FCT Relatório Científico 2011 Print: 08-11-2013 10:20:38 [Centro de Química]

General Information

Name of Research Unit:	(QUI-Norte-686) Centro de Química
Coordinator:	Maria João Ribeiro Peixoto de Queiroz
Main Scientific Domain:	Química
Other Subdomains:	n/a

Host Institutions

Leading Host Institution:	Universidade do Minho
Other Institutions Involved:	

Objectives & Achievements

Unit Description

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-022716 (refª FCT Pest-C/QUI/UI0686/2011) entitled "Projecto Estratégico-UI 686- 2011-2012". FCT gives also financial support through the Portuguese Nuclear Magnetic Resonance network.

The internal regulations of the centre determine the organization and management procedures of the research unit. The CQ members are either full-time equivalent researchers (FTERs - with a PhD degree) or associated members (PhD students, MSc students young graduate researchers supported by financed projects and undergraduate grant holders). In December 2011, the CQ/UM had 40.6 FTERs and 64 associated members.

The members of the Centre are distributed between 4 groups according to their scientific interests and affinities:

- Electrochemistry and Environment (EE) with 13 FTERs and 23 associated members;

- Synthesis and Application of Heterocycles (HC) with 15.6 FTERs and 18.5 associated members;

- Synthesis and Application of Amino Acids (AA) with 7 FTERs and 13.5 associated members;

- Biological Chemistry (BC) with 5 FTERs and 9 associated members.

The organization of the CQ/UM is based on a scientific council that includes all FTERs and a coordinating committee. The Director of the research unit presides over the coordinating committee that 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 unit Director officially represents the unit, convenes the committees meetings and implements the decisions of these bodies.

An advisory committee was created and will accompany and advise future research activities of the Centre, in accordance with FCT regulations.

General Objectives

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

Many of the projects under development within the EE group are based on the preparation or characterization of new materials which directly or indirectly reduce chemical impact on the environment. These materials or processes are applicable in domains of catalysis, environmental or food-related analytical chemistry, the implementation of environmentally-friendly synthetic methods, the recovery of energy from effluents, the application of safer and more efficient electrolyte components in electrochromic devices and the use of functionalized nanostructured components in optical and biological applications.

Most of the members of the HC group are dedicated to the synthesis of new drug candidates. The synthetic skills developed allow the preparation of novel heterocyclic molecules incorporating N, O, and/or S atoms, including carba-sugar and aza-sugar derivatives and macrocyclic complexes. The biological activity of the new compounds is tested through national and international collaborations, in particular as antioxidants, antipsychotics, anticancer, antiangiogenics, antitubercular, antifungal and antibacterial agents. Other interests of the HC group include the encapsulation of new anticancer compounds in nanoliposomes for drug delivery, the functionalization of carbon nanotubes (CNTs) for composite applications or as precursors of functionalized graphene nanoribbons and the synthesis and characterization of new heterocyclic materials for nonlinear optical, photochromic, catalytic and sensor applications.

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 2011 this work has been developed on new synthetic methods for the preparation of new N-alkyldehydroamino acids, beta-amidodehydroamino acids, the synthesis and application of alpha,alpha-dialkylglycines and new bis-amino acids; synthesis of new cyclic RGD-peptides; photocleavable protecting groups and phototriggers; synthesis and molecular modeling of antimicrobial peptaibols and development of new dehydropeptidic hydrogelators; synthesis of novel psoralen analogues and carboline derivatives containing amino acid residues; synthesis of alkynylamino acid derivatives as precursors of glycoconjugates using a click chemistry approach.

Within the BC group one of the objectives is the design, synthesis, characterization and in vivo and in vitro evaluation of novel metal complexes and nanostructures potentially useful for medical imaging. Development of aqueous two-phase systems (ATPS) for large-scale affinity purification of plasmid for molecular therapies is another goal of the BC group. The focus is now settled in using AAs as affinity ligands to increase the selectivity of the systems. Other interests include the application of molecular modelling for drug design and the simulation of DNA in room temperature ionic liquids (RTILs)

Main Achievements during the year of 2011

Objectives & Achievements

In the EE group catalysts of zeolite-encapsulated metal complexes for environmental applications and zeolite-based drug delivery systems (DDS) were prepared. Electrical properties of PVDF/zeolite nanocomposites were determined. Optical/electrochemical studies of metal-heterocyclic ligand complexes were done. Hybrid gels incorporating metal nanoparticles were prepared. Electrochemical studies of bioactive compounds were done. ABS compositions with photo-stabilizers and antioxidants were prepared. The degradation of polymers was studied. Novel SPEs were prepared using different strategies with various host/guest salt combinations, and were evaluated in prototype devices. Electrochemical mineralization of organic pollutants on CNT catalysts was done. A two-chamber electrolyser was developed as a MFC using wastewater samples. Electrochemical methods were used to cyclise glucose-based derivatives. Recently developed RACE was tested with solutions containing organic acids. Characterization using CNT-modified electrodes was done. GC/MS and LC/MS were applied to monitor products from electrochemical reactions.

The HC group developed new synthetic methods, including eco-friendly for purines and chromenes. Sugars with triazoles were obtained by click chemistry. Erythrose dienes were prepared and reacted with N- and C- dienophiles via Diels-Alder reactions using metal-ligand technology. Metal-catalyzed couplings were also used. Several molecules were submitted to virtual screening in receptors and enzymes. Biological tests identified as anticancer agents (adenines, chromeno-imidazo-pyridines, pyrimidopyrimidines, imidazoles, and thienopyridines), antioxidants (imidazo-pyrrolo-diazepines, purines, imidazoles, pyrimidopyrimidines and di(hetero)arylamines), antimicrobials (imidazolyltriazolones and 6-substituted purines), antipsychotics (chromenes, imidazoles and purines). Nanoliposomes with fluorescent anticancer compounds were prepared for DDS. Oligothienyl-BODIPY derivatives, azo dyes, pyrroles, thienylpyrroles, crown ethers, Ru complexes bearing thienyl and furyl-imidazo-phenanthrolines and modified AAs bearing heterocycles, fluorescent peptides based nanoparticles were prepared and their NLO, photochromic and sensor properties were evaluated. Benzothiazoles were also incorporated into nanofibers for NLO.

The AA group developed new cross-linking strategies for new bis-AAs and RGD peptides. The synthesis of non-proteinogenic AAs and heterocycles for application as UV and NIR fluorescent bio, imaging probes, chemosensors and bioactive compounds was continued. The preparation of new peptidic hydrogelators was initiated. The synthesis of fluorescent N-glycopeptides and glycoconjugates containing a 1,2,3-triazole was performed, as well as of novel xanthine oxidase inhibitors containing aminoacids. The synthesis of psoralenes based on dibenzofuran and carbazole was achieved, and the evaluation of their biological activity was done. Conformational (NMR and FTIR) and membrane activity studies of antimicrobial peptaibols started with the synthesis of peptaibolin and its mimetics and molecular dynamic simulations.The synthesis of α,α-dialkylglycines by solid phase Ugi reaction continued.

The BC group prepared, characterized and evaluated in vitro and in vivo, paramagnetic complexes (Mn(II) and Gd(III)) and Au nanoparticles functionalized with Gd(III) chelates as new contrast agents for MRI. The purification of plasmid DNA in ATPS using PEG-Arg and PEG-amine as affinity ligands was achieved. Molecular simulation of DNA in RTILs allowed a better a understanding of DNA solvation.

Activities

Integrative/multidisciplinary activities during the year of 2011

Various members of the EE group participated in multidisciplinary projects with colleagues from other groups within the centre, with scientists from other centres of the UMinho and with researchers from other national and international centres. A high percentage of the joint publications originated in these projects have been published in interdisciplinary journals that provide a high visibility to group members. These collaborations continue to provide new topics for future collaborative research in the domains of energy conversion, catalysis, environmental chemistry, nano-composite materials and polymer stabilization. Some examples of collaborative interactions include projects in which members of the HC group prepare 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 Málaga and Polytechnic Valência Univ. Spain and from UC, UTAD and UNLisboa.

The synthesis of drug candidates and imaging agents involves collaboration between the members of HC, AA and BC groups.

Testing the new compounds involves national and international collaborators (TAACF-USA for antituberculosis activity, the USC-Spain for antipsychotic activity, Universidade Fernando Pessoa- Porto, Fac. Pharmacy-UPorto, IPATIMUP, the Biology and Biological Engineering Dept.-UM for antifungal and antitumor activities and CBMA-UM for antioxidant activity at cellular level. Studies of encapsulation of new fluorescent antitumor compounds in liposomes for drug delivery are done in collaboration with CFUM. The isolation and characterization of bioactive molecules for studies of Immunology of Infection involves members of HC in collaboration with ICVS-UM. An open-source software (Chem T) for building template-based chemical libraries was developed with 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. 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 and the AA groups are also evaluated within national (UC) and international collaborations (Univ. Hospital, Basel and École Polytechnique Féderal de Lausanne, Switzerland; Centre de Biophysique Moléculaire CNRS, France). The development of protein based ligands for the affinity purification of plasmids in aqueous two-phase systems is carried out in collaboration with the Univ. of Aston, Cambridge and London.

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 Engeneering Department, involved in the preparation of new materials and composites.

Outreach activities during the year of 2011

In April of 2008, the Executive Committee of UNESCO approved the proposal presented by IUPAC, that 2011 should be proclaimed the International Year of Chemistry (IYC2011). This iniciative, with the motto "Chemistry, our life, our future", is a celebration of the contributions of chemistry to the well-being of humanity. This year coincides with the 100th aniversary of the Nobel Prize in Chemistry, awarded to Marie Curie and also with the 100th aniversary of the Portuguese Chemical Society.

During 2011 the members of the Centre of Chemistry organized seminars, exhibitions, cultural and artistic events, illustrating all aspects of Chemistry but with several centred on the iconic figure of Marie Curie in recognition of the important contribution made by women in this domain of Science. These activities were supported by the Portuguese Chemical Society, the University of Minho, the Curie Institute of Paris, the Maria Skłodowska-Curie Museum in Warsaw, the French and Polish Embassies, EDP, the Fundação Calouste Gulbenkian and FNAC.

The opening session of the IYC2011 took place in Braga on the 27th of January, at the same time as the inauguration ceremony in Paris. At this session the first two seminars of the annual program were presented, by Prof. Miguel Castanho and Profª. Raquel Gonçalves-Maia. In April two exhibitions were inaugurated, "the life and work of Maria Sklodowska-Curie" prepared by the AIQ committee of the Centre/Department with

Activities

financial support from the Polish Embassy, and "Marie Curie, 1867/1934, a life, itinerary of a woman" supported by the French Embassy. The first of these exhibitions was opened by Her Excellency Katarzyna Skórzynska, the Polish Ambassador to Portugal and was followed by a play (Radiation - the story of Marie Sklodowska-Curie), also financed by the Polish Embassy. Two further activities describing the research of Marie Curie took place in May with seminars presented by guest speakers Profª Raquel Gonçalves Maia and Prof. Décio Martins. Between May and July IYC2011 activities included a handicraft competition, a photografic exhibition, and a play enacted during the XXII National Meeting of the Portuguese Chemical Society.

The final two events that brought the IYC2011 activities to a close were a seminar entitled "Opera, poisons and other chemicals" in November and a piano concert and tasting of molecular gastronomic delicacies in December.

Naturally, in addition to specific IYC2011 iniciatives, the members of the Centre also participated in the traditional outreach activities that are included in the annual program. These are "Vamos Kimikar", "Olimpiadas de Química", "QSI - a closer look at Chemistry", visits of members of the centre to schools and participation of local schools in events and "open days" organized in the centre. In 2011 several short-duration courses were lectured by members for teachers as in-service training modules and two one-day meetings were held for Chemistry and Biochemistry degree course students.

Funding

	2008	2009	2010	2011
LA FCT	0,00	0,00		
Units FCT	143.775,00	192.500,00	138.600,00	58.307,55
Projects FCT	217.793,00	144.968,00	197.865,00	166.729,00
Other (National)	5.000,00	46.416,00	1.000,00	13.250,00
Other (International)	9.500,00	0,00	0,00	0,00
National Industry	0,00	0,00	1.000,00	0,00
International Industry	0,00	0,00	0,00	0,00
	376.068,00	**383.884,00**	**338.465,00**	**238.286,55**

General Indicators

	2007	2008	2009	2010	2011	Total
No. of Researchers Hired (Ciência Programme)	0,00	0,00	0,00	0,00	1,00	1,00
No. of Researchers integrated with PhD	0,00	0,00	0,00	0,00	41,00	
Training PhDs (PhD thesis completed)	0,00	0,00	0,00	0,00	5,00	5,00

Researchers Hired

Name	Start Date	End Date	Other Institution
César João dos Santos Oliveira	15-09-2011	14-09-2016	

Technical Personnel Hired

Name	Start Date	End Date	Other Institution
No technical personnel found...			

Additional Comments

Research Groups

Reference	Title / Principal Investigator
RG-Norte-686-1064	Biological Chemistry (Joao Carlos Ramos Nunes Marcos)
RG-Norte-686-1656	Electrochemistry and Environment (EE) (Michael John Smith)
RG-Norte-686-1733	Heterocyclic Compounds (HC) (Maria Fernanda de Jesus Rego Paiva Proença)
RG-Norte-686-1930	Amino Acids (AA) (Paula Margarida Vidigal Soares Teixeira Ferreira)

Strategic Project Adjustments

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Group Description

Title of Research Group:	(RG-Norte-686-1930) Amino Acids (AA)
Principal Investigator:	Paula Margarida Vidigal Soares Teixeira Ferreira
Main Scientific Domain:	n/a
Group Host Institution:	Universidade do Minho

Funding, source, dates

Funding, source, dates

PTDC/QUI/69607/2006 titled "New photolabile groups as phototriggers and protecting groups: synthesis, photophysical and photorelease studies"; (PI/AA), total funding 97 000 €, AA: 8083 €.

PTDC/QUI/66250/2006 titled "Development of new heterocyclic compounds as luminescent and colorimetric chemosensors: metallic anion and cation detection"; (PI/HC), total funding 110 100 €, AA: 5505 €.

PTDC/QUI/81238/2006 (PI/CF-UM), titled "Interaction of new fluorescent biologically active heterocyclic compounds with DNA, lipid membranes and membrane proteins" total funding 89 325 €, AA: 1489 €.

PTDC/QUI/70063/2006 (PI/CNBC-UC), titled "Target nanoconstructs for multimodal medical molecular imaging" total funding 150 600 €, AA: 5020 €.

PTDC/CTM/105597/2008 (PI/CF-UM), titled Nonlinear spectroscopy of push-pull organic molecules" total funding 165 000 €, AA: 1000 €.

Total FCT Projects 2011: 21097 €

FCT fees for PhD students: 16612€

Bilateral colaboration under "Acções Integradas Luso-Espanholas" intitled with Prof. Rámon Martínez-Mánez from the Institute of Molecular Recognition and Technological Development (IDM), Polytechnic University of Valencia/University of Valencia (Spain), 375€

Objectives & Achievements

Objectives

The main objective of the Synthesis and Applications of Amino Acids group (AA) group in this project is finding new applications of amino acid and peptide chemistry in frontier areas of medicinal chemistry and advanced nanomaterials. Therefore, the AA group is committed to 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. Based on the expertise of the AA group, the areas to be developed include new synthetic methods for the preparation of non proteinogenic amino acids, namely dehydroamino acids, alpha,alpha-dialkylglycines, bis-amino acids and heterocyclic alanine derivatives, and their application in the synthesis of new cyclic peptides and antimicrobial peptide mimetics, small peptide hydrogelators, new peptide-based fluorimetric chemosensors and metal chelators for imaging purposes, fluorescent UV and NIR probes (using amino acid/peptide conjugates with heterocycles), and photoactive peptide prodrugs. In addition, protecting group chemistry research by using electrochemically or photochemically cleavable protecting groups as green alternatives to classical protecting groups will be pursued.

In recent years, the AA group has managed to establish a network of national and international collaborative interactions with other research groups, thus the maintenance and expansion of this network is also a fundamental objective.

Main Achievements

During 2011, the AA group was engaged in the development of new methods and new intermediates for peptide synthesis and their application in the production of peptides, peptide analogues and peptidomimetics with biological activity and potential application in the fields of drug discovery and in interfacial areas of biomedical and nanomaterials sciences. The main achievements include:

- the synthesis of new amino acid derivatives and heterocycles for application as UV and NIR fluorescent probes (in biomolecules and membranes), imaging probes, chemosensors and bioactive compounds;

- the development of new amino acid cross-linking strategies and their application to the cyclization of peptides. These compounds were tested in vitro for their ability and selectivity to bind specific targets. Some of these peptides were conjugated with bifunctional metal chelators to give imaging probes for PET, SPECT and MRI;

- the preparation of new small peptide hydrogelators with new dehydroamino acids to be used as surrogates of the extracellular matrix. The physicochemical and rheological properties for tissue engineering were evaluated;

- the development of new peptide fluorimetric chemosensors based on new unnatural amino acids with O, S and N heterocycles for the recognition of ions and bioactive molecules. Also, the assembly of Au and Si nanoparticles based on emissive peptide metallic complexes were used for biomolecule sensing studies;

- the synthesis of phototriggers for caging applications by testing novel heterocycles and their corresponding conjugates with model biomolecules under irradiation at different wavelengths in a photochemical reactor. The design and synthesis of new photoactivable prodrugs that allow the temporal and spatially controlled release of the bioactive compound was pursued. The synthesis of novel fluorescent heterocycles and their application in the preparation of prodrugs of 5-aminolevulinic acid, butyric acid was investigated with photoactivation by one- and two-photon excitation;

- the synthesis and application of highly hindered dialkylglycines (DAGs) with a new target, namely the synthesis of peptaibol mimetics, a class of natural antibiotic peptides. The substitution of selected residues by more structurally constrained and hydrophobic DAGs was directed by MD simulations. The membrane permeating activity of the mimetics was evaluated in model vesicles through fluorescence spectroscopy;

- the design and synthesis of novel heterocyclic photocleavable protecting groups by 1- and 2-photon excitation for the caging of amino acids (including neurotransmitters), biogenic amines and its biosynthetic precursors;

Objectives & Achievements

- the preparation of new carboline and psoralen derivatives containing amino acid residues and of new alkynylamino acid derivatives as precursors of glycoconjugates containing a 1,2,3-triazole unit. The evaluation of the biological activity of the new compounds was carried out;

- the synthesis of fused heterocycles based on oxazine systems displaying NIR fluorescence in order to obtain novel mono- and bifunctionalised derivatives possessing a combination of substituents that allow their application in labeling of biomolecules either alone or in conjugation with other photoactive entities;

- the study of the electrochemical behavior of new amino acid derivatives.

Group Productivity

Publications in peer review Journals

AA1 P.M.T. Ferreira, L.S. Monteiro, E.M.S. Castanheira, G. Pereira, C. Lopes, H. Vilaça "Electrochemical reduction of dehydroamino acids: synthesis and photophysical properties of β, β-diarylalanines", Tetrahedron, 2011, 67, 193-200. (IF10 = 3.011).

AA2 S. Naik, C.M.A. Alves, P.J.G. Coutinho, M.S.T. Gonçalves, "N-(Di)icosyl-substituted benzo[a]phenoxazinium chlorides: synthesis and evaluation as near-infrared membrane probes", European Journal of Organic Chemistry, 2011, 2491-2497. (IF10 = 3.206).

AA3 A.M. Piloto, A.M.S. Soares, G. Hungerford, S.P.G. Costa, M.S.T. Goncalves, "Long wavelength photolysis of amino acid 6-(methoxy-2-oxo-2H-naphtho[1,2-b]pyran-4-yl)methyl esters", Eur. J. Org. Chem., 2011, 5447-5451. (IF10 = 3.206).

AA4 C.M.A. Alves, S. Naik, P.J.G. Coutinho, M.S.T. Gonçalves, "Novel DNA fluorescence probes based on N-[5-(11-functionalised-undecylamino)-9H-benzo[a]phenoxazin-9-ylidene]propan-1-aminium chlorides: synthesis and photophysical studies", Tetrahedron Letters, 2011, 52, 112–116. (IF10=2.618)

AA5 M.J.G. Fernandes, S.P.G. Costa, M.S.T. Gonçalves, "Phototriggering of neuroactive amino acids from 5,6-benzocoumarinyl conjugates", Tetrahedron 2011, 67, 2422-2426. (IF10 = 3.011)

AA6 A.M. Piloto, A.M.S. Soares, G. Hungerford, S.P.G. Costa, M.S.T. Gonçalves, "Long-wavelength photolysis of amino acid 6-(methoxy-2-oxo-2H-naphtho[1,2-b]pyran-4-yl)methyl esters", European Journal of Organic Chemistry, 2011, 5447-5451. (IF10 = 3.206)

AA7 M.M. Fernandes, A.C. Gomes, A. Vasconcelos, F.-D. Munteanu, T. Tzanov, M.S.T. Gonçalves, N. End, K.-U. Schoening, G.M. Guebitz, A. Cavaco-Paulo, "Protein disulphide isomerase-assisted functionalization of keratin-based matrices", Applied Microbiology and Biotechnology, 2011, 90, 1311–1321. (IF10 = 3.28)

AA8 M. J. G. Fernandes, M. S. T. Gonçalves, S. P. G. Costa, "Phototriggering of neuroactive amino acids from 5,6-benzocoumarinyl conjugates", Tetrahedron, 2011, 67, 2422-2426. (IF10 = 3,011)

AA9/HC21 E.M.S. Castanheira, M.S.D. Carvalho, D.J.G. Soares, P.J.G. Coutinho, R.C. Calhelha, M.-J.R.P. Queiroz "Fluorescence studies on new potential antitumoral benzothienopyran-1-ones in solution and in liposomes", J. Fluorescence, 2011, 21, 911-922. (IF2010=1.966)

AA10/HC22 B.F. Hermenegildo, G. Pereira, A.S. Abreu, E.M.S. Castanheira, P.M.T. Ferreira, M-J.R. P. Queiroz, "Phenanthrenyl-indole as a fluorescent probe for peptides and lipid membranes", J. Photochem. Photobiol. A: Chem., 2011, 221, 47-57. (IF10=2.243)

AA11/HC23 A.S. Abreu, E.M. S. Castanheira, M-J.R. P. Queiroz, P.M.T. Ferreira, L.A. Vale-Silva, E. Pinto, "Nanoliposomes for encapsulation and delivery of the potential antitumoral methyl 6-methoxy-3-(4-methoxyphenyl)-1H-indole-2-carboxylate", Nanoscale Research Letters, 2011, 6:482. (IF10 = 2.560)

AA12/HC24 J. Gomes; L.O. Lunardi, F.H. Caetano, A.E.H. Machado, A.M.F. Oliveira Campos, L.M. Bendhack, C.N. Lunardi, "Biodegradable nanoparticles containing benzopsoralens: An attractive strategy for modifying vascular function in pathological skin disorders", Journal of Applied Polymer Science 2011, 121: 1348–1354. (IF10 = 1.203)

AA13/HC25 A.M. F. Oliveira-Campos, A.M. Salaheldin, F.A. Almeida Paz, L.M. Rodrigues "Synthesis of 3-indolylazoles and meridianin derivatives from indolyl enaminonitriles" ARKIVOC, 2011, XI, 121-133 (IF10=1.096)

AA14/ HC26 R.M.F. Batista, E. Oliveira, S.P.G. Costa, C. Lodeiro, M.M.M. Raposo, "Imidazo-benzo-15-crown-5 ether bearing arylthienyl and bithienyl moieties as novel fluorescent chemosensors for Pd2+ and Cu2+", Tetrahedron, 2011, 67, 7106-7113. (IF10 = 3.011).

AA15/HC27 E. Oliveira, S.P.G. Costa, M.M.M. Raposo, O.N. Faza, C. Lodeiro, "Synthesis, characterization, fluorescence and DFT studies of new Cu2+, Ni2+ and Hg2+ complexes with emissive thienylbenzoxazolyl-alanine ligands", Inorg. Chem. Acta, 2011, 366, 154-160. (IF10 = 1.899)

AA16/ HC28 C.I.C. Esteves, M.M.M. Raposo, S.P.G. Costa, "Novel highly emissive non proteinogenic amino acids: synthesis of 1,3,4-thiadiazolyl asparagines and evaluation as fluorimetric chemosensors for biologically relevant transition metal cations", Amino Acids, 2011, 40, 1065-1075. (IF10 = 4.106).

AA17/HC29 E. Oliveira, D. Genovese, R. Juris, N. Zaccheroni, J.L. Capelo, M.M.M. Raposo, S.P.G. Costa, L. Prodi, C. Lodeiro, "Synthesis of new emissive peptides probes based on benzo[d]oxazol derivatives and their gold and sílica nanoparticles", Inorg. Chem., 2011, 50, 8834-8849. (IF10 = 4.325)

AA18/ HC30 R.M.F. Batista, E. Oliveira, S.P.G. Costa, C. Lodeiro, M.M.M. Raposo, "(Oligo)thienyl-imidazo-crown ether derivatives: synthesis, photophysical studies and evaluation of their chemosensory properties", Talanta, 2011, 85, 2470-2478. (IF10 = 3.722).

27 communications to international congresses

- 4th Iberian Meeting on Colloids and Interfaces, 13-15 July, 2011,Porto (Portugal),

- 23rd International Congress of Heterocyclic Chemistry, ICHC2011, 31 July-4 August, 2011, Glasgow(UK).

- Glupor 9 - 9th International Meeting of the Portuguese Carbohydrate Chemistry Group/5th Iberian Carbohydrate Meeting, 4-7 September 2011,Vila Real (Portugal)

- International Conference on Applications of Optics and Photonics (AOP2011), 3-7 May 2011, Braga (Portugal)

- Twelfth Tetrahedron Symposium, 21 - 24 June 2011,Sitges (Spain)

- 17th European Symposium on Organic Chemistry (ESOC 2011), 10-15 July 2011,Hersonissos (Greece)

- European Catalysis X Congress (EuropaCat X), Catalysis across the disciplines, 28 August- 2 September 2011, Glasgow (UK)

- 12th Conference on Methods and Applications of Fluorescence, Spectroscopy, Imaging and Probes, 11-14 September 2011, Starsbourg (France)

- 15th International Electronic Conference on Synthetic Organic Chemistry (ECSOC-15), 1 - 30 November 2011.

- HORIBA Scientific workshop series, 29 November- 1 December 2011,Munich (Germany)

Group Productivity

- 13th European Symposium on Organic Reactivity, 11-16 September 2011, Tartu (Estonia)

- COST Chemistry D38: Metal-based systems for molecular imaging applications, joint WG 2 and WG 6, 24-26 March 2011,Torino (Italy)

- COST Chemistry D38: Metal-based systems for molecular imaging applications, Final Meeting, 13-15 September2011,Oxford (UK)

24 communications to national congresses

- XXII Encontro Nacional da Sociedade Portuguesa de Química (SPQ), 3-6 july 2011,Braga.

-MicroBiotec 2011, 11th National Congress,1-3 December2011, Braga.

Other international publications

AA1. A. M. S. Soares, S. P. G. Costa, M. S. T. Gonçalves, "Novel fused oxobenzopyrano[6,7-d]oxazoles as light-triggered protecting groups for carboxylic acids", Proceedings of ECSOC-14, 14th International Electronic Conference on Synthetic Organic Chemistry, http://www.mdpi.net /ecsoc/, J.A. Seijas e M. P.V. Tato (Eds), MDPI, Basel, 2011 (ISBN: 3-906980-24-3).

AA2. A. M. Piloto, S. P. G. Costa, M. S. T. Gonçalves, "Release of model amino acids by ester linkage photolysis from fused 2-oxo-2H-benzopyranyl conjugates", Proceedings of ECSOC-14, 14th International Electronic Conference on Synthetic Organic Chemistry, http://www.mdpi.net/ecsoc/, J.A. Seijas e M. P.V. Tato (Eds), MDPI, Basel, 2011 (ISBN: 3-906980-24-3).

AA3. R. M. F. Batista, S. P. G. Costa, M. Belsley, M. M. M. Raposo, "Synthesis and characterization of novel push-pull thiophene and thienylpyrrole derivatives functionalized with indanonedicyanovinyl acceptor moiety as efficient NLO-chromophores", 8001-186, Proceedings of the International Conference on Applications of Optics and Photonics (AOP2011), SPIE, , 2011 (ISBN: 9780819485755).

Ph.D. thesis completed

- Rosa Batista, intitled "Synthesis and characterization of heterocyclic compounds and modified amino acids with application in nonlinear optics and/or as fluorimetric and colorimetric sensors for anions and cations", FCT grant (SFRH/BD/36396/2007), Department of Chemistry, concluded in 22nd December 2011, co-supervisors: Susana Costa (Amino Acids group) and Manuela Raposo (Heterocycles group).

Organization of conferences

Organization of "XXII National Meeting of the Portuguese Chemical Society – A hundred years of Chemistry in Portugal", Braga, from 3rd to 6th July 2011 (Susana Costa, member of the Organizing Comittee).

Organization of "International Year of Chemistry" in Braga with several events during 2011 (Luís Monteiro and Paula Margarida Ferreira, members of the organizing comittee).

Internationalization

- Doctor Graham Hungerford, HORIBA Jobin Yvon IBH Ltd, Glasgow, UK.

- Prof. Ramón Martinez-Mañez, from the Institute of Molecular Recognition and Technological Development (IDM), Polytechnic University of Valencia/University of Valencia, Spain.

- Doctor Carlos Lodeiro, BIOSCOPE Group, Department of Physical Chemistry, Sciences Faculty of Ourense, University of Vigo, Ourense, Spain.

- Professor Bing Xu, Department of Chemistry, University of Brandeis, Massachusetts, USA.

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Group Description

Title of Research Group:	(RG-Norte-686-1064) Biological Chemistry
Principal Investigator:	Joao Carlos Ramos Nunes Marcos
Main Scientific Domain:	n/a
Group Host Institution:	Universidade do Minho

Funding, source, dates

Funding, source, dates

Projects funded by FCT:

PTDC/QUI/70063/2006 "Targeted nanoconstructs for multimodal medical imaging" Coordinated by Prof. Carlos Geraldes (CNC-UC). JAM and JPA team

members (01/01/08-31/12/11) 25000

PTDC/QUI/67407/2006 Coordinated by Prof. Maria José Alves (HC/CQ-UM). JAM team member (01/01/09-31/12/11)

Ph.D. Students funded by FCT:

Sandra Barros SFRH/BD/36522/2007 (01/04/09-01/03/12) 2750€

Miguel Filipe M. M. Ferreira (SFRH/BD/63994/2009) (01/03/10-28/02/13) 2750€ BC/AA

André Fontes(SFRH/BD/63676/2009) (01/03/10-28/02/13) 2750€ BC/ AA

Arsénio Sá (SFRH/BD/63639/2009) (01/01/10-31/12/12) 2750€ (BC/AA)

Objectives & Achievements

Objectives

The Biological Chemistry group encompasses several chemical studies related to biological systems:

Task 1- Design, synthesis, physico-chemical characterization and pharmacological evaluation (in vivo – biodistribution and in vitro - cell line studies) of new metal complexes (Gd(III), Mn(II) and Ga(III)) and nanostructures (gold nanoparticles, iron oxide) functionalized with metal complexes as potential agents for medical imaging (MRI, gamma scintigraphy and PET).

Task 2- Development of aqueous two-phase systems (ATPS) for the affinity purification of plasmid to be used on molecular therapies. In this year it was continued to be tested the possibility of using amino acids as affinity ligands.

Task 3 – Development of new human neutrophil elastase inhibitor-peptides, derived from endogenous proteins. Activity and kinetic studies on the system composed by elastase/N-succinyl-Ala3-pNA/inhibitor-peptides, to determine the applicability of the selected peptides as elastase inhibitors and determine inhibition type present in the given system. Structural determinations on the inhibitor peptides, in conditions that mimic the physiologic settings. Development of methodologies to study protein oxidative damages.

Task 4 - The main objective is to improve the state-of-the-art of computer-aided drug design methodologies in collaboration with medicinal chemistry groups from CQ-UM and other research groups outside the centre. Furthermore structural, dynamics and functional studies of biomolecules in ionic liquids will be performed.

Main Achievements

Task 1- Synthetic routes for novel triaza- and tetraaza-based chelators for Ga(III), Mn(II) and Gd(III) have been developed. Mn(II) chelates of bifunctional triaza ligands have been characterized by relaxometry as potential contrast agents for MRI.

Biodistribution and γ-scintigraphic studies with 67Ga(III) labeled chelates of tetraaza-based ligands functionalized with PEG moieties were performed on Wistar rats.

In the near future we intend to couple the bifunctional ligands to RGD peptides and to evaluate the pharmacological properties of these 67Ga(III) labeled chelates as potential radiopharmaceutical agents.

The synthetic rote, proposed previously, for DO3A-N-(α-amido)propionate chelators has been validated and extended to NO3A-N-(α-amido)propionate chelators. The Ga(NO3A-N-(α-amino)propionate) chelate and a model amide conjugate, Ga(NO3A-N-(α-benzoylamido)propionate) chelate, have been characterized by 1H and 69Ga NMR.

The Gd(DO3A-N-(α-benzoylamido)propionate) chelate, characterized before by relaxometry, has been evaluated as a potential CA by MRI studies in rats.

A new DO3A-N-(α-mercaptoundecanamido)propionate conjugate has been prepared for decorating gold nanoparticles with Gd3+ chelates. Gold nanoparticles functionalized with Gd3+ chelates have been characterized by 1H NMRD and 17O NMR, and MRI studies as potential CAs for MRI.

The functionalization of gold nanoparticles decorated with Gd3+ chelates with (bio)epitopes (folic acid, cyclic RGD peptides, etc) to target cancer cells is underway. The preparation of conjugates porfirin/ftalocyanin - Gd3+ chelates is underway for evaluation as novel theragnostics-Photodynamic Therapy / MRI.

Task 2 – It was tested the possibility of using Polyethylene glycol amine as as affinity ligands for plasmid DNA (pDNA) purification from bacterial alkaline lysates in Polyethylene glycol (PEG)/dextran (DEX) systems. As previously observed with PEG-Lysine and PEG-Arginine the pDNA was steered to the PEG phase but only with desalted lysate. However a higher concentration of the ligand (4%) was needed to recover all the pDNA

Objectives & Achievements

in the PEG phase. Mixing the PEG phase of this system with a 30% solution of (NH4)2SO4 another ATPS was obtained with pure pDNA in the bottom phase. The interaction of the free aminoacids lysine, arginine and histidine, with pDNA was studied using a fluorescent intercalator method. Histidine show the highest affinity with a maximum value at pH 8.5, while for both Lysine and Arginine the affinity decreased between pH 7.5 and 9.5.

Task 3 – In collaboration with the EE group a methodology was developed for the electrochemical generation of hydroxyl radicals, and applied to the study of oxidative modification on proteins. A platinum anode and a boron dopped diamond (BDD) anode were used . Both were effective in generating hydroxyl radicals although the BDD anode was more effective in protein oxidation. It was also concluded that while the BDD anode promotes the fragmentation of the protein the platinum anode oxidizes mainly the side chains of the protein.

Task 4 – It was disclosed novel insights concerning the understanding of DNA in ten room temperature ionic liquids (RTILs) with different representative chemical moieties. RTILs are drawing great attention from many chemical scientific communities as a media to perform a growing number of processes such as, catalysis, separation and materials, just to name a few. Our findings provide a significant step forward in several chemical research areas were DNA is used, and will be a reference for the future understanding and development of novel RTILs specific for nucleic acids solutes.

Group Productivity

Publications in peer review Journals

BC1 L. Cardoso, N.M. Micaelo, "DNA Molecular Solvation in Neat Ionic Liquids", ChemPhysChem, 2011, 12, 275 – 277. (IF10 3.339)

BC2 A. Fontes, M.I.M. Prata, C.F.G.C. Geraldes, J.P. André, "Ga(III) chelates of amphiphilic DOTA-based ligands: synthetic route and in vitro and in vivo studies", NuclEEr Medicine and Biology, 2011, 38, 363-370. (IF 2.620)

BC3 J.M.C. Teixeira, D.M. Dias, F.J. Cañada, J.A. Martins, J.P. André, J.J. Barbero, C.F.G.C. Geraldes, "The Interaction of La3+ Complexes of DOTA/DTPA Glycoconjugates with the RCA120 lectin: A Saturation Transfer Difference (STD) NMR Spectroscopic Study", Journal of Biological Inorganic Chemistry, 2011, 16, 725-734. (IF 3.287)

BC4 C. Caramelo-Nunes, T. Tente, P. Almeida, J.C. Marcos, C.T. Tomaz, "Specific berenil–DNA interactions: An approach for separation of plasmid - Isoforms by pseudo-affinity chromatography", Analytical Biochemistry, 2011, 412, 153–158. (IF10 3.236)

BC5/HC15 M.J. Alves, F.T. Costa, V.C.M. Duarte, A. Gil Fortes, J.A. Martins, N.M. Micaelo, "Advances in the synthesis of homochiral (−)-1-azafagomine and (+)-5-epi-1-azafagomine. 1-N-phenyl carboxamide derivatives of both enantiomers of 1-azafagomine: leads for the synthesis of active α-glycosidase inhibitors", J. Org. Chem., 2011, 76, 9584-9592. (IF10 4.002)

Other national publications

BC - J.P. André, A. de Sá, "Radioisótopos e sociedade: O legado de Marie Curie 100 anos depois", Química (Boletim da Sociedade Portuguesa de Química), 2011, 120, 31-37.

FCT Relatório Científico 2011 Print: 08-11-2013 10:21:34 [Centro de Química]

Group Description

Title of Research Group:	(RG-Norte-686-1656) Electrochemistry and Environment (EE)
Principal Investigator:	Michael John Smith
Main Scientific Domain:	n/a
Group Host Institution:	Universidade do Minho

Funding, source, dates

Funding, source, dates

Research stimulation program (Programa de Estimulo à Investigação) 10.000 Euros Fundação Calouste Gulbenkian.

Projects FCT and FEDER:

- "Thienylpyrroles as building blocks for the synthesis of organic and coordination compounds with non-linear optical (NLO) applications", with financial support from FCT through PTDC/QUI/66251/2006, 7 670 euros in 2011.

- "Nanostructured catalysts based on carbon nanofibres for environmental applications" within the Capacitation program in Nanotechnology, with financial support through FCT. Researcher responsable José Luis Figueiredo (UPorto). NANO/NTec-CA/0122/2007. Total financial support of 111 984,00 euros with a UMinho component of 55 992,00 euros of which 19 926,00 euros were provided in 2011.

- "ELECTRA – Transístores de filme fino electrocrómicos para aplicação em janelas inteligentes" with reference PTDC/CTM/099124/2008 and a total financial support of 180 000 euros. The UMinho component was 27.480 euros (MMS) and 9 160 euros in 2011.

- Support for the Ações Integradas Luso-Espanholas program in 2011/12, reference E-136/12 (with a contribution of 2 500 € for the year 2011).

- FCT Human Resources Grants to 8 PhD research students provided a total of 25 300 euros.

Objectives & Achievements

Objectives

In 2011 the members of the research group continued to focus their activity on areas of intersection between the environment and electrochemistry with particular attention being devoted to the development of clean chemical processes, materials with improved energy-efficiency and novel analytical methods. The research portfolio of the group was also extended to include the preparation, characterization and exploitation of properties of new materials.. The objectives described in this section were originally defined in 2010 for research that was planned for 2011. For this reason all objectives are identified in the future tense.

Low environmental-impact heterogeneous catalysts based on encapsulated metal complexes in nanostructures will be developed for oxidation of organic pollutants in aqueous media. Nanostructured drug delivery systems represent an important emerging domain of medical research with particular relevance for administration of anticancer drugs. New nanostructured encapsulating materials will be prepared and evaluated by collaborators in cell-strain testing.

Organometallic compounds will be prepared, characterized and optimized for use as components with nonlinear optical properties for applications in signal transmission and energy-light conversion (LEDs).

Polymeric materials with improved mechanical and thermal properties will be developed for specific applications in the automotive industry. Polymer nanocomposites will be prepared and evaluated as biodegradable engineering materials.

Solid polymer electrolytes are materials with potential technological application in energy conversion (batteries and capacitors) and displays (electrochromic devices). The objective of research in this field is to prepare and characterize new electrolyte systems and, in collaboration with other groups, evaluate potential applications.

Properties of protective coatings and active filters may be significantly improved by the incorporation of nanoparticles within the component structure. The sol-gel synthetic strategy will be applied in the preparative process in order to introduce important advantages in relation to conventional procedures.

Cyclization reactions involving ester and glucose derivatives are of synthetic importance as a route to useful intermediates. The objective of this sub-project is to elucidate the mechanism of relevant reactions and optimize the experimental conditions.

Organic pollutants and nitrates will be removed from wastewater using paired electrolyses with electrocatalysts based on carbon nano-tubes. The effect of cell geometry on the operational parameters of a microbial fuel cell will be evaluated. The laboratory-scale cell will be subjected to scale-up and re-evaluation.

Systematic electrochemical studies of novel compounds with anti-cancer or anti-oxidant activity will continue in order to establish a structure-activity relationship and to synthesize compounds with enhanced biological performance.

An electrochemical method will be applied to generate hydroxyl radicals and oxidize proteins under conditions of simulated "in vivo" oxidative stress. Experimental variables will be studied to identify the parameters that determine the reactivity and the quantity of radicals produced. Antioxidant activity of phenolic compounds will be evaluated with microfluidic electrochemical devices.

Advanced chromatographic methods (GC-MS and LC-MS) will be used to monitor products from electrochemical reactions and analytical tools will be developed to improve the efficiency and precision of methods currently applied to the quantification of pesticides in wines, soils, water and biological matrices. These procedures will also be adapted to characterize the organic content of archaeological artifacts.

Main Achievements

During 2011 the members of the E&E group contributed to many multidisciplinary projects in collaboration with colleagues from other groups within the centre, with members of other centres within the UMinho and also with other national and international researchers from external institutions. This broad-based collaboration is one of the strengths of the group and has led to opportunities for new projects, particularly in domains at the interface between Chemistry and other natural and physical sciences or between Chemistry and Engineering. As the group develops to take advantage of new research opportunities, projects based on preparation, characterization and application of novel materials have been included in the research portfolio.

Objectives & Achievements

New molybdenum complexes with heterocyclic ligands were found to show alterred electrochemical behavior and a significant improvement in optical characteristics. The hyper-Rayleigh scattering technique was used to evaluate hyperpolarizabilities of these compounds.

Encapsulation of metal complexes in nanoporous NaY was achieved by two different synthetic methods. The catalytic behavior of metal complexes in NaY was evaluated by oxidation of organic compounds.

Anticancer drugs applied in colorectal cancer therapy were encapsulated in zeolite structures and the effect of the zeolite and DDS on HCT-15 human colon carcinoma cell line viability was evaluated. Encapsulation of the drug was shown to significantly increased its potency.

ABS compositions containing light stabilizers and antioxidants were prepared to study the effectiveness of additives in protecting the chemical structure and macroscopic properties of the polymer against UV radiation under natural and accelerated weathering conditions. The influence of parameters on the degradation of electrospun poly(L-lactic acid) and chitosan membranes was reported.

In the domain of solid polymer electrolytes new spectroscopic and electrochemical characterization of organic-inorganic hybrid networks was carried out, electrolytes based on novel guest ionic species in complex host systems were studied and various multi-functional electrolyte components were evaluated in small-scale prototype electrochromic devices.

Hybrid gel materials with improved optical transparency, reduced shrinkage and very low surface roughness were obtained by the sol-gel method using alternative precursors and catalysts. New methods were implemented to reproduce imprinted gratings on monolith surfaces demonstrating the production of difraction lenses with a wide range of forms.

Electrochemical carboxylation of allylic acetates and carbonates and the electroreductive intramolecular cyclization of bromoalkoxylated derivatives were successfully accomplished with the use of nickel catalysts. These procedures contribute to an improved approach to key-compound synthesis in "green" media.

Electrochemical evaluation of substituted imidazopyrrolodiazepine scaffolds was performed as a preliminary screening test of potential anti-cancer activity of the compounds.

A new method for evaluation of antioxidant capacity was developed based on the simulation of oxidative attack of specific reactive oxygen species. The ability of Pt to produce hydroxyl radicals was characterized following the production of hydroxylated products from a non-electroactive species.

The electrochemical mineralization of organic acids in aqueous medium was achieved with excellent yields on metal-modified electrocatalysts based on carbon nanotubes (M/CNT). The reduction of nitrate to nitrogen was carried out on M/CNT, while nitrite and ammonia appear as by-products. Very satisfactory performance of the filter press Microbial Fuel Cell in bioelectricity production and carbon removal was achieved by high electrode area/electrolyte volume ratio. The electrochemical behavior of proteins isolated from Geobacter was studied and an active redox center/oxidation potential relationship for a microbial fuel cell was established.

Group Productivity

Publications in peer review Journals

EE1 R Magalhães, N Durães, J Silva, M Silva, V Sencadas, G Botelho, JL Gómez Ribelles, S Lanceros-Méndez, "The role of solvent evaporation in the microstructure of electroactive b-poly(vinylidene fluoride) membranes obtained by isothermal crystallization", Soft Materials, 2011, 9, 1-14. (IF10 2.088)

EE2 R Oliveira, J Marques, F Bento, D Geraldo, P Bettencourt, "Reducing Antioxidant Capacity Evaluated by means of a Controlled Potential Electrolysis", Electroanalysis, 2011, 23, 692–700. (IF10 2.721)

EE3 AP Samantilleke, MF Cerqueira, SH Evens, P Warren, IM Dharmadasa, GEA Muftah, CJR Silva, B Marí, "Analysis of the chemical bath deposition of CdS thin films on different substrates using electrolyte contacts", Thin Solid Films, 2011, 519, 7583-7586.

EE4 FM Gray, MJ Smith, MV Borges Silva, "Identification and characterization of textile fibers by thermal analysis", J. Chem. Educ., 2011, 67, 476 – 479. (IF08 0.300)

EE5 PC Barbosa, M Fernandes, SMF Vilela, A Gonçalves, MC Oliveira, E Fortunato, MM Silva, MJ Smith, R Rego, V de Zea Bermudez, "Di-ureasil hybrids doped with LiBF4: Attractive candidates as electrolytes for smart windows", Int. J. Electrochem. Sci., 2011, 6, 3355-3374. (IF10 2.808)

EE6 PC Barbosa, M Fernandes, SMF Vilela, MM Silva, MJ Smith, V de Zea Bermudez, "Di-ureasil hybrids doped with LiBF4: Spectroscopic study of the ionic interactions and hydrogen bonding", Materials Chemistry and Physics, 2011, 129, 385-393, (IF10 2.353)

EE7 P.C. Barbosa, L.C. Rodrigues, M.M. Silva, M.J. Smith, "Characterization of pTMCnLiPF6 solid polymer electrolytes", Solid State Ionics, 2011, 193, 39-42 (IF10 2.491).

EE8 A Gonçalves, C Costa, S Pereira, N Correia, MM Silva, PC Barbosa, LC Rodrigues, I Henriques, R Martins, E Fortunato, "Study of electrochromic devices with nanocomposites polymethacrylate hydroxyethylene resin based electrolyte", Polymers for Advanced Technologies, 2011, 22, 1-5. (IF10 1.532)

EE9 AV Machado, G Botelho, MM Silva, IC Neves, AM Fonseca, "Stability of nanocomposites of poly(ε-caprolactone) with tungsten trioxide", J. Polymer Research, 2011, 18, 1743-1749 (IF10 1.532)

EE10 E Lima, R Mattos, F Sentanin, LC Rodrigues, MM Silva, RAS Ferreira, LD Carlos, A Pawlicka, "Functional novel polymer electrolytes containing europium picrate", Materials Research Innovations, 2011, 487-497 (IF10 1.723)

EE11 M Fernandes, SS Nobre, LC Rodrigues, A. Gonçalves, R. Rego, MC Oliveira, RAS Ferreira, E Fortunato, MM Silva, LD Carlos, V de Zea Bermudez, "Li+- and Eu3+- doped poly(e-caprolactone)/siloxane biohybrid electrolytes for electrochromic devices", ACS Applied Materials & Interfaces, 2011, 3, 2953-2965. (IF10 = 2.925)

EE12 I Kuźniarska-Biernacka, K.Biernacki, AL Magalhães, AM Fonseca, IC Neves, "Catalytic behaviour of 1-(2-pyridylazo)-2-naphthol transition metal complexes encapsulated in Y zeolite", Journal of Catalysis, 2011, 278, 102-110. (IF10=5.415)

EE13 N Vilaça, R Amorim, O Martinho, RM Reis, F Baltazar, AM Fonseca, IC Neves, "Encapsulation of alfa-cyano-4-hydroxycinnamic acid into a NaY zeolite", Journal of Materials Science, 2011, 46, 7511-7516. (IF10 1.855)

EE14 B Silva, H Figueiredo, V P Santos, MFR Pereira, JL Figueiredo, AE Lewandowska, MA Bañares, IC Neves, T Tavares, "Reutilization of Cr-Y zeolite obtained by biosorption in the catalytic oxidation of volatile organic compounds", Journal of Hazardous Materials, 2011, 92, 545-553 (IF10 4.144).

EE15 A C Lopes, CM Costa, CJ Tavares, IC Neves, S Lanceros-Mendez, "Nucleation of the Electroactive γ Phase and Enhancement of the Optical Transparency in Low Filler Content Poly(vinylidene)/Clay Nanocomposites", Journal Physical Chemistry C, 2011, 115 (37) 18076-18082. (IF10 = 4.524)

Group Productivity

EE16 L Peixoto, B Min, G. Martins, AG Brito, P Kroff, P Parpot, I Angelidaki, R Nogueira, "In situ microbial fuel cell-based biosensor for organic carbon" Bioelectrochemistry, 81 (2) (2011) 99. (IF10 3.520).

EE17 O Carvalho, D Soares, A Fonseca, FS Silva, "Comparative study of tarnishing resistance of several coloured gold based alloys", Corrosion Engineering, Science and Technology, 2011, 46, 271-276. (IF10 0.495)

EE18 MJ Medeiros, C Pintaric, S Olivero, E Dunach, "Nickel-catalysed electrochemical carboxylation of allylic acetates and carbonates", Electrochimica Acta, 2011, 56, 4384–4389. (IF10 3.642)

EE19 MJ Medeiros, CSS Neves, AR Pereira, E. Duñach, "Electroreductive intramolecular cyclisation of bromoalkoxylated derivatives catalysed by nickel(I) tetramethylcyclam in "green" media", Electrochimica Acta, 2011, 56, 4498–4503. (IF10 = 3.642)

EE20 M. Fernandes, L.C. Rodrigues, R.A. Ferreira, A. Gonçalves, E. Fortunato, M.M. Silva, M.J. Smith, L.D. Carlos, V. de Zea Bermudez, "K+-doped poly(epsilon-caprolactone)/siloxane biohybrid electrolytes for electrochromic devices", Solid State Ionics, 2011, 204-205, 129-139 (IF10 = 2.491)

EE21 LC Rodrigues, MM Silva, MJ Smith, A Gonçalves, E Fortunato, "Preliminary characterisation of LiAsF6 hybrid polymer electrolytes for electrochromic devices", Electrochimica Acta, 2011, 57, 52-57. (IF10 3.642).

EE22 AP Samantilleke, MF Cerqueira, S Heavens, P Warren, IM Dharmadasa, GEA Muftah, CJR Silva, B Marí – Characterization of chemical bath deposited CdS thin films on different substrates using electrolyte contacts, Thin Solid Films, 2011, 519 7583-7586.

EE23 A. California, V.F. Cardoso, C.M. Costa, V. Sencadas; G. Botelho, J.L. Gómez-Ribelles, S. Lanceros-Mendez, "Tailoring porous structure of electroactive poly(vinylidene fluoride-trifluoroethylene) by controlling solvent/polymer ratio and solvent evaporation rate", European Polymer Journal, 2011, 47, 2442-2450 (IF10 2.517)

EE24/HC16 AJ Mendonça, M Inês, AP Esteves, DI Mendonça, MJ Medeiros, "Kolbe electrosynthesis of 1,2-di(bicyclo[2.2.1]heptan-2-yl)ethane and 1,2-diphenylethane", Synthetic Communications, 2011, 41, 820–825. (IF10 0.937)

EE25/HC17 MMM Raposo, AMC Fonseca, MCR Castro, M Belsley, MFS Cardoso, LM Carvalho, PJ Coelho, "Synthesis and characterization of novel diazenes bearing pyrrole, thiophene and thiazole heterocycles efficient photochromic and nonlinear optical (NLO) materials", Dyes Pigments, 2011, 91, 62-73. (IF10 2.635)

EE26/HC18 MMM Raposo, MCR Castro, AMC Fonseca, P. Schellenberg, M Belsley, "Design, synthesis and characterization of the electrochemical, nonlinear optical properties and theoretical studies of novel thienylpyrrole azo dyes bearing benzothiazole acceptor groups", Tetrahedron, 2011, 67, 5189-5198. (IF10 3.011)

EE27/HC19 MMM Raposo, MCR Castro, M Belsley, AMC Fonseca, "Push-pull bithiophene azo-chromophores bearing thiazole and benzothiazole acceptor moieties: synthesis and evaluation of their redox and nonlinEEr optical properties", Dyes Pigments, 2011, 91, 454-465. (IF10 2.635)

EE28/HC20 PJ Coelho, MCR Castro, AMC Fonseca, M.M. Raposo, "Photoswitching in azo dyes bearing thienylpyrrole and benzothiazole heterocyclic systems", Dyes Pigments, 2011, 92, 745-748. (IF10 2.635)

Other international publications

EE1. M.C.R. Castro, A.M.C. Fonseca, M. Belsley, M.M.M. Raposo, "Highly efficient and thermally stable NLO organic materials based on pyrrole and thiophene heterocycles", Atas do International Conference on Applications of Optics and Photonics (AOP2011), Universidade do Minho, Braga, Portugal, 3 a 7 de maio de 2011. Proc. SPIE, 2011, 8001, 80012U1-80012U10.

EE2. J.F. Ribeiro, M.F. Silva, L.M. Gonçalves, J. P. Carmo, J. H. Correia, M.M. Silva, F. Cerqueira, P. Alpuim, J. E. Bourée, "Thin-film solid-state rechargeable lithium battery", Proceedings of MME 2011, 22nd Micromechanics and Micro Systems Europe Workshop (MME2011), Toensberg, Norway, 19 a 22 de junho de 2011(ISBN 978-82-7860-224-9).

EE3. F. Vieira, J.C. Morgado, J. Almeida, M.M. Silva, J. Sá, "Representações da vida académica: o papel do ensino na Universidade", Actas do congresso II Congreso Internacional de Docencia Universitaria, Vigo, Espanha, 30 de Junho a 2 de julho de 2011.

EE4. S. Devesa, J.L.C. Silva, M.M. Silva, "Um contributo da universidade na aproximação do cidadão à ciência", Actas do congresso II Congreso Internacional de Docencia Universitaria, Vigo, Espanha, 30 de junho a 2 de julho de 2011.

EE5. C.M. Costa, A. California, V.F. Cardoso, V. Sencadas, L.C. Rodrigues, M.M. Silva, S. Lanceros-Méndez, "Electroactive Poly(Vinylidene Fluoride – Trifluorethylene) (PVDF-TrFE) microporous membranes for Lithium-ion battery applications", Proceedings of EMF-12, Bordeús, França, 26 de junho a 02 de julho de 2011.

Other national publications

EE- I. Kuźniarska-Biernacka, "Obchody stulecia przyznania Marii Skłodowskiej-Curie nagrody Nobla w zakresie chemii, w Portugalii", Orbital, 2011, 143-144.

Ph.D. thesis completed

Paula Cristina Vieira Barbosa, "Desenvolvimento de novos electrólitos poliméricos sólidos", oral Fev 2011, orientadores M.J. Smith e M.M. Silva.

Organization of conferences

Six members of the Electrochemistry and Environment group participated in the organization of XXII Meeting of the Portuguese Society of Chemistry held in Braga from the 3rd to 6th of July, as members of the organizing and scientific committees. This meeting was a combined event of the Analytical, Physical, Inorganic, Organic and Free Radical Chemistry groups and included 7 plenary and 34 keynote lectures, 82 oral and 383 poster presentations with a total of 600 national and foreign participants.

The one-day meeting, "Jornadas de Química 2011", was co-organized by one of the group members (ICN). The objective of this meeting was to provide students of various chemistry-related courses with information about the professional and scientific activity of chemists in industry.

Industry contract research

- Preliminary studies were performed for NewTextiles, Vinália, Yazaki Saltano and other external institutes (3B´s). These exploratory studies using GC/MS and LC-MS, were supported by analytical costs levied on samples submitted with funding of about 500 euros in 2011. These additional funds were classified as national industry.

Group Productivity

Internationalization

The research carried out by the Electrochemistry and Environment group during 2011 has resulted in the publication of 28 papers in international journals and the acceptance or publication of a further 13 papers in 2012. The impact of both international and interdisciplinary scientific exchange within this group is evident in the high percentage of this academic production (almost 30%) that is co-authored with researchers from foreign research centres. This interaction with collaborators based in other centres, located within both Portuguese and foreign institutions, certainly provides additional inspiration for new projects developed within the centre. During 2011 members of the group presented a total of 51 poster or oral sessions at 23 international conferences and 22 communications at 3 national meetings.

Members of this group continue to participate in a Cost Action ("MP0803 PLASMONICS" CJS) and in the Eliare Network SUDOE Project (Health Theme, CJS). The main objective of the COST network is to form a European-wide scientific and technological platform of knowledge dedicated to the study and development of plasmonic components and devices. The Elliare Network Sudoe is a 3-year project financed through Interreg IV involving 10 universities and R&D institutions from France, Spain and Portugal. The principal objective of this latter iniciative is to stimulate scientific exchange between public and private research institutions, and to foster the creation of networks within the European Research Community in programmatic areas of Materials, Health, Environment and Information Technologies

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Group Description

Title of Research Group:	(RG-Norte-686-1733) Heterocyclic Compounds (HC)
Principal Investigator:	Maria Fernanda de Jesus Rego Paiva Proença
Main Scientific Domain:	n/a
Group Host Institution:	Universidade do Minho

Funding, source, dates

Funding, source, dates

PhD fees (FCT)

R.Araújo SFRH/BD/38318/2007(Supervisors HC/EE) Dec07 – Nov11, 1260€

M. Solange Carvalho SFRH/BD/47052/2008 (Supervisors HC/ CFUM) Feb09 1375€

V. Duarte SFRH/BD/61290/2009 Feb10 2750

N. Senhorães SFRH/BD/73721/2010 April11 2062€

Elina Marinho SFRH/BD/73659/2010 April11 2062€

Sandrina Heleno SFRH/BD/70304/2010 April 11 2062€

Cátia Esteves (SFRH/BD/68360/2010) Jul11 (AA/HC) 687€

Projects FCT/FEDER

PTDC/QUI-QUI/111060/2009 (PI/HC; IPBragança, Fac.Med.-UPorto, T=134529 €) 12.792 €

PTDC/CTM/105597/2008(HC,AA; PI/CFUM 01/04/10-31/03/13 T=165000€) 2000 €

PTDC/QUI/66250/2006 (PI/HC; AA,UNLisboa 01/01/08-30/06/11 T=110100€) 4587 €

PTDC/QUI/66251/2006 (PI/HC,EE,CFUM,UTAD 01/01/09-31/12/12 T= 159486€) 13533 €

PTDC/QUI/81238/2006(HC,AA,PI/CFUM 1/11/08-31/10/11 T= 89325€) 2000€

PTDC/QUI/68382/2006(HC,U.Coimbra, PI/Biol-UM 01/01/09-31/12/11 T=108 042€) 1000€

PTDC/QUI/67407/2006(HC,UAlg,UP,U Santiago 04/01/09-03/07/12, T=159 882€) 47 964.60€

Total Projects: 83876€

Acções Integradas Luso-Espanholas: 375€

Objectives & Achievements

Objectives

The researchers of this group are mainly dedicated to the synthesis of new heterocyclic compounds and to the search for new synthetic methods including eco-friendly approaches. Part of these molecules can be considered drug candidates and their biological activity was tested by national/international experts.

The search for new materials is an equally important subject, developed in collaboration with national/international partners for the study of optoelectronic, photochromic, DNA intercalation and chemosensor properties.

The synthesis of potentially bioactive heterocycles was pursued with the preparation and testing of:

-Antitubercular agents in particular compounds incorporating hydrazides, 6-triazolopurines, imidazolyl-triazoles, 5-amino-4-amidinoimidazoles and hydrazidopurines.

-Antipsychotics namely flexible analogs of clozapine, novel chromene, imidazole and purine scaffolds were tested on adenosine receptors.

-Antifungal and antibacterial agents namely pyrimidopyrimidine, imidazole and purine derivatives.

-Anticancer agents such as imidazole, purine and pyrimidopyrimidine derivatives, chromeno-imidazo-pyridines, bi(hetero)aryls, di(hetero)arylalkynes and di(hetero)arylether derivatives of thieno[3,2-b]pyridines obtained by Pd or Cu –catalyzed, C-C (Sonogashira, Suzuki) C-N (Buchwald-Hartwig) and C-O couplings.

-Encapsulation of fluorescent antitumorals in nanoliposomes for drug delivery purposes.

-Antioxidants/pro-oxidants including imidazo[4,5-d]pyrrolo[3,2-f][1,3]diazepine, benzo[b]thiophene-based di(hetero)arylamines, phenolic purines and imidazole.

The synthesis of new compounds and heterocyclic/organic-based materials includes:

-acetylenic derivatives of amino acids and coumarin, substituted tetrahydrofurans, including some linked to acetylated D-Glucose, by reductive electrocyclisation in "green media", 1,2,3-triazoles linked to D-glucose, esters derived from sugars, substituted pyrido[2,3-b]indolizines, 2-aryl-1,9-dihydrochromeno[3,2-d]imidazoles from salicylaldehydes and arylideneaminoacetonitriles, imidazopyridine-fused chromones, 6-cyano and 6-unsubstituted 2-aryl-8-oxopurine from a common 2-oxoimidazole precursor, 2- and 8- amino purines, 2- imidazolyl benzimidazoles, pyrimidine and quinazoline derivatives by 1,3-cycloaddition reactions.

-new functionalized oligothienyl-BODIPY dyes, pyrroles, thienylpyrroles, azo dyes, crown ethers, Ru complexes bearing thienyl and furyl-imidazo-phenanthrolines and modified AAs bearing heterocycles, peptides based nanoparticles.

-homochiral Azafagomine and analogues by a diastereoselective Diels-Alder methodology, deoxy-azasugars by two diastereoselective strategies, azasugars from dienes bearing a hydroxyl group by enantioselective Diels-Alder methodology, chiral amino acid included in a polyalcohol structure, azamacrocylic compound,

-Some 1,3-dipolar cycloadditions were found to be stereo-selectives using a dienophile derivative of D-eritrose.

Objectives & Achievements

-Covalent and non-covalent functionalization of MWCNTs for composite applications and preparation of functionalized graphene nanoribbons.

Main Achievements

Results on the synthesis of new drug candidates include:

-Phenol-substituted imidazoles, purines and pyrimidopyrimidines, fused heterocyclic N-oxides and benzo[b]thiophene-based diarylamines as antioxidants. Some of this compounds were active on colorectal cancer cell lines.

-Pyrimidopyrimidines and 6-substituted purines to be tested against Mtb, fungi and bacteria.

- Pyridoindolizines, aryl-chromenoimidazoles, imidazopyridine-fused chromones, 2-, 6- and 9-substituted purines. Some compounds were active on adenosine receptors.

-Thieno[3,2-b]pyridine derivatives, bi(hetero)aryls, di(hetero)arylalkynes, di(hetero)arylamines and di(hetero)arylethers were obtained by metal-catalyzed couplings and were evaluated as anticancer agents using human tumor cell lines: breast adenocarcinoma (MCF-7), melanoma (A-375), non-small cell lung cancer (NCI-H460) and heptacelular carcinoma (HepG2). The evaluation on non-tumor cells was done using a porcine liver primary cell line. For the most active and less toxic compounds effects on the cellular cycle and on apoptosis were determined on the NCI-H460 cell line. This work was done in collaboration with the Fac. Pharmacy-Univ. Porto, IPBragança and IPATIMUP-Univ. Porto.

- Tri and tetra heterocyclic fluorescent compounds from benzo[b]thiophene and thienopyridines using Pd/Cu-assisted reaction, were evaluated as antitumorals, encapsulated in nanoliposomes and their interaction with DNA was studied.

-Broad scope enantioselective Diels-Alder methodology to the synthesis of 1-azafagomine derivatives and other aza-sugars. Glycosidase inhibition tests gave very good results with some compounds.

The synthesis of new materials contemplates:

-Oligothienyl-BODIPY dyes, pyrroles, thienylpyrroles, azo dyes, crown ethers, Ru complexes bearing thienyl and furyl-imidazo-phenanthrolines and modified amino acids bearing heterocyclic moieties and their gold and silica nanoparticles. Evaluation of their photophysical, thermal, NLO and sensor properties indicates that they may be used as solvatochromic probes and efficient DNA intercalators, photochromic, NLO materials and as ion sensors. Other materials were evaluated through theoretical and experimental studies concerning their optical and sensor properties.

-Non-covalent functionalization of CNT with perylene derivatives and covalent functionalization by cycloadditions. Graphene formation by unzipping of functionalized CNT.

New synthetic methods were developed for the preparation of:

-Pyridoindolizines by a cascade reaction using unsaturated carbonyl compounds and a dimmer of 1-(cyanomethyl)pyridinium chloride.

-Aryl-chromenoimidazoles and imidazopyridine-fused chromones from salicylaldehydes and arylideneaminoacetonitriles or 1-(cyanomethyl)pyridinium chloride respectively.

- Pyrroles and isoguanines, 2,6- and 6,8-diaminopurines from 4-substituted imidazole precursors.

-Tetrahydrofurans by electrosynthesis in non-toxic microemulsions or in non-polluting solvents from unsaturated substrates some bearing acetylated D-glucose.

-Fluorescent N-glycopeptides from sugar azide and acetylenic heteroaromatic compounds.

-Glycoconjugates containing a 1,2,3-triazole unit.

-1-Azafagomine, hydroxy-dienes and t-butil 2H-azirines 3-carboxylate from penta-2,4-dieno-1-ol and 3,5-dihydro-4-phenyl-4H-triazol-3,5-dione in the presence of several R- and S-BINOL with excellent enantio-selectivities.

-1-Azafagomine derivatives from D-eritrose.

Group Productivity

Publications in peer review Journals

HC1 N Senhorães AM Dias LM Conde MF Proença One-Pot Regioselective Synthesis of 2,6,9-Trisubstituted Adenines Synlett 2011, 181-186. IF2010 2.447

HC2 X. García-Mera J.E. Rodríguez-Borges MLC Vale, MJ Alves Highly diastereoselective synthesis of 2-azabicyclo[2.2.1]hept-5-ene derivatives: Bronsted acid catalyzed aza-Diels Alder reaction between cyclopentadiene and imino-acetates with two chiral auxiliaries Tetrahedron 2011, 67, 7162-7172. IF 3.011

HC3 MJRP Queiroz RC Calhelha LAVale-Silva E Pinto GM Almeida MH Vasconcelos Synthesis and Evaluation of Tumor Cell Growth Inhibition of Methyl 3-Amino-6-[(hetero)arylethynyl]thieno[3,2-b]pyridine-2-carboxylates. Structure-Activity Relationships, Effects on the Cell Cycle and Apoptosis Eur J Med Chem 2011, 46, 236-240. IF 3.193

HC4 RMV Abreu HJC Froufe POM Daniel MJRP Queiroz ICFR Ferreira Chem T, an open-source software for building template-based chemical libraries, SAR QSAR Environ. Res. 2011, 22, 603-610. IF1.560

HC5 EMS Castanheira MSD Carvalho ARO Rodrigues RC Calhelha MJRP Queiroz New potential antitumoral fluorescent tetracyclic thieno[3,2-b]pyridine derivatives: Interaction with DNA and nanosized liposomes, Nanoscale Res Lett 2011, 6, 379. IF 2.560

HC6 A Begouin MJRP Queiroz Tandem Pd/C-CuI catalyzed Sonogashira coupling and intramolecular cyclization from 2-bromonicotinic acid and arylacetylenes to 4-azaphthalides and 5-azaisocoumarins Helv Chim Acta 2011, 94, 1792-1801. IF 1.284

HC7 M Zaki MF Proença Synthesis of 6-cyano and 6-unsubstituted 2-aryl-8-oxopurine from a common 2-oxoimidazole precursor Tetrahedron 2011, 67, 755-762.

HC8 M Costa MF Proença A one-pot synthesis of substituted pyrido[2,3-b]indolizines Tetrahedron 2011, 67, 1071-1075.

HC9 M Costa F Proença 2-Aryl-1,9-dihydrochromeno[3,2-d]imidazoles: a facile synthesis from salicylaldehydes and arylideneaminoacetonitriles Tetrahedron 2011, 67, 1799-1804.

HC10 M Costa F Areias M Castro J Brea MI Loza F Proença Synthesis of novel chromene scaffolds for adenosine receptors Org Biomol Chem 2011, 9, 4242 -4249.IF 3.451

HC11 M Costa F Proença Selective synthesis of some imidazopyridine-fused chromones Tetrahedron, 2011, 67, 8622 – 8627.

HC12 D Collado J Casado SR González JT López-Navarrete R Suau E Perez-Inestrosa TM Pappenfus MMM Raposo Enhanced functionality for

Group Productivity

donor-acceptor oligothiophenes via inclusion of BODIPY: synthesis, electrochemistry, photophysics and model chemistry Chem Eur J 2011, 17, 498-507. IF 5.476

HC13 AM Dias AS Vila-Chã AL Costa DP Cunha N Senhorães MF Proença Versatile Synthesis of 5-Aminoimidazole-4-carboxylic Acid Derivatives Synlett 2011, 2675-2680.

HC14 RMV Abreu ICFR Ferreira RC Calhelha RT Lima MH Vasconcelos F Adega R Chaves MJRP Queiroz Anti-hepatocellular carcinoma activity using human HepG2 cells and hepatotoxicity of 6-substituted methyl 3-aminothieno[3,2-b]pyridine-2-carboxylate derivatives: in vitro evaluation, cell cycle analysis and QSAR studies Eur J Med Chem 2011, 46, 5800-5806.

HC15/ BC5 MJ Alves FT Costa VCM Duarte A Gil Fortes JA Martins NM Micaelo Advances in the synthesis of homochiral (−)-1-azafagomine and (+)-5-epi-1-azafagomine. 1-N-phenyl carboxamide derivatives of both enantiomers of 1-azafagomine: leads for the synthesis of active α-glycosidase inhibitors J Org Chem 2011, 76, 9584-9592. IF 4.002

HC16/EE24 AJ Mendonça M Inês AP Esteves DI Mendonça MJ Medeiros Kolbe electrosynthesis of 1,2-di(bicyclo[2.2.1]heptan-2-yl)ethane and 1,2-diphenylethane Synth Commun 2011, 41, 820–825. IF 0.937

HC17/EE25 MMM Raposo AMC Fonseca MCR Castro M Belsley MFS Cardoso LM Carvalho PJ Coelho Synthesis and characterization of novel diazenes bearing pyrrole, thiophene and thiazole heterocycles efficient photochromic and nonlinear optical (NLO) materials Dyes Pigments 2011, 91, 62-73. IF 2.635

HC18/EE26 MMM Raposo MCR Castro AMC Fonseca P. Schellenberg M Belsley Design, synthesis and characterization of the electrochemical, nonlinear optical properties and theoretical studies of novel thienylpyrrole azo dyes bearing benzothiazole acceptor groups Tetrahedron 2011, 67, 5189-5198.

HC19/EE27 MMM Raposo MCR Castro M Belsley AMC Fonseca Push-pull bithiophene azo-chromophores bearing thiazole and benzothiazole acceptor moieties: synthesis and evaluation of their redox and nonlinEEr optical properties Dyes Pigments 2011, 91, 454-465.

HC20/EE28 PJ Coelho MCR Castro AMC Fonseca MMM Raposo Photoswitching in azo dyes bearing thienylpyrrole and benzothiazole heterocyclic systems Dyes Pigments 2011, 92, 745-748.

HC21/AA9 EMS Castanheira MSD Carvalho DJG Soares PJG Coutinho RC Calhelha MJRP Queiroz Fluorescence studies on new potential antitumoral benzothienopyran-1-ones in solution and in liposomes J Fluoresc 2011, 21, 911-922. IF 1.966

HC22/AA10 BF Hermenegildo G Pereira AS Abreu EMS Castanheira PMT Ferreira, MJRP Queiroz Phenanthrenyl-indole as a fluorescent probe for peptides and lipid membranes J Photochem Photobiol A:Chem 2011, 221, 47-57. IF 2.243

HC23/AA11 AS Abreu EMS Castanheira MJRP Queiroz PMT Ferreira LA Vale-Silva E. Pinto Nanoliposomes for encapsulation and delivery of the potential antitumoral methyl 6-methoxy-3-(4-methoxyphenyl)-1H-indole-2-carboxylate Nanoscale Res. Lett. 2011, 6:482.

HC24/AA12 J Gomes LO Lunardi FH Caetano AEH Machado AMF Oliveira Campos LM Bendhack CN Lunardi Biodegradable nanoparticles containing benzopsoralens: An attractive strategy for modifying vascular function in pathological skin disorders J Appl Polym Sci 2011, 121:1348–1354.IF 1.203

HC25/AA13 AMF Oliveira-Campos AM Salaheldin FA Almeida Paz LM Rodrigues Synthesis of 3-indolylazoles and meridianin derivatives from indolyl enaminonitriles ARKIVOC, 2011, XI, 121-133. IF 1.096

HC26/AA14 RMF Batista E Oliveira SPG Costa C Lodeiro MMM Raposo Imidazo-benzo-15-crown-5 ether bearing arylthienyl and bithienyl moieties as novel fluorescent chemosensors for Pd2+ and Cu2+ Tetrahedron 2011, 67, 7106-7113.

HC27/AA15 E Oliveira, SPG Costa MMM Raposo ON Faza C Lodeiro Synthesis, characterization, fluorescence and DFT studies of new Cu2+, Ni2+ and Hg2+ complexes with emissive thienylbenzoxazolyl-alanine ligands Inorg Chem Acta 2011, 366, 154-160. IF 1.899

HC28/AA16 CIC Esteves MMM Raposo SPG Costa Novel highly emissive non proteinogenic amino acids: synthesis of 1,3,4-thiadiazolyl asparagines and evaluation as fluorimetric chemosensors for biologically relevant transition metal cations, Amino Acids 2011, 40, 1065-1075. IF 4.106

HC29/AA17 E Oliveira D Genovese R Juris N Zaccheroni JL Capelo MMM Raposo, SPG Costa L Prodi C Lodeiro Synthesis of new emissive peptides probes based on benzo[d]oxazol derivatives and their gold and sílica nanoparticles Inorg Chem 2011, 50, 8834-8849. IF 4.325

HC30/AA18 RMF Batista E Oliveira SPG Costa C Lodeiro MMM Raposo (Oligo)thienyl-imidazo-crown ether derivatives: synthesis, photophysical studies and evaluation of their chemosensory properties Talanta 2011, 85, 2470-2478. IF 3.722

Ph.D. thesis completed

- Carla Bernardete Barbosa Correia Pereira supervisor: M. Alice Carvalho"Síntese e avaliação da actividade antioxidante e micobacteriana de novos derivados de imidazole e purina", Fev. 2011.

- Alexandra Emanuela Ribas Ribeiro supervisor: M. Alice Carvalho "Síntese de imidazoles substituídos e N-óxidos heterocíclicos com potencial actividade antioxidante", Apr. 2011.

- Marta Sílvia Freitas Costa (SFRH/BD/31531/2007) supervisor M. Fernanda Proença), "Síntese de derivados de cromeno para screening como agentes antipsicóticos", Apr 2011.

- Rosa Maria Ferreira Batista (SFRH/BD/36396/2007) supervisors: HC/AA M. Manuela Raposo and Susana P. G. Costa "Synthesis and characterization of heterocyclic compounds and modified amino acids with application in nonlinear optics and/or as fluorimetric and colorimetric sensors for anions and cations", Dec. 2011.

Organization of conferences

Some members of the Heterocyclic Compounds group participated in the organization of XXII Meeting of the Portuguese Society of Chemistry held in Braga from the 3rd to 6th of July, as members of the organizing and scientific committees. This meeting was a combined event of the Analytical, Physical, Inorganic, Organic and Free Radical Chemistry groups and included 7 plenary and 34 keynote lectures, 82 oral and 383 poster presentations with a total of 600 national and foreign participants.

Internationalization

The work on synthetic heterocyclic chemistry developed by most members of this group is complemented with the collaboration of international experts, in particular to study the biological and physical properties of the new compounds.

-Research on anti-tubercular agents has the collaboration of the Tuberculosis Antimicrobial Acquisition & Coordinating Facility (TAACF-USA) for

Group Productivity

screening the new compounds against Mtb strain H37Rv.

-The search for new antipsychotics has the collaboration of members of the IMIM – Barcelona, Spain for in silico screening and of the Faculty of Pharmacy-Univ. Santiago Compostela, Spain for in vitro screening.

-Theorectical, photophysical and Raman spectroscopic studies of functionalized heterocyclic materials and metallic complexes bearing heterocyclic ligands for nonlinear optics (NLO), DNA intercalation and as sensors of cations and anions were done at University of Málaga, University of Madrid and Polytechnic University of Valencia-Spain.

- Theoretical rationalization of transition states in the Diels-Alder, were made at Universidad Central de Las Villas, Cuba.

- The Biological studies of the macrocyclic-metal complex as antioxidants will be done at the Robert Gordon University, Aberdeen, UK.