of a new arylalkylamine by C-N

coupling as a potential inhibitor of VEGFR-2 " 1st Symposium on Medicinal Chemistry of University of Minho, Braga, 17 de Maio de 2013.

**HC28** - Begouin, A.; Campos, J.F.; Queiroz, M.-J.R.P. "Synthesis of new di(hetero)aryl amide or triazole thienopyridine thioethers through Cu-catalysed reactions as potential inhibitors of VEGFR2" 10º Encontro Nacional de Química Orgânica, 1º Simpósio Luso Brasileiro de Química Orgânica, 4-6 Set 2013, Lisboa, Portugal

**HC29** - Queiroz, M.-J.R.P.; Begouin, A.; Peixoto, D. "New strategies for the synthesis of 2-(hetero)arylthieno[2,3-b] or [3,2-b]pyridine scaffolds from 2,3-dihalopyridine", selected for oral communication (OC1), 10º Encontro Nacional de Química Orgânica-1º Simpósio Luso-Brasileiro de Química Orgânica (10ENQO-1SLB), Fac. Farmácia, Univ. de Lisboa, 4-6 Sept. 2013 Lisboa, Portugal

**HC30** - Begouin, A.; Campos, J.F.; Queiroz, M.-J.R.P. "Synthesis of new di(hetero)aryl amide or triazole thienopyridine thioethers through Cu-catalysed reactions as potential inhibitors of VEGFR2" 10º Encontro Nacional de Química Orgânica, 1º Simpósio Luso Brasileiro de Química Orgânica, 4-6 sept. 2013, Lisboa, Portugal

**HC31** - Guimarães, R.; Barros, L.; Calhelha, R.C.; Dueñas, M.; Carvalho, A.M.; Queiroz, M.J.R.P. Santos-Buelga, C.; Ferreira, I. C.F.R. Bioactivity and chemical characterization of phenolic and anthocyanin extracts of *Arbutus unedo* L. wild fruits. 1st Symposium on Medicinal Chemistry of University of Minho. 17 de Maio de 2013, Braga, Portugal; PC-39; 56p.

**HC32** - Abreu, R.M.V.; Froufe, H.J.C.; Queiroz, M.-J.R.P.; Ferreira, I.C.F.R. Aplicação de ferramentas de quimioinformática no desenvolvimento de novos fármacos: tienopiridinas como inibidores de VEGFR-2. V Workshop em Bioinformática. Escola Superior Agrária de Bragança, 15 e 16 de Maio de 2013, Bragança, Portugal.

**HC33** - Guimarães, R.; Barros, L.; Calhelha, R.C.; Carvalho, A.M.; Queiroz, M.J.R.P.; Ferreira, I. C.F.R. Phytochemicals and bioactivity in wild German and Roman chamomiles infusions. 1st Symposium on Medicinal Chemistry of University of Minho. 17 de Maio de 2013, Braga, Portugal; PC-40; 57p.

**HC34** - Heleno, S.A.; Ferreira, I.C.F.R.; Esteves, A.P.; Ćirić, A.; Glamočlija, J.; Martins, A.; Soković, M.; Queiroz, M.J.R.P. Antimicrobial activity of *Ganoderma lucidum* extract, p-hydroxybenzoic and cinnamic acids and their synthetic acetylated glucuronide methyl esters. 1st Symposium on Medicinal Chemistry of University of Minho. 17 de Maio de 2013, Braga, Portugal; PC-41; 58p.

**HC35** - Heleno, S.A.; Barros, L.; Martins, A.; Queiroz, M.J.R.P.; Ferreira, I.C.F.R. Chemical characterization and antioxidant activity of phenolic, polysaccharidic and lipidic fractions of *Coprinopsis atramentaria*, a wild edible mushroom from Northeast Portugal. 1st Symposium on Medicinal Chemistry of University of Minho. 17 de Maio de 2013, Braga, Portugal; PC-42; 59p.

**HC36** - Heleno, S. A.; Ferreira, I.C.F.R.; Calhelha, R.C.; Martins, A.; Esteves, A.P.; Queiroz, M.J.R.P. Growth inhibitory activity of *Coprinopsis atramentaria* extract, phenolic acids and protected acetylated

glucuronides on human tumor and non-tumor cell lines. XXIII Encontro Nacional da SPQ, 12 a 14 de Junho de 2013, Aveiro, Portugal. P2.35., 199p.

**HC37** - Heleno, S.A.; Stojković, D.; Barreira, J.C.M.; Glamočlij, J.; Soković, M.; Martins, A. Queiroz, Maria João R.P. Isabel C.F.R. Ferreira. Chemical composition of *Morchella esculenta* (L.) Pers. from Portugal and Serbia: A comparative study based on chromatographic techniques. 8º Encontro Nacional de Cromatografia, 2 a 4 de dezembro de 2013, Covilhã. P011, 145-146p

**HC38** - Castro, M. C. R.; Belsley, M., Raposo, M. M. M., "Synthesis and nonlinear optical properties of heterocyclic cationic chromophores containing piridinium, quinolinium and benzothiazolium acceptor groups", PC26, 10º Encontro Nacional de Química Orgânica, 1º Simpósio Luso-Brasileiro de Química Orgânica, 4-6 September 2013, Lisboa, Portugal.

**HC39** - Fernandes, S. S. M.; Raposo, M. M. M., "Novel donor-acceptor heterocyclic systems bearing phthalazine, thiophene and furan groups for DSSC: Synthesis and characterization", PC71, 10º Encontro Nacional de Química Orgânica, 1º Simpósio Luso-Brasileiro de Química Orgânica, 4-6 September 2013, Lisboa, Portugal.

**HC40** - Francisco C.; Rodrigues L.; Esteves A. "Synthesis and characterization of psoralen analogues based on dibenzothiophenes", 10º Encontro Nacional de Química Orgânica, 2013, Lisbon – Portugal.

**HC41** - Francisco, C. S.; Rodrigues, L.M.; Cerqueira, N.M.F.S.A.; Oliveira-Campos, A.M.F.; Rodrigues, L.M.; Esteves, A.P. "Synthesis and characterization of novel psoralen analogues derived from 2-hydroxycarbazole and 2-hydroxydibenzofuran", 1st Symposium on Medicinal Chemistry, 2013, Braga - Portugal

**HC42/AA15** - Esteves, C. I. C.; Raposo, M. M. M.; Costa, S. P. G., "Unnatural amino acids based on 2,4,5-triarylimidazoles as fluorescent labels for peptides", PC 32, 1st Symposium on Medicinal Chemistry, 17 May 2013, Braga, Portugal.

**HC43/AA16** - Esteves, C. I. C.; Raposo, M. M. M.; Costa, S. P. G., "Amino acid based hydrazones: synthesis and evaluation as new chemosensors for ion recognition", PC25, 10º Encontro Nacional de Química Orgânica, 1º Simpósio Luso-Brasileiro de Química Orgânica, 4-6 September 2013, Lisboa, Portugal.

**HC44/AA18** - Ferreira, R. C. M.; Dias, C. P. R.; Costa, S. P. G.; Belsley, M.; Raposo, M. M. M., "Synthesis and characterization of novel thiazolo[5,4-d]thiazoles as two photon absorbers (TPA)", PC30, 10º Encontro Nacional de Química Orgânica, 1º Simpósio Luso-Brasileiro de Química Orgânica, 4-6 September 2013, Lisboa, Portugal.

**HC45/AA17** - Batista, R. M. F.; Pina, J.; Seixas de Melo, J.; Costa, S. P. G. Raposo, M. M. M., "Synthesis and photophysical characterization of novel triphenylamine-benzimidazole derivatives", PC69, 10º Encontro Nacional de Química Orgânica, 1º Simpósio Luso-Brasileiro de Química Orgânica, 4-6 September 2013, Lisboa, Portugal.

**HC46/BC5** - Barroso C, André J, Esteves A, "Synthesis of glyconjugates as precursors of targeted Mn(II)-based MRI contrast agents", 10<sup>o</sup> Encontro Nacional de Química Orgânica, 2013, Lisbon – Portugal.

**HC47/BC6** - Barroso, C.R.; André, J.P.; Esteves, A.P. "Synthesis of macrocyclic ligands as precursors of targeted Mn(II)-based MRI contrast agents", 1st Symposium on Medicinal Chemistry, 2013, Braga – Portugal

**HC48/EE25** - Rui F. Araújo, Carlos J. Silva, M. Conceição Paiva, M. Fernanda Proença, Efficient dispersion of multiwalled carbon nanotubes in aqueous solution by non-covalent interaction with perylene bisimides, NanoPortugal 2013, 13-15 February, Porto, Portugal

**HC49/EE22** – Leite, A.C.; Lobo, F.; Correia, C.; Carvalho, M.A.; Proença, M.F.; Bettencourt, A.P. "Evaluation of the antioxidant activity of new phenolic imidazole derivatives by cyclic voltammetry", 18th Meeting of the Portuguese Electrochemical Society, Porto, Portugal, 25 a 27 de março de 2013.

**HC50/EE23** – Bettencourt, A.P.; Lobo, F.; Leite, A.C.; Correia, C.; Carvalho, M.A.; Proença, M.F. "New phenolic imidazole derivatives: evaluation of antioxidant activity", E-NOV 2013, Jornadas de Eletroquímica e Inovação, Vila Real, Portugal, 16 a 17 de Novembro de 2013.

**HC 51/EE24** – Gusmão, R.; Fortes M.; Oliveira, R.; Bento, F.; Geraldo, D.; Proença, F., Paiva, C. "Screen Printed Electrodes Modified with Carboxylated Multiwall Carbon Nanotubes for the Analysis of Hydroquinone and Ascorbic Acid", Jornadas de Eletroquímica e Inovação 2013, Vila Real, September, 2013.

**HC52/ EE26/AA13** - Pasquier, A.;Gellé, F.;Kuzniarska-Biernacka, I.;Batista, R. M. F.;Costa, S. P. G.;Raposo, M. M. M.;Fonseca, A. M.;Neves, I. C., "Encapsulated Cu(II) complex as heterogeneous catalyst for limonene oxidation", poster communication (P41), 9th National Meeting of the Catalysis and Porous Materials Division, 6-7th May 2013, Porto, Portugal.

**HC53/EE27/AA14** - Gellé, F.; Pasquier, A.; Kuzniarska-Biernacka, I.; Batista, R. M. F.; Costa, S. P. G.;Raposo, M. M. M.; Fonseca, A. M.; Neves, I. C., "Phenol oxidation catalysed by copper(II) complex encapsulated on ZMS-5 zeolite", poster communication (P19), 9th National Meeting of the Catalysis and Porous Materials Division, 6-7th May 2013, Porto, Portugal.

## **7. Livros e Capítulos de livros internacionais**

**BC** - João Paulo André, NMR Spectroscopy of Gallium in Biology, in "Encyclopedia of Metalloproteins", R. H. Kretsinger, V. N. Uversky, E. A. Permyakov (Eds.); Springer, 2013

## **8. Livros e Capítulos de livros nacionais**

**EE1** - Neves, I. C; Fonseca, A. M; Oliveira, C; Parpot, P; Kuzniarska-Biernacka, I; Morais, R; "Characterization of ceramic fragments from Esposende´s Bético Augustano shipwreck by XRD and SEM-



EDS”, O Irado Mar Atlântico, Ed. R Morais, H. Granja, A.M. Cerdán, 2013, pp. 247-261. ISBN:978-989-97443-1-8.

**EE2** - Oliveira, C; Kuźniarska-Biernacka, I; Parpot, P; Neves, I. C; Fonseca, A. M; Morais, R; “Chemical analysis of organic residues in anphorae from the Baetica shipwreck of Esposende”, O Irado Mar Atlântico, Ed. R Morais, H. Granja, A.M. Cerdán, 2013, pp. 263-281. ISBN:978-989-97443-1-8.

## 9. Patentes

### 10. Spin-offs, start-ups e outras empresas

M.F. Proença, Promotora da Spin-off da Universidade do Minho “EARTH ESSENCES, LDA” aprovada em Maio de 2013.

### 9.3. Números globais da produtividade científica da subunidade

Artigos em revistas		Atas de congressos		Comunicações em congressos		Livros e Cap. De Livros		Patentes	Spin-offs, start-ups e outras empresas
Intern.	Nacion.	Intern.	Nacion.	Intern.	Nacion.	Intern.	Nacion.		
89	-	25	-	53	93	1	2	-	1

### 9.4. Reconhecimento científico

#### 1. Prémios e distinções atribuídas

#### 2. Palestras a convite em conferências

**AA1** - Paula Ferreira "Dehydropeptide based hydrogels for controlled release of anticancer drugs" "2h 19th July, Advanced Course in the scope of the Programa Doutoral em Biologia Molecular e Ambiental in the Centro de Biologia Molecular e Ambiental (CBMA/UM)- Cancer therapy: from basic research to clinic, 15-24 July 2013, Escola de Ciências-Univ. do Minho Portugal

**EE1** - Amaral L.; Coelho P; Santana F.I; Brito A.G; Peixoto L; Ribeiro D; Martins G; Parpot P; “Restaurative Water Technologies: From an Old Tradition to a New Paradigm”, 44th World Chemistry Congress (IUPAC), Istanbul, Symposium I, Turkey, 11 - 16 August, 2013 (Keynote lecture).

**EE2** - Pinto, M.F; Ferreira, M; Neves, I.C; Fonseca, A.M.; Peixoto, L; Brito, A.G; Nogueira, R; Soares, O.S.G.P; Órfão, J.J.M; Pereira, M.F.R; Figueiredo J.L; Parpot, P; “Electrocatalysts based on carbon nanotubes: application to wastewater treatments” , 3rd Forum on Electrochemistry and Innovation, Vila Real, Portugal, 16-17 September 2013 (Keynote lecture).

**EE3** - Gabriela Botelho “Química e Ambiente-atividades experimentais com polímeros” 3º Encontro de professores de Ciências experimentais, Areal Editores, Culturgest, Lisboa, 16 de fevereiro de 2013.

**EE4** - Gabriela Botelho “Química e Ambiente-atividades experimentais com polímeros” 3º Encontro de professores de Ciências experimentais, Areal Editores, Exponor, Porto, 9 de março de 2013.

**HC1** - Eunice Cunha, Helena Rocha, M. Fernanda Proença, Rui Araújo, Natália Alves, João F. Mano, Diogo Mata, Manuel Melle-Franco, Manuel Bañobre-López, Francis Leonard Deepak, José Rivas, Joaquín Fernandez-Rossier and M. Conceição Paiva, Polymer composites with graphene nanoribbons formed by the unzipping of carbon nanotubes, CNPComp2013 – 6th International Conference on Carbon Nanoparticle Based Composites, September 22nd-25th, 2013, Dresden, Germany.

**HC2** - M. Fernanda Proença, “A procura de novos fármacos”, lição convidada apresentada no I Workshop Luso-Brasileiro de Ciências do Instituto Federal Goiano, 17-19 de julho, 2013.

**HC3** - M. Fernanda Proença, “New drug candidates for cancer therapy: a chemist’s perspective”, lição convidada apresentada no curso Cancer therapy: from basic research to clinic, Universidade do Minho, 23 Junho, 2010.

**HC4** - Raposo, M. M. M., “2,4,5-Tri(hetero)arylimidazoles: design, synthesis and characterization as novel TPA chromophores and optical chemosensors”, SLB-IOC2, 10º Encontro Nacional de Química Orgânica, 1º Simpósio Luso-Brasileiro de Química Orgânica, 4-6 September 2013, Lisboa, Portugal.

**HC5** - Queiroz, M.J.R.P. "New heterocyclic compounds as antitumorals and antiangiogenics", 2h 17th july, Advanced Course in the scope of the Programa Doutoral em Biologia Molecular e Ambiental in the Centro de Biologia Molecular e Ambiental (CBMA/UM)- Cancer therapy: from basic research to clinic, 15-24 July 2013, Escola de Ciências-Univ. do Minho Portugal

**HC6** - Queiroz, M.J.R.P. “New thienopyridine and thienopyrimidine derivatives as antitumorals and/or antiangiogenics with tyrosine kinase membrane receptors as targets”- 2nd workshop on Medicinal Chemistry- Dept de Química e Bioquímica, Fac. Ciências, Universidade do Porto, 9 de janeiro 2013, Porto, Portugal.

**HC7** - Queiroz, M.J.R.P."Evaluation of the antitumor and/or antiangiogenic potential of new heterocyclic compounds"- IV Jornadas Nacionais de Ciências Biomédicas, Universidade de Aveiro 14-16 de March 2013, Aveiro, Portugal.

**HC8** - Queiroz, M.J.R.P."Synthesis and evaluation of the antitumor/antiangiogenic potential of new heterocyclic compounds" - Universidade de Évora 5 Abril 2013, Évora Portugal.

**HC9** - Queiroz, M.J.R.P. “Synthesis and evaluation of the antitumor and/or antiangiogenic potential of new heterocyclic compounds” VI Jornadas de Bioquímica Univ. de Trás-os Monte e alto Douro 10 de Abril 2013, Vila Real, Portugal.

**HC10** - Queiroz, M.J.R.P. “Aplicações práticas da cultura de células em estudos do potencial anti-tumoral e/ou antiangiogénico e avaliação da toxicidade em culturas de células primárias, de novos compostos sintéticos.” 2h, Instituto politécnico de Bragança, Curso de Linhas Celulares 19 de Abril 2013

**HC11** - Queiroz, M.J.R.P. “Synthesis and evaluation of the antitumor and/or antiangiogenic potential of new heterocyclic compounds”- IV Jornadas de Farmácia , in the scope of the 1st Annual Meeting Coimbra Health School, 20th april 2013, Coimbra, Portugal.

**HC12** - Queiroz, M.J.R.P. “Synthesis and evaluation of the antitumor and/or antiangiogenic potential of new heterocyclic compounds” 1º Simpósio de Química Medicinal da Universidade do Minho, 17th may 2013, Braga, Portugal

### **3. Participação em corpos editoriais de revistas científicas**

**EE** - Maria Manuela Silva, faz parte do painel editorial da revista Challenges of Modern Technology desde 2011 até à presente data.

**EE** - Maria Manuela Silva, faz parte do painel editorial da revista Journal of Chemistry desde 2013 até à presente data.

**EE** - António Maurício Fonseca, Editorial Board of journal ISRN Inorganic Chemistry. (<http://www.isrn.com/journals/ic/editors>)

**EE** - Gabriela Botelho faz parte do corpo editorial das revistas Cientificas da Hindawi Publishing Corporation

**HC** - Raposo, M.M.M.- Member of the editorial board of American Journal of Optics and Photonics

### **4. Organização de conferências nacionais**

- 1st Symposium on Medicinal Chemistry of University of Minho was organized in the scope of the Medicinal Chemistry MSc by the course directive committee, 17 de may de 2013, University of Minho.

Membros de comissões organizadoras de congressos nacionais:

**EE** - M. F. Bento e M. D. Geraldo, membros da comissão organizadora das III Jornadas de Electroquímica e Inovação, Vila Real, 16, 17 de setembro, 2013.

Membros de comissões científicas de congressos nacionais

**EE** - Pier Parpot, membro da comissão científica de 18th Meeting of the Portuguese Electrochemical Society. 25-27th March 2013, Porto, Portugal.

**HC** - M. Fernanda Proença, Membro da comissão científica do 10º Encontro Nacional de Química Orgânica, Lisboa, 4-6 September 2013.

### **5. Organização de conferências internacionais**

## **9.5. Internacionalização**

### **1. Publicações em colaboração com parceiros internacionais**

AA-3

BC/AA-2

BC-4

EE-11

HC-10

### **2. Projetos de I&D em colaboração com parceiros internacionais**

### **3. Participação em redes de investigação**

The CQ/UM is integrated in the National NMR network (coordinator in the CQ/UM Maria João Queiroz)

### **4. Investigadores estrangeiros na subunidade orgânica**

Issam Oueslati – from Tunísia;

Iwona Kuzniarska – Biernacka from Poland

### **5. Estudantes estrangeiros de pós-graduação na subunidade orgânica**

Agathe Begouin Post-Doc– French

Juliana Andrade PhD Student – Brazilian

**PARTE II****10. Medidas implementadas na sequência do relatório produzido pela Comissão de Acompanhamento Externo em 2012 (anexar o relatório da CAE, relativo ao ano de 2012).**

- The collaborations with industry were increased.
- More PhD theses were concluded.

**11. Análise SWOT**

<b>Strengths</b>	<b>Threats</b>
<ul style="list-style-type: none"> <li>- Scientifically mature team of researchers with a good output record of publications in ISI/SCOPUS indexed journals.</li> <li>- Multidisciplinary collaborations within the CQ, other research centres of UM and other Nat. and Int. Universities.</li> <li>- Consolidated International cooperation.</li> <li>- Membership of the national NMR network (RNNMR/PTNMR)</li> </ul>	<ul style="list-style-type: none"> <li>- Limited financial support:               <ul style="list-style-type: none"> <li>to improve laboratory infrastructures and safety conditions.</li> <li>to maintain research equipment.</li> </ul> </li> <li>- Dispersion between teaching/administrative activities.</li> <li>- The current University policy does not reward research quality.</li> <li>- The funding from FCT is not done regularly affecting the correct functioning of the CQ/UM</li> </ul>
<b>Opportunities</b>	<b>Weaknesses</b>
<ul style="list-style-type: none"> <li>- Growing PhDs and Master Students.</li> <li>- Recent Master degree courses are a source of new researchers.</li> <li>- New PhD course in Chemistry was approved by the Ministry.</li> <li>- Collaborations with Iberian Nanotechnology Lab (Braga) are being developed.</li> </ul>	<ul style="list-style-type: none"> <li>- Insufficient technical and administrative support that unable the possibility of responding to European project funds.</li> <li>- Insufficient collaborations with industry.</li> <li>- Some of the scientific equipment and infrastructures require extra maintenance/replacement.</li> </ul>