FCT Relatório Científico 2010 Print: 08-11-2013 10:18:06 [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 financed by the Portuguese Foundation for Science and Technology (FCT) through the pluriannual Support Programme and recently also 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 2009, the CQ/UM had 37 FTERs and 63.5 associated members.

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

Electrochemistry and Environment (EE) with 12 FTERs and 26 associated members;

Synthesis and Application of Heterocycles (HC) with 13.5 FTERs and 18.6 associated members;

Synthesis and Application of Amino Acids (AA) with 6.5 FTERs and 15.5 associated members;

Biological Chemistry (BC) with 5 FTERs and 5.4 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 sugar and aza-sugar derivatives. The biological activity of the new compounds is tested through national and international collaborations, in particular as antioxidants, antipsychotics, anticancer, antitubercular, antifungal and antibacterial agents. Other interests of the HC group include the encapsulation of anticancer compounds in nanoliposomes for drug delivery, the functionalization of carbon nanotubes (CNTs) for composite applications and the synthesis and characterization of new heterocyclic materials for nonlinear optical, photochromic and sensor applications.

The main objective of the AA group is the development of new methods and intermediates for peptide synthesis and to apply them to 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. This work has been developed on new synthetic methods for the preparation of non-proteinogenic amino acids; new photocleavable protecting group chemistry based on N, S and O heterocycles; synthesis and application of alpha,alpha-dialkylglycines; development of new bis-amino acids and their application in establishing new cross-links between peptide chains; synthesis, structure and molecular modeling of peptides; synthesis of new cyclic RGD-peptides.

Within the BC group one of the objectives is the design, synthesis, physico-chemical characterization and pharmacological evaluation (in vivo and in vitro) of new metal complexes (Gd3+, Ga3+, Al3+) as potential agents for medical imaging (MRI, γ-scintigraphy and PET). 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 2010

Achievements of the Electrochemistry and Environment group include the development of methods for evaluating antioxidant capacity using microelectrodes and cyclic voltammetry, procedures for preparation of zeolite-encapsulated metal complex catalysts, hybrid gels containing semiconductors, new organometallic compounds for NLO applications and novel solid polymer electrolytes. These materials were characterized with appropriate techniques.

Objectives & Achievements

Photo-oxidative degradation of ABS was studied under controlled conditions. The effect of operating parameters on microbial fuel cell efficiency was characterized. A clean electrosynthetic procedure was used to obtain heterocyclic compounds from D-glucose-based derivatives. Electro-oxidative degradation of organic pollutants using CNTs-based catalyst was optimized.

The HC group developed new synthetic methods, including eco-friendly for purine and chromene derivatives. Esters derived from sugars were prepared and sugars with triazoles were obtained by click chemistry. Erythrose dienes were prepared and reacted with nitrogen and carbon dienophiles via Diels-Alder reactions. Metal-catalyzed couplings were used to prepare benzo[b]tiophene and thieno[3,2-b]pyridine derivatives. Several molecules were submitted to virtual screening in receptors and enzymes. The biological activity of some compounds was evaluated: -chromenes and purines were active on adenosine and serotonine receptors; imidazolyltriazolones and 6-substituted purines were active against Mtb; 2-oxo-6-amidrazono purines and imidazoles were active as antimicrobials; purines, pyrimidopyrimidines and benzo[b]thiophene-based diarylamines showed antioxidant properties at nM range at cellular level; some thieno[3,2-b]pyridines were active as antitumorals; azafagomine derivatives were highly active against alpha-glucosidases.

(Oligo)thiophenes, pyridazines, imidazoles, anthraquinones, azo dyes, crown ethers and modified AAs bearing heterocycles, emissive metallic complexes bearing AAs, fluorescent peptides based nanoparticles were prepared and their NLO and sensor properties were evaluated. The latter referred moieties were also incorporated into nanofibers for NLO.

The AA group developed new cross-linking strategies for the preparation of new bis-AAs and some of them were applied to the cyclization of RGD peptides. The synthesis of unnnatural AAs and heterocycles for application as UV and NIR fluorescent probes (in biomolecules and membranes), imaging probes, chemosensors and bioactive compounds was carried out. Their peptides afforded emissive metallic complexes and fluorescent peptide Au and Si nanoparticles. Heterocyclic photocleavable protecting groups were used for caging of amino acids (including neurotransmitters), biogenic amines and its biosynthesis precursors, with cleavage by one- and two-photon excitation. Fluorescent N-glycopeptides and glycoconjugates containing a triazole were synthesized, as well as psoralen derivatives containing amino acids based on dibenzofuran and carbazole.

In the BC group two novel amide conjugates of the (DO3A-N-α-aminopropionate) synton have been prepared and characterised as novel contrast agents for MRI. The Gd3+ chelates of the amide conjugates have the ideal properties: fast water exchange and inertness towards transmetallation. Successful purification of plasmid DNA in ATPS using lysine and arginine as affinity ligand was achieved. Molecular simulation of DNA in RTILs allowed a better a understanding of DNA solvation in these media.

Activities

Integrative/multidisciplinary activities during the year of 2010

The multidisciplinary character of the topics developed within the CQ/UM result in a strong interaction between the members of the different research groups and stimulate collaborative research with national and international partners. This is reflected in joint publications, supervisions (PhD and MSc students) and research projects.

The EE group collaborates essentially in the domains of Fundamental and Applied Physics, Environmental Science and Polymer Engineering with both national and international laboratories and research centres. 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 easy-to-use software tool (MOLA) that performs parallel virtual screening of compound databases against protein receptors was developed in collaboration 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.

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 2010

During 2010 the researchers of the Chemistry Research Centre invested a sustained effort in outreach activities in order to promote a favorable public image of Chemistry within the local school population and the general public. Various projects were implemented in 2010. These projects include presentations centred on specific themes requested by secondary school teachers involving organized day-visits to the installations of the Centre or Department. Several lecturers/researchers were also invited to present lectures in local schools. The principal objective of these activities was to support local schools by providing specialist knowledge on topics of interest, and ultimately to encourage the study of Chemistry and attract students to the degree courses available in the University of Minho.

Other outreach activities were prepared for the secondary school population and include "Vamos Kimikar" (laboratory classes for 11-13 year olds), "Olimpíadas de Química" (a team competition for 13-14 year olds), "QSI - a closer look at Chemistry" (a week-long chemistry activity for 16-18 year olds hosted by the Chemistry Department) and "Science in the summer" (project placement for 16-18 year olds). Some of these initiatives were supported by external funds that were used to provide prizes and special offers to participants in the activities. During the year more than 1200 school-children of ages between 12 and 17 and almost 120 school-teachers were directly involved in one or more of these activities.

Members of the teaching staff of the Department of Chemistry and researchers of the Chemistry Research Centre prepared several 25 hour course units for school-teachers as in-service training activities. These courses were formally recognized by the Portuguese commission for

Activities

continuing education and made available to teachers in order to allow them to obtain supplementary training in key areas. These courses are also intended to strengthen secondary school-university interaction, intended to reinforce links with the secondary school community.

New course units were prepared for introduction in 2011, based on the accumulated experience and feedback from teachers. In 2010, once again, approximately 60% of the in-service training within the departments of the Science Faculty took place in the Chemistry Department.

Based on the practical experience obtained during the academic year 2009/10, a new course was prepared and presented to the University authorities for approval. This course is a re-structured "broad-band" version of the existing course in further education for school-teachers. A formal presentation of the course to the Portuguese Ministry of Education for approval and authorization to admit students will take place in 2011.

Plenary lectures were delivered by guest speakers from nanotechnology, archeology, pulp paper, marine and textiles industries. In addition, there was also the public oral presentations of the research results of the "Integration Research Grants BII-FCT", 2009, Chemistry Center, by newly graduates in Chemistry.

Funding

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

General Indicators

	2007	2008	2009	2010	2011	Total
No. of Researchers Proposed	0,00	0,00	0,00	0,00	0,00	0,00
No. of Researchers Hired (LA)	0,00	0,00	0,00	0,00	0,00	0,00
Balance	0,00	0,00	0,00	0,00	0,00	0,00
No. of Researchers Hired (Ciência Programme)	0,00	0,00	0,00	0,00	0,00	0,00
No. of Researchers integrated with PhD	0,00	0,00	0,00	37,00	0,00	
Training Masters (Master thesis completed)	0,00	0,00	0,00	0,00	0,00	0,00
Training PhDs (PhD thesis completed)	0,00	0,00	0,00	1,00	0,00	1,00

Researchers Hired

Name	Start Date	End Date	Other Institution
No researchers found...			

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)

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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:	Química
Group Host Institution:	Universidade do Minho

Funding, source, dates

Funding, source, dates

Current FCT Funding:

PTDC/QUI/69607/2006 (PI/AA), 97 000 €, AA: 32333 €.

PTDC/QUI/66250/2006 (PI/HC), 110 100 €, AA: 11010 € .

PTDC/QUI/81238/2006 (PI/CF-UM), 89 325 €, AA: 1489 €.

PTDC/QUI/70063/2006 (PI/CNBC-UC), 150 600 € AA: 5020 €.

PTDC/CTM/105597/2008 (PI/CF-UM), 165 000 € AA: 5500 €.

Total: 55352 €

Projects funded by the Council of Rectors of the Portuguese Universities (CRUP):

Ac. Integ. Luso-Espanholas Nº E-144/10, 1000 €.

FCT PhD grants:

A. Fonseca, SFRH/BD/32664/2006, Sep 2007, (11 000 €) AA: 2750 €.

M. Fernandes, SFRH/BD/36695/2007, Sep 2008 (11 000 €) AA: 2750 €.

G. Pereira, SFRH/BD/38766/2007, Sep 2008 (11 000 €) AA: 2750 €.

A. Cerqueira, SFRH/BD/61459/2009, Oct 2009 (11 000 €) AA: 2750 €.

C. Francisco, SFRH/BD/48636/2008, Dec 2009 (11 000 €) AA: 2750 €.

R. Batista, SFRH/BD/36396/2007, co-sup. HC, Feb 2007 (5 500 €) AA: 1375 €.

A. Fontes, SFRH/BD/63676/2009 co-sup. BC, March 2010 (5500€) AA: 1375 €.

A. Sá SFRH/BD/63639/2009 co-sup. BC, Jan 2010 (5500 €) AA: 1375 €.

Total: 17875 €

Portuguese National NMR network funding from FCT (total CQ/UM 18.100€)

Objectives & Achievements

Objectives

- Synthesis of new amino acids and new heterocyclic compounds (oxazoles and indoles) using dehydoamino acids as substrates. Application of the new compounds as fluorescent probes and in conformational studies.

- Study of the electrochemical behaviour of dehydroamino acid derivatives: reduction of the alpha,beta double bond. Synthesis of new beta,beta-disubstituted alanines.

- Synthesis of new metal chelators using N,N-diacyldehydroalanines that can be used in the development of imaging probes for the nuclear imaging modalities, positron emission tomography (PET) and single photon emission computed tomography (SPECT) and for magnetic resonance imaging (MRI).

- Development of new strategies for the synthesis of orthogonally protected bis-amino acids and application in the cyclization of RGD peptides.

- Synthesis of new N-ethyldehydroamino acids.

- Evaluation of the biological activities and photophysical properties of the new amino acid derivatives prepared.

- Structure-based design, synthesis and membrane activity studies of peptide mimetic of antimicrobial peptaibols bearing unnatural symmetrical alpha,alpha-dialkylglycines.

- Evaluation of conditions necessary to achieve the synthesis of a,a-dialkylglycines by a Ugi reaction/TFA cleavage procedure performed on solid-phase media.

- Application of the a,a-dialkylglycine synthetic strategy based on an Ugi reaction/TFA cleavage procedure to the “in situ” formation of novel peptide bonds.

- Synthesis of fluorescent heterocycles for application as photocleavable protecting groups for biomolecules, namely amino acids, including neurotransmitter amino acids, and peptides (C-, N- and O-protection) and as photocleavable dual-linkers for solid phase peptide synthesis.

- Investigation of the photochemical stability of the amino acid-fluorophore linkage. Kinetics studies of the photocleavage reaction of several fluorescently bioconjugates of amino acids.

- Synthesis of novel unnatural amino acids functionalized with sulfur, oxygen and nitrogen heterocycles [benz-X-azoles (X= S, O and N), thiophene, furan, pyrrole, carbazole, indole, (aza)crown-ether] and short peptides incorporating the novel amino acids, as well as emissive metallic complexes and fluorescent peptide based nanoparticles.

- Evaluation of the photophysical and chemosensory properties of the novel heterocyclic amino acids and peptides as fluorescent chemosensors for ions with biological, environmental and analytical relevance.

Objectives & Achievements

- Synthesis of fluorescent benzo[a]phenoxazines and naphtho[2,3-a]phenoxazines for biomedical applications.

- Evaluation of the biological activities and photophysical properties of the new amino acid derivatives prepared.

- Synthesis of novel psoralen derivatives containing nitrogen sulfur, oxygen and heterocycles and amino acid residues. Purification, characterization and evaluation of biological activity..

-Collaborative work on synthesis of carboline derivatives containing amino acid residues and on the synthesis of alkynylamino acid derivatives as precursors of glycoconjugates containing a 1,2,3-triazole unit.

Main Achievements

The study of the reactivity of dehydroamino acid and dehydropeptide derivatives was continued with the aim of obtaining new amino acids and heterocycles. The fluorescent properties of some of the compounds prepared allowed their application as fluorescent probes in peptides and lipid membranes and also their use in conformational studies (2 papers).

The development of new strategies for the synthesis of orthogonally protected bis-amino acid derivatives using several types of reactions was continued. Some of these strategies were applied in the synthesis of cyclic RGD peptides (1 PhD thesis is ongoing and 1 MSc concluded).

The study of the electrochemical behaviour of dehydroamino acid derivatives by cyclic voltammetry and controlled potential electrolysis was continued. This allowed the synthesis of the E-isomers of dehydroamino acids and the synthesis of beta,beta-diarylalanines from the corresponding dehydroalanine derivatives (2 papers, 1 proceeding 1 MSc thesis).

The N-alkylkation of non-proteinogenic amino acids was initiated. The procedure developed allowed the synthesis of N-ethyldehydroamino acid derivatives (1 paper, 1 proceeding and 1 Msc thesis ongoing).

Several N,N-diacyldehydroalanines and cyclic RGD peptides were prepared and used in the synthesis of new metal chelators for the development of imaging probes (1 paper).

The work on the synthesis and characterization of new fluorescent probes, namely benzo[a]phenoxazines (1 MSc thesis, 1 Post-PhD, 1 paper, accepted), pyranones, benzopyranones, quinolones, benzoquinolones, benzooxazoles and benzopyranooxazole was continued, as well as the covalent and non-covalent fluorescent labeling of material of biological interest (neurotransmitters, DNA and membranes). With the aim of developing efficient phototriggers for caging applications of neurotransmitter amino acids, amines and nucleotides and its biosynthesis precursors, and dual-linkers for the solid phase synthesis of peptide analogues and/or mimetics, photophysical studies of tags and conjugates and photocleavage experiments by one- and two-photon excitation, including kinetic studies, of selected fluorescent conjugates were carried out (3 PhD thesis on going and 1 MSc thesis, 4 proceedings, 4 papers).

Several novel unnatural amino acids modified at their side chain with sulfur, oxygen and nitrogen heterocycles were obtained and their photophysical properties evaluated for application as fluorescent probes within peptidic structures. The novel amino acids were also evaluated as fluorescent chemosensors for metallic cations and incorporated into di and tripeptides. These short peptides were used for the preparation of silica and gold nanoparticles with application as MALDI-TOF-MS active matrices for metal ions (1 PhD and 3 MSc ongoing, 4 papers). Some of the new compounds were also evaluated for materials science applications due to their optical properties (2 proceedings, 2 papers).

The membrane activity studies of antimicrobial peptaibols started with the synthesis of peptaibolin and peptaibolin mimetics (1 Msc thesis initiated).

Studies on the conditions necessary to perform the synthesis of a,a-dialkylglycines by solid phase Ugi reaction were performed (1 MSc thesis is ongoing).

The application of the synthetic strategy based on an Ugi reaction/TFA cleavage procedure to "in situ" formation of novel peptide bonds is ongoing.

The synthesis of novel psoralen derivatives based on dibenzofuran was completed. The derivatives based on carbazole are on the way. The results were communicated at international and national Symposia (1 PhD thesis are ongoing).

The collaborative work on heterocyclic chemistry was continued on synthesis, purification and characterization of several heterocycles containing amino acids, (new novel xanthine oxidase inhibitors, carbolines) and glycoconjugates containing a 1,2,3-triazole unit. The results were presented at several Meetings (4 papers and 1 proceeding).

Group Productivity

Publications in peer review Journals

AA1- L.S. Monteiro, J. Kołomańska, A.C. Suarez "Synthesis of novel non-proteinogenic amino acids: N-ethyl-alpha,beta-dehydroamino acid methyl esters" Eur. J. Org. Chem., 2010, 6731-6735 (IF3.096).

AA2 - P.M.T. Ferreira, E.M.S. Castanheira, L.S. Monteiro, G. Pereira, H. Vilaça "A mild high yielding synthesis of oxazole-4-carboxylate derivatives", Tetrahedron, 2010, 66, 8672-8680 (IF3.219).

AA3- P.M.T. Ferreira, L.S. Monteiro, G. Pereira, "Synthesis and electrochemical behaviour of beta-halodehydroamino acid derivatives", Amino Acids, 2010, 37, 499-513 (IF 3.877).

AA4- A.M.S. Soares, S.P.G. Costa, M.S.T. Gonçalves,"2-Oxo-2H-benzo[h]benzopyran as a new light sensitive protecting group for neurotransmitter amino acids", Amino Acids, 2010, 39, 121-133. (IF 3.877)

AA5- A.S.C. Fonseca, M.S.T. Gonçalves, S.P.G. Costa, "Light-induced cleavage of phenylalanine model conjugates based on coumarins and quinolones", Amino Acids, 2010, 39, 699-712. (IF 3.877)

AA6- A.M.S. Soares, S.P.G. Costa, M.S.T. Gonçalves, "Oxazole light triggered protecting groups: synthesis and photolysis of fused heteroaromatic conjugates", Tetrahedron, 2010, 66, 8189-8195. (IF 3.219)

AA7- G. Hungerford, L. Ryderfors, M.J.G. Fernandes, M.S.T. Gonçalves, S.P.G. Costa, "One- and two-photon time-resolved fluorescence study of neurotransmitter amino acid – 5,6-benzocoumarin conjugates", J. Photochem. Photobiol. A: Chemistry, 2010, 215, 214–222. (IF 2.553)

AA8/BC3 - A. de Sá, Á.A. Matias, M.I.M. Prata, C.F.G.C. Geraldes, P.M.T. Ferreira, J.P. André, "Gallium labeled NOTA-based conjugates for peptide receptor-mediated medical imaging", Bioorg. Med. Chem. Lett., 2010, 20, 24, 7345-7348 (IF2.650).

AA9/HC23 - G. Pereira, E.M.S. Castanheira, P. M.T. Ferreira, M.-J. R.P. Queiroz, "Synthesis and photophysical studies of new fluorescent indole derivatives obtained from beta-bromodehydroamino acids. Interaction with fluoride anion", Eur. J. Org. Chem., 2010, 3, 464-475 (IF- 3.096).

AA10/HC27- J. Pina, J. Seixas de Melo, R. M. F. Batista, S. P. G. Costa, M. M. M. Raposo, "Synthesis and characterization of the ground and

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excited states of tripodal-like oligothienyl imidazoles", J. Phys. Chem B, 2010, 114, 4964-4972. (IF3.471)

AA11/HC28- J. Pina, J. Seixas de Melo, R. M. F. Batista, S. P. G. Costa, M. M. M. Raposo, "The influence of the relative position of the thiophene and pyrrole rings in donor-acceptor thienylpyrrolyl benzothiazole derivatives. A photophysical and theoretical investigation", Phys. Chem. Chem. Phys. 2010, 12, 9719-9725. (IF4.116)

AA12/HC30- C.I.C. Esteves, M. M. M. Raposo, S. P. G. Costa, "Synthesis and evaluation of benzothiazolyl and benzimidazolyl asparagines as amino acid based selective fluorimetric chemosensors for Cu2+", Tetrahedron, 2010, 66, 7479-7486. (IF 3.219)

AA13/HC31- E. Oliveira, R. M. F. Batista, S. P. G. Costa, M. M. M. Raposo, C. Lodeiro, "Exploring the emissive properties of new azacrown compounds bearing aryl, furyl or thienyl moieties: a special case of Chelation Enhancement of Fluorescence upon interaction with Ca2+, Cu2+ or Ni2+", Inorg. Chem., 2010, 49, 10847-10857. (IF4.657)

AA14/HC20/EE24- A.M. Salaheldin, A.M.F. Oliveira-Campos, P. Parpot, L.M. Rodrigues, M.M. Oliveira, F.P. Feixoto, "Synthesis and Biological Evaluation of New Tacrine Analogues from 4-Aminopyrrole-3-carbonitrile", Helv. Chimica, Act, 2010, 93(2), 242-248. (IF 1.435).

AA15/HC21/EE25 –A.M. F. Oliveira-Campos, J.M.O. Ribeiro, L.M. Rodrigues, P. Parpot, P.E. Lopes, "3-[1-(4-Methylphenylsulfonyl)-1,4-dihydropyridin-4-yl]-1H-indole", Acta Cryst., 2010, E66, o915 (IF-0.411).

AA16/HC22 –A.M.F. Oliveira-Campos, L.M. Rodrigues, A.P. Esteves, M.E. Silva, A. Sivasubramanian, R. Hrdina, G.M.B.Soares, T.A.D. Pinto, O. Machalicky, "Naphthotriazole derivatives: synthesis and fluorescence properties" Dyes & Pigments, 2010, 87, 188-193 (IF2.855).

Other international publications

AA1 - P.M.T. Ferreira, L.S. Monteiro, E.M.S. Castanheira, G. Pereira, C. Lopes, "Electrochemical reduction of β-aryldehydroamino acid derivatives", Proceedings of the 31st European Peptide Symposium, M. Lebl, M. Meldal, K.J. Jensen, T. Hoeg-Jensen (Eds.) European Peptide Society, 2010, pp. 102-103 (ISBN 0-9715560-5-9).

AA2 - L.S. Monteiro, J. Kołomańska, A.C. Suarez, "Synthesis of novel non-proteinogenic amino acids: N-ethyldehydroamino acids", Proceedings of the 31st European Peptide Symposium, M. Lebl, M. Meldal, K.J. Jensen, T. Hoeg-Jensen (Eds.) European Peptide Society, 2010, pp. 128-129 (ISBN 0-9715560-5-9).

AA3- M.J.G. Fernandes, M.S.T. Gonçalves, S.P.G. Costa, "Photo-uncaging of neurotransmitter amino acids from fluorescent 5,6-benzocoumarinyl precursors", "Peptides 2020, Tales of Peptides" - Proceedings of the 31st European Peptide Symposium, Copenhaga, Dinamarca, M. Lebl, M. Meldal, K. J. Jensen, T. Hoeg-Jensen (Eds), European Peptide Society, 2010, 82-83 (ISBN 0-9715560-5-9).

AA4- A. Fonseca, M.S.T. Gonçalves, S.P. G. Costa, "Photolabile protecting goups based on novel thiocoumarins and thioquinolones: synthesis and photorelease of a model amino acid conjugates", "Peptides 2020, Tales of Peptides" - Proceedings of the 31st European Peptide Symposium, Copenhaga, Dinamarca, M. Lebl, M. Meldal, K. J. Jensen, T. Hoeg-Jensen (Eds), European Peptide Society, 2010, 8-9 (ISBN 0-9715560-5-9).

AA5- 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, The 14th International Electronic Conference on Synthetic Organic Chemistry, J. A. Seijas and M. P. V. Tato (Eds), 2010, in press, MDPI, Basel, Switzerland.

AA6- A. Piloto, S. 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, The 14th International Electronic Conference on Synthetic Organic Chemistry, J. A. Seijas and M. P. V. Tato (Eds), 2010, in press, MDPI, Basel, Switzerland.

AA7/HC. R. M. F. Batista, S. P. G. Costa, M. Belsley, M. M. M. Raposo, "Synthesis and characterization of novel donor-acceptor oligothiophenes as efficient and thermally stable second-order nonlinear optical chromophores", Adv. Mat. Forum V, 2010, 636-637, 380-386 (ISSN: 1662-9752).

AA8/HC. R. M. F. Batista, S. P. G. Costa, M. Belsley, M. M. M. Raposo, "Synthesis and characterization of new push-pull anthraquinones bearing an arylthienyl-imidazo conjugation pathway as efficient nonlinear optical chromophores", Adv. Mat. Forum V, 2010, 636-637, 387-391 (ISSN: 1662-9752).

AA9/HC - A.M.F. Oliveira-Campos, J.C.O. Gonçalves, L. M. Rodrigues, A.P. Esteves, "Synthesis of 5H-pyrido[4,3-b]indole by a modification of Pomeranz-Fritsch isoquinoline synthesis", Proceedings of ECSOC-14, The 14th International Electronic Conference on Synthetic Organic Chemistry, J. A. Seijas and M. P. V. Tato (Eds), 2010, in press, MDPI, Basel, Switzerland.

Book chapter

AA1 - M.S.T. Gonçalves, in "Advanced Fluorescence Reporters in Chemistry and Biology I. Fundamentals and Molecular Design", Demchenko A.P. (Volume Ed.), O.S. Wolfbeis (Series Ed.), Springer Series on Fluorescence, Vol. 8, Chapter 2, "Optimized UV/Visible Fluorescent Markers", pages 27-64, Springer, Heidelberg, 2010 (ISBN 978-3-642-04700-8).

FCT Relatório Científico 2010 Print: 08-11-2013 10:18:36 [Centro de Química]

Group Description

Title of Research Group:	(RG-Norte-686-1064) Biological Chemistry
Principal Investigator:	Joao Carlos Ramos Nunes Marcos
Main Scientific Domain:	Química
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 (01/01/08-31/12/10) 22692

PTDC/QUI/69607/2006 "New photolabile groups as phototriggers and protecting groups: synthesis, photophysics and photorelease studies"

Coordinated by Prof. Susana Costa . JCM team member. (01/01/08-31/12/10)

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)

Portuguese National NMR network funding from FCT (total CQ/UM 18.100€)

Objectives & Achievements

Objectives

The Biological Chemistry group encompasses several chemical studies connected with biological systems. Until last year the different lines of research were divided in three tasks. This year it was decided to created another task for the molecular modeling and simulation studies previously included in task 3.

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), Ga(III), Mn(II), Al(III)) and nanostructures 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 tested the possibility of using amino acids as affinity ligands.

Task 3 – Development of new human neutrophilelastase 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- Efficient synthetic routes for new triaza- and tetraaza-based amphiphilicchelators for Ga(III) have been developed.The Ga(III) and Al(III) chelates of the triaza-based ligands were studied by multinuclear NMR spectroscopy. The critical micelle concentration values of the Ga(III) chelates of the triaza and tetraaza-based ligands were determined. Biodistribution and γ-scintigraphic studies of the 67Ga(III) labeled chelates were performed on Wistar rats.

The orthogonal protection strategy for the synthesis of these ligands allows their covalent coupling to targeting peptides. Three NOTA-based ligands were coupled to a RGD peptide. The radiolabelling with 67Ga allowed studying their binding to the receptors in a U87MG-gliobastoma cell line, demonstrating a weak but specific interaction.

A new synthetic route for amide conjugates of the ligand DO3A-N-(α-amino)propionate has been established. The physical-chemical and relaxometric characterization (1H NMRD and 17O NMR) of Gd3+ chelates of two novel amide ligands has been performed in collaboration with Prof. C. Geraldes from FCTUC, Coimbra, and Dr. E. Toth from CBM, CNRS, Orleans, France. The Gd3+chelates of the amide conjugates retain the accelerated water exchange and the inertness of the parent amine. The pyrenyl conjugate [Gd(DO3A-N-(α-pyrenebutanamido)propionate)], self-assembles in solution leading to high relaxivities due to simultaneous optimization of kex and τR. This conjugate is able to sensitize the NIR emitting lanthanide ions Nd3+ and Y3+. These chelates are promising agents for NIR imaging in vivo.

Gold nanoparticles (NP) functionalized with Gd3+ chelates of the ligands DO3A-N-(α-lipoamido)propionate and DO3A-N-(α-cystamido)propionate have been prepared, purified and characterized by DLS and Zeta potential measurements. The Au/Gd ratio on the NP has been determined by ICP-MS. The full relaxometric characterization of the NP as CA for MRI is underway in collaboration with Prof. Lothar Helm from EPF, Lausanne. The NP are exceptionally stable displaying very high relaxivities. In vivo MRI studies in rats are scheduled at the CIB "Alberto

Objectives & Achievements

Sols", Madrid. Vectorization of the NP with peptide (bio)epitopes (RGD peptides) is underway.

Task 2 – The amino acids lysine and arginine were tested as affinity ligands for plasmid DNA (pDNA) purification from bacterial alkaline lysates in Polyethylene glycol (PEG)/dextran (DEX) systems. Both ligands were tested free and bound to PEG. The free amino acids had no effect on pDNA partitioning but the PEG conjugates were able to steer the pDNA to the PEG phase where less contaminants accumulate. However this was only observed with desalted lysate. It was concluded that the high concentration of salts in the alkaline lysates impaired the interaction of both aminoacids with pDNA. In fact the addition of several salts (NaCl, KCl and (NH4)2SO4) to systems with desalted lysate reverts the partition of pDNA to the dextran phase. The ligands were tested in PEG 3350/ DEX 40 and PEG 600/DEX 100 systems where it was observed that very low amounts of PEG conjugates were needed to completely steer the pDNA to the PEG phase. In the first system only 0.7% of both conjugates in relation to total polymer was needed. In the second system this value decreased to 0.2%. 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.

Task 3 – The evaluation of the stability of the selected peptides in the presence in the presence of elastase, for different periods of incubation, was performed by Mass Spectrometry. The degradation studies reveal that both inhibitor-peptides are degraded by elastase and therefore might be used safely in the formulation of wound dressings. Bidimensional NMR studies on these inhibitor-peptides are still ongoing. The influence of ROS (oxygen reactive species: H2O2; HClO; ONOO- and •O2-) on the inhibitory properties of these peptides on Elastase, was also evaluated.A modified version of the common DNPH (2,4 –dinitrophenylhidrazine) assay for quantification of carbonyls in oxidized proteins was developed. The method does not required protein precipitation, is faster and less prone to interferences, while maintaining similar sensibility.

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 - C. Gonçalves, M.F.M. Ferreira, A.C. Santos, M.I.M. Prata, C.F.G.C. Geraldes, J.A. Martins, F.M. Gama, "Studies on the biodistribution of dextrin nanoparticles", Nanotechnology, 2010, 21(29), article number: 295103. (IF 2009 =3.315)

BC2 - A. de Sá, M.I.M. Prata, C.F.G.C. Geraldes, J.P. André, "Triaza-based amphiphilic chelators: synthetic route, in vitro characterization and in vivo studies of their Ga(III) and Al(III) chelates", Journal of Inorganic Biochemistry, 2010, 104, 1051-1062.(IF 2009=3.252)

BC3/AA8- A. de Sá, Á.A. Matias, M.I.M. Prata, C.F.G.C. Geraldes, P.M.T. Ferreira, J.P. André, "Gallium labeled NOTA-based conjugates for peptide receptor-mediated medical imaging", Bioorganic and Medicinal Chemistry Letters, 2010, 20, 7345-7348. (IF 2009 = 2.650)

BC4 - L. Cardoso, N.M. Micaelo, "DNA Molecular Solvation in Neat Ionic Liquids", ChemPhysChem, 2010, 11, 1- 3. (IF 2009 = 3.453)

BC5 - H. Barbosa, A.V. Hine, S. Brocchini, N.K.H. Slater, J.C. Marcos, "Dual Affinity Method for Plasmid DNA Purification in Aqueous Two-Phase", Journal of Chromatography A, 2010, 1217, 1429-1436. (IF 2009 = 4.101)

Other international publications

BC1- Barbosa, H. Marcos, J.C. in Encyclopedia of Industrial Biotechnology Bioprocess, Bioseparation, and Cell Technology," M. C. Flickinger (editor), Vol 6, pp 3953-3965, "Plasmid Purification, Therapeutic Applications", John Wiley & Sons: London, 2010.

Internationalization

The research work is carried out through collaboration with well established and reputed international institutions:

- Institute of Nuclear Medicine of University Hospital Basel, Switzerland (group of Prof. H. Maecke)

- Laboratoire de Chimie Inorganique et Bioinorganique, École Polytechnique Fédérale de Lausanne, Switzerland (groups of Prof. André Merbach and Prof. Lothar Helm)

- Centre de Biophysique Moléculaire, CNRS, Orleans, France (group of Dr. Éva Tóth)

- Instituto de Investigaciones Biomédicas "Alberto Sols", CSIC-UAM, Madrid, Spain (group of Prof. Sebastián Cerdán)

- Department of Chemical Engineering , University of Cambridge (group of Prof. Nigel Slater) – Joint Ph.D. student

- School of Pharmacy, University of London (group of Prof. Steve Brocchini)

FCT Relatório Científico 2010 Print: 08-11-2013 10:19:02 [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:	Química
Group Host Institution:	Universidade do Minho

Funding, source, dates

Funding, source, dates

66 169 Euros were received from the following independently-financed projects:

PTDC/AMB/73854/2007: 18 130 Euros attributed in 2010. (total project funding 181 389 Euros).

PTDC/QUI/66251/2006 – 13 533 Euros attributed in 2010, (total project funding 159 486 Euros).

PTDC/CTM/099124/2008 - 6 510 Euros attributedin 2010, (total project funding 180 000 Euros).

NANO/NTec-CA/0122/2007 - Capacitation program in Nanotechnology: 27 996 Euros attributed in 2010, (total project funding 55 992 Euros).

FCT-Human Resources grants to 13 PhD students provided a total of 22 175 Euros.

Materials and chemical reagents corresponding to a total value of approximately1 000 euros were provided for analytical services under contract to the academic spin-off "Vinalia" in an on-going industrial-academic collaboration. Other occasional analytical tasks were carried out for Research Centers of Minho University.

Objectives & Achievements

Objectives

Studies of nickel-catalyzed cyclization of different D-glucose-based derivatives in environmentally-friendly media will continue. The influence of experimental conditions will be characterized in order to elucidate the reaction mechanism.

Metal complexes encapsulated/immobilized in nanostructured supports will be developed as environmentally-friendly catalysts. Catalytic materials prepared by biosorption or ion exchange will be evaluated using specific reactions. Nanocomposites will be developed using polymers with nanostructures for electronic devices and nanocomposites based on hybrid materials will be developed to reduce the environmental impact caused by waste packaging.

Polymer formulations with improved electrical, mechanical and thermal properties will be developed using nano-particle structures. ABS stability to photodegradation by ultraviolet radiation will be optimized using a combination of UV/light stabilizers and antioxidants in order to understand the UV degradation mechanism that seems to be different under natural or accelerated conditions.

The study of TEMPO-mediated electro-oxidation of carbohydrates will be extended to include new ionic liquids.

The electroreactivity of organic pollutants in aqueous medium at functionalized or non-functionalized carbon nanofibers will be studied. Oxidation products will be determined by long-term electrolysis.

The power output of microbial fuel cells will be optimized using different cell configurations.

The evaluation of the antioxidant activity of families of new compounds by electrochemical methods will be continued. These data will be used to establish the identity and location of the functional groups that lead to an increase in antioxidant activity.

The scavenging ability of different classes of antioxidants towards electrogenerated HO• will be studied. Antioxidants such as polyphenols, tocopherols and thiols will be tested in order to verify the absence of specific interactions with the anode material and confirm the involvement of HO• in the antioxidants oxidation reaction. Experiments to be performed include cyclic voltammetry, controlled electrolyses and the analysis of electrolyzed solutions.

Encouraging results have been obtained using host networks with a variety of chemical compositions and architectures, formulated with different guest salt combinations. Evaluation of relevant performance parameters of new formulations will continue and electrochromic displays using the most promising electrolyte compositions will be assembled and characterized.

Synthesis of various functional nanoparticles including carbon-based materials, semiconductors (CdSe, CdS@ZnS and CdSe@ZnS), metals (Au and Ag) and manganite (AaBbMnO3), is being developed. Characterization of physical and chemical properties will carried out to evaluate potential applications in optics and life sciences

Main Achievements

The members of the Electrochemistry and Environment group continue to develop synthetic and analytical methods of low environmental impact and to prepare and characterize new materials with potential for application in a variety of commercial devices and processes.

A new method for the evaluation of antioxidant capacity was developed based on the simulation of the oxidative attack of specific ROS and validated in single antioxidant solutions and in mixtures at different pHs. In this study organic acid concentrations were determined using microelectrodes. The antioxidant activity of several families of new compounds was evaluated by electrochemical methods particularly cyclic voltammetry. The electrochemical oxidation mechanisms of various compounds were determined. The cyclic voltammetric data obtained was used to establish structure – activity relationships. Heterogeneous catalysts based on metal complexes encapsulated in zeolites were obtained by biosorption or ion exchange methods and their activity was evaluated. Electrical properties of nanocomposites based on PVDF/zeolites were determined. The optical and electrochemical properties of thiophenes, heterocyclic azo dyes and coordinated compounds were evaluated. Hybrid gels incorporating semiconductor and metal nanoparticles were prepared and characterized. The procedures necessary for the production of high-resolution gratings for optical applications were optimized. The photo-oxidative degradation of ABS was studied under natural and accelerated weathering conditions. Novel solid polymer electrolytes, prepared using different strategies and with various host/guest salt combinations, were prepared and evaluated in prototype devices. The performance of small-scale prototypes confirmed that multi-functional polymer components provide significant advantages in these devices. The electroreactivity of some organic pollutants at catalysts

Objectives & Achievements

based on carbon nanotubes was investigated and the kinetic parameters of the reactions were determined. The effect of choice of anode material and temperature on microbial fuel cell efficiency was investigated. The conditions for direct and indirect high yield transformation of carbohydrates were determined. Electrosynthesis of heterocyclic compounds from D-glucose-based derivatives was achieved in non-toxic media.

Group Productivity

Publications in peer review Journals

EE1 - G. Botelho, R. Santos, A.V. Machado, Materials Science Forum, 2010, 636-637, 772-778.

EE2 - G. Botelho, R.M. Santos, A.V. Machado, Journal of Applied Polymer Science, 2010, 116, 2005-2015.

EE3 - G. Botelho, M.P. Silva, V. Sencadas, A.V. Machado, A.G. Rolo, J.G. Rocha, S. Lanceros-Mendez, Materials Chemistry & Physics, 2010, 122, 87-92.

EE4 - G. Botelho, M.P. Silva, J.G. Rocha, S. Lanceros-Mendez, Polymer Testing, 2010, 29, 613.

EE5 - V.F. Cardoso, G. Minas, P. Martins, L. Rebouta, S. Lanceros-Mendez, G. Botelho, Science and Technology of Advanced Materials, 2010, 11, 045006.

EE6 - P.C. Barbosa, L.C. Rodrigues, M.M. Silva, M.J. Smith, A. Gonçalves, E. Fortunato, J. Mater. Chem., 2010, 20, 723-730. (IF4.795)

EE7 - M.M. Silva, P.C. Barbosa, L. C. Rodrigues, A. Gonçalves, C. Costa, E. Fortunato, Optical Materials, 2010, 32, 719-722. (IF 1.728)

EE8 - M.C. Gonçalves, V. de Zea Bermudez, M.M. Silva, M.J. Smith, E. Morales, R.A. Sá Ferreira, L.D. Carlos, Ionics, 2010, 16 193-201. (IF0.899)

EE9 - P.C. Barbosa, L.C. Rodrigues, M.M. Silva, M.J. Smith, A.J. Parola, F. Pina, C. Pinheiro, Electrochimica Acta, 2010, 55, 1495-1502. (IF3.325)

EE10 - J.C.S. Teixeira, M. Fernandes, V. de Zea Bermudez, P.C. Barbosa, L.C. Rodrigues, M.M. Silva, M.J. Smith, Electrochimica Acta, 2010, 55, 1328-1332. (IF3.325)

EE11 - P.C. Barbosa, L.C. Rodrigues, M.M. Silva, M.J. Smith, M. Costa, ECS Transactions, 2010, 25(35) 383-394. (IF10 = 0.233)

EE12 - M.J. Smith, F.M. Gray, J. Chem. Educ., 2010, 87 162-167. (IF0.300)

EE13 - H. Figueiredo, B. Silva, C. Quintelas, M.F.R. Pereira, I.C. Neves, T. Tavares, Environmental Engineering and Management Journal, 2010, 9, 3, 305-311. (IF0.885)

EE14 - I.C. Neves, C. Cunha, M.R. Pereira, M.F.R. Pereira, A.M. Fonseca, Journal Physical Chemistry C, 2010, 114 (24), 10719-10724. (IF4.224)

EE15 - A.C. Lopes, M.P. Silva, R. Gonçalves, M.F.R. Pereira, G. Botelho, A.M. Fonseca, S. Lanceros-Mendez, I.C. Neves, Journal Physical Chemistry C, 2010, 114 (34), 14446-14452. (IF4.224)

EE16 - H. Figueiredo, B. Silva, C. Quintelas, I.C. Neves, T. Tavares, Chemical Engineering Journal, 2010, 163 22–27. (IF 2.816)

EE17 - M. Curras, M. Branco, I.C. Neves, M.A. Sanromán, T. Tavares, Chemical Engineering & Technology, 2010, 33 1-8. (IF09 = 1.266)

EE18 - A. Soloviev, A.G. Rolo, D.J. Barber, M.J.M. Gomes, C.J.R. Silva, Journal of Nanoscience and Nanotechnology, 2010, 10, 2858–2862.

EE19 - K. De, A. Roy, C.J.R. Silva, M.J.M. Gomes, Solid State Communication, 2010, 150, 1187-1191.

EE20 - M. Matos, C. Canhoto, F. Bento, M.D. Geraldo, J. Electroanal. Chem., 2010, 647, 144 - 149.

EE21 - P. Parpot, V.P. Muiuane, V. Defontaine, A.P. Bettencourt, Electrochimica Acta, 2010, 55, 3157 – 3163. (IF3.325)

EE22 - G. Martins, L. Peixoto, D.C. Ribeiro, P. Parpot, A.G. Brito, R. Nogueira, Bioelectrochemistry, 2010, 78 (1) 67. (IF 2.652)

EE23 - P. Parpot, K. Servat, A.P. Bettencourt, H. Huser, K.B. Kokoh, Cellulose, 2010, 17, 815. (IF2.156)

EE24/AA14/HC20 - A.M. Salaheldin, A.M.F. Oliveira-Campos, P. Parpot, L.M. Rodrigues, M.M. Oliveira, F.P. Feixoto, Helv. Chim. Acta, 2010, 93, 242-248. (IF = 1.396)

EE25/AA15/HC21- A.M.F. Oliveira-Campos, J.M.O. Ribeiro, L.M. Rodrigues, P. Parpot, P.E. Lopes, Acta Cryst. 2010, E66, o915. (IF0.411).

EE26/HC24 - P.J. Coelho, L.M. Carvalho, L.F.F.F. Gonçalves, C.J.R. Silva, A.M. Campos, M.J. Gomes, " J Sol-Gel Sci Technol, 2010, 56, 203–211. (IF1.393).

EE27/HC19 - M.C. Paiva, R.M. Novais, R.F. Araújo, K.K. Pederson, M.F. Proença, C.J.R. Silva, C.M. Costa, S. Lanceros-Méndez, Polymer Composites, 2010, 31, 3, 369-376.

EE28/HC25 - H. Figueiredo, B. Silva, M.M.M. Raposo, P. Parpot, A.M. Fonseca, A.E. Lewandowska, M.A. Bañares, I.C. Neves, T. Tavares, Applied Catalysis B: Environmental, 2010, 94(1-2), 1-7. (IF5.252).

EE29/HC26 - C. Herbivo, A. Comel, G. Kirsch, A.M.C. Fonseca, M. Belsley, M.M.M. Raposo, Dyes Pigments, 2010, 82(3), 217-226. (IF2.855)

EE30/HC29 - A.F. Fonseca, M. Belsley, E.M. Gomes, M.C.R. Castro, M.M.M. Raposo, Eur. J. Inorg. Chem. 2010, 19, 2998-3004. (IF2.941)

The titles of the articles are not presented due to the lack of characteres.

Other international publications

Book chapters

EE1 - V. de Zea Bermudez, M.M. Silva, in "Polymer electrolytes: Fundamentals and applications", D.M.F. Santos, C.A. Sequeira (Ed.), Chapter 12, "Lithium-doped Hybrid Polymer Electrolytes", Woodhead Publishing Limited, Portugal, 2010.

Proceedings of conferences

EE1 - A. Cunha, A. Nobre, A.M. Gonçalves, C. Aguiar, I.C. Neves, I. Mina, J. Pamplona, L. Gonçalves, M.A. Forjaz, S. Franco, T. Viseu, A.M. Almeida, "Sentir a Ciência' - actividades multidisciplinares em interacção com escolas do ensino básico e secundário: uma parceria natural para a construção do pensamento científico", Actas do Congresso do Ensino Superior em Mudança: Tensões e Possibilidades, Universidade do Minho, Braga 25 e 26 de Fevereiro de 2010.

EE2 - M.M. Silva, "Ensinar/Aprender no estrangeiro: uma experiência nova", Actas do Congresso Ensino Superior em Mudança: Tensões e Possibilidades, Congresso Ibérico, Universidade do Minho, Braga, 2010.

EE3 - F. Vieira, J. Sá, J.C. Morgado, J. Almeida, M.M. Silva, "Representações da Vida Académica: Tensões e Paradoxos", Actas do Congresso Ensino Superior em Mudança: Tensões e Possibilidades, Congresso Ibérico, Universidade do Minho, Braga, 2010.

Group Productivity

EA4 - M.M. Silva, "Centrar a docência no aluno: reflexão sobre questões éticas", Actas do VI Congreso Iberoamericano de Docencia Universitaria, Lima Peru, 2010.

Other national publications

EE1 - G. Botelho, R.M. Santos, A.V. Machado, "Avaliação da fotodegradação de ABS exposto a condições naturais", Ciência e Tecnologia dos Materiais, 2010, 22, 87-90.

EE2 - A.M. Fonseca, "A importância dos trabalhos de projecto na promoção de competências de investigação a sua ligação á comunidade escolar", Actas do Seminário "A formação inicial de professores na Universidade do Minho: Que (Des)Continuidade?", Universidade do Minho, Braga, 2010, pp. 1-8.

Ph.D. thesis completed

Although 1 PhD thesis was completed within the year 2010 the oral exam took place in 2011.

Organization of conferences

One of the members of the group (MFB) participated in the organization of the XII Iberic Meeting of Electrochemistry & XVI Meeting of the Portuguese Electrochemical Society, ISEL, held in Lisboa, in September of 2010. The program of this three-day meeting included 5 plenary and 6 keynote lectures with 39 oral and 42 poster communications.

Two members of the group (DG and APB) collaborated in the organization of the 1st Meeting of Techniques of Characterization and Analysis held in The University of Minho on the 7th of May. The program included two plenary lectures, eight keynote presentations and about 50 poster presentations delivered by the 150 participants.

The one-day meeting "Jornadas de Química" 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. The program of the meeting included 5 invited lectures and 4 presentations by BII student-grant holders.

Industry contract research

One of the members (GB) of the Electrochemistry and Environment group participated as co-supervisor of an industrial PhD project, in collaboration with the Department of Polymer Engineering (UM). The industrial sponsorship for this industrial-academic project is provided by a Portuguese company (Poliversal) and also involves a Dutch company, DSM Research, as an external consultant. The objective of this project is to improve the UV radiation resistance of ABS terpolymers.

The collaborative interaction supported by a Portuguese analytical company (Vinalia) was continued as a MSc research project in 2010 (PP). The results of the research, describing new methods using GC-MS and LC-MS instruments for chemical analysis of pesticide content of wines, were submitted in the form of a thesis by the student this year. New informal contacts with other analytical laboratories are being explored with a view to establishing other similar academic-industrial exchanges.

A previously established relationship has been continued with a technological interface company, Simbiente - Environmental Engineering and Management, Ltd. This company maintains an interest in the development of a microbial fuel cell (PP) with a view to eventual exploitation of practical commercial devices. This research has been carried out by students in the Chemistry and Biological Engineering laboratories at the University of Minho.

Internationalization

The research carried out by the Electrochemistry and Environment group during 2010 has resulted in the publication of 30 papers in international journals and the publication/acceptance of a further 8 papers in 2011. The impact of interdisciplinary and international scientific exchange within this group is evident through the high percentage (more than 60%) of publications that are co-authored with researchers from other centres/scientific domains and that involve collaboration with foreign institutions (30%). Participation in multi-disciplinary projects with collaborators based in other centres, located within both Portuguese and foreign institutions, continues to provide inspiration for new projects carried out within the centre. During 2010 members of the group presented about 46 papers in poster or oral sessions at international conferences and 25 papers at national meetings.

Members of this group participate in Cost Actions ("MP0701-Composites with novel functional and structural properties by nanoscale materials". The main objective of this COST network is to form a European-wide scientific and technology knowledge platform based on polymer nanocomposites. These materials are blends of different polymer matrices with nanometer-sized functional particles.

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 objective of this project is to promote collaboration 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. Within this research program, exchange between participants has led to the presentation of new trans-national projects for support.

Previous collaborations within CRUP-sponsored projects have led to student and staff exchange with foreign universities. Within Erasmus projects these links have been exploited to provide opportunities for three-month undergraduate student placements and have also led to collaboration in the supervision of master degree students in collaborative research projects

FCT Relatório Científico 2010 Print: 08-11-2013 10:19:28 [Centro de Química]

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:	Química
Group Host Institution:	Universidade do Minho

Funding, source, dates

Funding, source, dates

Projects funded by FCT and FEDER:

PTDC/QUI/81238/2006(HC,AA,PI/CFUM 1/11/08-31/10/11 total 89325€) 6000€

PTDC/QUI/68382/2006(HC,Univ.Coimbra,PI/BioI-UM 01/01/09-31/12/11 total 108 042€) 6000€

PTDC/QUI/66250/2006(PI/HC,AA,UNLisboa 01/01/08-31/12/10 total 110100€)9175€

PTDC/QUI/66251/2006 (PI/HC,EE,CFUM,UTAD 01/01/09-31/12/11 total 159486€)13533€

PTDC/CTM/105597/2008(HC,AA,PI/CFUM 01/11/09-01/10/12 total 165000€)1000€

PTDC/QUI/67407/2006 (HC, UAlg; UP; U Santiago 09/01/04-12/01/03, total: 159 882€) 47 964.60 valor recebido em 2010

PhD students funded by FCT:

R.Calhelha SFRH/BD/29274/2006 Oct06- Sep10 2750€

M.Costa SFRH/BD/31531/2007 May07 2750€

R.Araújo SFRH/BD/38318/2007(Supervisors HC/EE) Dec07 1375€

R.Batista SFRH/BD/36396/2007(Supervisors HC/AA) Oct07 1375€

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

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

Post-Doc researchers funded by FCT:

M.Zaki SFRH/BPD/27029/2006, Feb07

A.Salaheldin SFRH/BPD/31490/2006 Feb07-Jan10

A.Abreu SFRH/BPD/24548/2005, (HC/AA and CFUM) May06

A.Begouin SFRH/BPD/36753/2007 Nov07

Portuguese National NMR network funding from FCT (total CQ/UM 18.100€)

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. These include eco-friendly approaches to prepare molecules incorporating nitrogen, oxygen and sulfur heteroatoms. Part of these molecules can be considered drug candidates and their biological activity was tested by national and international experts.

The search for new materials is an equally important subject, developed in collaboration with national and international partners for the study of their optoelectronic properties or the preparation of composites with improved physical/electronic properties.

The synthesis of new heterocycles with potential biological activity was pursued with the preparation and testing of:

- Antitubercular agents in particular compounds incorporating hydrazides (including Isoniazid and analogues for SAR studies), imidazolyl-triazoles, 5-amino-4-amidinoimidazoles and hydrazidopurines.

- Antipsychotics namely flexible analogs of clozapine, chromene derivatives, substituted imidazoles and purines.

- Antifungal and antibacterial agents namely imidazole and purine derivatives.

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

-Encapsulation of the fluorescent antitumor in nanoliposomes for drug delivery purposes.

- Antioxidants including benzo[b]thiophene-based di(hetero)arylamines at cellular level (nM range), phenolic purines and imidazole-based heterocycles.

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

- Binding of sugars to heterocycles by click chemistry.

- Synthesis of esters derived from sugars.

- Synthesis of 2-oxoimidazole derivatives.

- Synthesis of substituted tetrahydrofurans, including some linked to acetylated D-Glucose, by reductive electrocyclisation in “green media”.

- Synthesis of 1,2,3-triazoles linked to D-glucose.

- Development of diastereoselective Diels-Alder methodology which will lead to the synthesis of L- and D- aza-sugar analogs of Azafagomine and Deoxymannojirimycine.

Objectives & Achievements

- New functionalized heterocyclic derivatives such as (oligo)thiophenes, azo dyes, pyridazines, imidazoles, anthraquinones, crown ethers and modified amino acids bearing heterocyclic moieties and their gold and silica nanoparticles as solvatochromic and fluorescence probes, NLO and photochromic materials, sensors of cations and anions for analytical, medicinal and environmental applications.

- Covalent organic functionalization of MWCNTs for composite applications. Synthesis of pyrene and perylene derivatives for non-covalent functionalization of CNTs.

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 these compounds were evaluated for their potential against induced oxidative stress at cellular level.

-N-heterocycles were assessed against Mtb (185 new compounds: 15 active, 59 weakly active).

-4-Substituted imidazoles, namely 5-amino-4-amidino imidazoles and imidazolyl-triazoles, pyrimido[5,4-d]pyrimidines, pyrimido[4,5-e][1,2,4]triazolo [1,5-c]pyrimidines and 6-substituted purines, to be tested against Mtb, fungi and bacteria.

-2-, 6- and 9-substituted purines, triazolopurines, anthranilonitrile derivatives, fused chromeno-imidazoles and pyrido-indolizines to be tested on adenosine, serotonine, dopamine and metabotropic glutamate receptors. Part of the 6-aminopurines and substituted 8-oxopurines, proved to be active on serotonine and adenosine receptors.

-Thieno[3,2-b]pyridine derivatives, bi(hetero)aryls, 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) and non-small cell lung cancer (NCI-H460). For the most active compounds (GI50<10 microM) their effects on the cellular cycle and on apoptosis were determined on the NCI-H460 cell line. The antitumoral activities were evaluated collaboration with the Fac. Pharmacy-Univ. Porto and the effects on the cell cycle and induction of apoptosis were determined in collaboration with IPATIMUP-Univ. Porto

-Heteroaromatic fluorescent compounds from dehydroAAs and heterocycles using Pd/Cu-assisted reactions, as antitumorals or as fluorescent probes for biological systems. The interaction with fluoride ions was followed by photophysical methods

-Azafagomine derivatives, highly active against alfa-glucosidases.

Research on natural products includes:

-Isolation of Mycolactone D from M.Ulcerans strain 98-912. This compound was purified, characterized and used in studies of the immunology of infection.

The synthesis of new materials contemplates:

-(Oligo)thiophenes, pyridazines, anthraquinones, imidazoles, heterocyclic azo dyes, crown ethers and modified amino acids bearing (oligo)thiophenes, benzoxazole and thiadiazole moieties and their gold and silica nanoparticles. Evaluation of their photophysical, thermal, NLO and sensor properties indicates that they may be used as solvatochromic and fluorescence probes, as efficient and thermally stable catalysts, photochromic, NLO materials and as ion sensors. Other materials prepared by HC and AA groups are evaluated through theoretical and experimental studies concerning their optical (linear, nonlinear) and sensor properties by researchers of other Universities.

-Covalent functionalization of MWCNT using Diels-Alder and 1,3-dipolar cycloadditions. Graphene formation by unzipping of the external layer of functionalized CNT. New pyrene and perylene derivatives for the non-covalent functionalization of CNT.

New synthetic methods were developed for the preparation of:

-1-Azafagomine, starting from penta 2,4-dieno-1-ol and 3,5-dihydro-4-phenyl-4H-triazol-3,5-dione in the presence of several catalysts. This new methodology gave only poor enantio-selectivities.

-Novel 12H-chromeno-imidazo-pyridines and 2-aryl-1,9-dihydrochromeno-imidazoles, by one-pot procedures in aqueous media.

-Substituted 2-oxoimidazoles, used as precursors of bi-imidazoles, bi-imidazolodiazepines and 6-amidino-8-oxopurines.

-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.

Group Productivity

Publications in peer review Journals

(IF2009)

HC1-L. Assunção, E. Marinho, F. Proença, Arkivoc, 2010(v),82-91.(IF1.090)

HC2-M.C. Paiva, W. Xu, M.F. Proença, R. Novais, E. Lægsgaard, F. Besenbacher, Nano Letters, 2010, 10, 1764-1768.(IF9.991)

HC-3-M.F. Proença, M. Costa, Tetrahedron, 2010, 66, 542-4550.(IF3.219)

HC4-E. Marinho, R. Araújo, F. Proença, Tetrahedron, 2010, 6(45),8681-8689.(IF3.219)

HC-5-A.M. Dias, I.M. Cabral, A.S.Vila-Chã, D. Cunha, N. Senhorães, S. Nobre, C. Sousa, M.F. Proença, Synlett, 2010, 2792-2796.(IF2.718)

HC6-A.H. Bacelar, M.A. Carvalho, M.F. Proença, Eur.J.Med.Chem, 2010, 45,3234-3239.(IF3.269)

HC7-F. Areias, J. Brea, E. Gregori-Puigjané, M.E.A. Zaki, M.A. Carvalho, E. Domínguez, H. Gutiérrez-de-Terán, M.F. Proença, M.I. Loza, J. Mestres, Bioorg.Med.Chem., 2010, 18,3043-3052.(IF2.882)

HC8-E. Torrado, A.G. Fraga, E. Logarinho, T.G. Martins, J.A. Carmona, J.B. Gama, M.A. Carvalho, F. Proença, A.G. Castro, J. Pedrosa, The Journal of Immunology, 2010, 184, 947-955.(IF5.646)

HC9-M.M. Oliveira, L. Carvalho, F. Peixoto, A.M. Oliveira-Campos, A. Reis, P. Domingues, M. Domingues, Rapid Communications in Mass Spectrometry, 2010, 24(14), 2171-2174.(IF2.695)

HC10-S.M. Marques, C.J. Tavares, L.F. Oliveira, A.M.F. Oliveira-Campos, Journal of Molecular Structure 983(2010), 147–152.(IF 1.551)

HC11-M.J. Alves, V.C. M. Duarte, H. Faustino, A.G. Fortes, Tetrahedron: Asymmetry, 2010, 21, 1817-1820.(IF2.625)

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HC12-R.C. Calhelha, M.-J.R.P. Queiroz, Tetrahedron Lett. 2010, 51, 281-283.(IF2.660)

HC13-J.P. Silva, V.A. Machado, R.C. Calhelha, M.-J.R.P. Queiroz, O.P.Coutinho, Drug Discoveries and Therapeutics, 2010, 4(4), 246-256.(New Journal)

HC14-M.-J.R.P. Queiroz, R.C. Calhelha, L.A. Vale-Silva, E. Pinto, R.T. Lima, M.H. Vasconcelos, Eur.J.Med.Chem., 2010, 45, 5628-5634.(IF3.269)

HC15-M.-J.R.P. Queiroz, R.C. Calhelha, L.A. Vale-Silva, E. Pinto, M.S.-J.Nascimento, Eur.J.Med.Chem., 2010, 45, 5732-5738.(IF3.269)

HC16-R.M.V. Abreu, H.J.C. Froufe, M.-J.R.P. Queiroz, I.C.F.R. Ferreira, J. Cheminf.2010,2:10, (New Journal)

HC17-M.M.M. Raposo, B. García-Acosta, T. Ábalos, R. Martínez-Manez, J.V. Ros-Lis, J. Soto, J.Org.Chem., 2010, 75(9), 2922–2933.(IF4.219)

HC18-M.C. Paiva, F. Simon, R. Novais, T. Ferreira, M.F. Proença, W. Xu, F. Besenbacher, ACS Nano 2010, 4(12), 7379-7386.(IF7.493)

HC19/EE27-M.C. Paiva, R.M. Novais, R.F. Araújo, K.K. Pederson, M.F. Proença, C.J.R. Silva, C.M. Costa, S.Lanceros-Méndez, Polymer Composites, 2010, 31, 3, 369-376.(IF1.194)

HC20/AA14/EE24-A.M. Salaheldin, A.M.F. Oliveira-Campos, P. Parpot, L.M. Rodrigues, M.M. Oliveira, F.P. Feixoto, Helv.Chim.Acta (93), 2010, 242-248.(IF1.396)

HC21/AA15/EE25-A.M.F. Oliveira-Campos, J.M.O. Ribeiro, L.M. Rodrigues, P. Parpot, P.E. Lopes, Acta Cryst.(2010) E66, o915. (IF0.411)

HC22/AA16-A.M.F. Oliveira-Campos, L.M. Rodrigues, A.P. Esteves, M.E. Silva, A. Sivasubramanian, R. Hrdina, G.M.B. Soares, T.A.D. Pinto, O. Machalicky, Dyes and Pigments, 2010, 87, 188-193.(IF2,855)

HC23/AA9-G. Pereira, E.M.S. Castanheira, P.M.T. Ferreira, M.-J.R.P. Queiroz, Eur.J.Org.Chem. 2010, 464-475.(IF3.096)

HC24/EE26-P.J. Coelho, L.M. Carvalho, L.F.F.F. Gonçalves, C.J.R. Silva, A.M. Campos, M.J. Gomes, J Sol-Gel Sci Technol (2010) 56:203–211.(IF1.393)

HC25/EE28-H. Figueiredo, B. Silva, M.M.M. Raposo, P. Parpot, A.M. Fonseca, A.E. Lewandowska, M.A. Bañares, I.C. Neves, T. Tavares, Applied Catalysis B: Environmental 2010, 94(1-2), 1-7.(IF5.252)

HC26/EE29-C. Herbivo, A. Comel, G. Kirsch, A. Maurício, C. Fonseca, M. Belsley, M.M.M. Raposo, Dyes Pigments 2010, 82(3), 217-226.(IF2.855)

HC27/AA10–J. Pina, J.S. Seixas de Melo, R.M.F. Batista, S.P.G. Costa, M.M.M. Raposo, J. Phys.Chem B 2010, 114(15), 4964-4972.((IF3.471)

HC28/AA11–J. Pina, J.S. Seixas de Melo, R.M.F. Batista, S.P.G. Costa, M.M.M. Raposo, Phys.Chem.Chem.Phys., 2010, 12(33), 9719-9725.(IF4,116)

HC29/EE30–A.F. Fonseca, M. Belsley, E.M. Gomes, M.C.R. Castro, M.M.M. Raposo, Eur.J.Inorg.Chem. 2010, 19, 2998-3004.(IF2,941)

HC30/AA12–C.I.C. Esteves, M.M.M. Raposo, S.P.G. Costa, Tetrahedron 2010, 66(38), 7479-7486.(IF3.219)

HC31/AA13–E. Oliveira, R.M.F. Batista, S.P.G. Costa, M.M.M. Raposo, C. Lodeiro, Inorg.Chem., 2010, 49, 10847-10857.(IF4.657)

The titles of the articles are not presented due to the lack of characteres.

Other international publications

- Proceedings of conferences (with referees)

HC1- E.M.S. Castanheira, A.S. Abreu, M.-J.R.P. Queiroz, P.M.T. Ferreira, "Studies of Encapsulation of a New Potential Antitumoral Indole Derivative in Nanoliposomes for Drug Delivery Applications", Proceedings of the 3rd International NanoBio Conference 2010, European Cells & Materials, Volume 20, Supplement 3, 2010, Page 35; ISSN 1473-2262.

HC2/AA7 – R.M.F. Batista, S.P.G. Costa, M. Belsley, M.M.M. Raposo, "Synthesis and characterization of novel donor-acceptor oligothiophenes as efficient and thermally stable second-order nonlinear optical chromophores", L. G. Rosa, F. Margarido (Eds), V International Materials Symposium/XIV Encontro da Sociedade Portuguesa de Materiais, Instituto Superior Técnico, Universidade Técnica de Lisboa, Lisboa, Portugal, 5-8 de Abril de 2009, Mater. Sci. Forum, 2010,636-637, 380-386.

HC3/AA8 – R.M.F. Batista, S.P.G. Costa, M. Belsley, M.M.M. Raposo "Synthesis and characterization of new push-pull anthraquinones bearing an arylthienyl-imidazo conjugation pathway as efficient nonlinear optical chromophores ", V International Materials Symposium/XIV Encontro da Sociedade Portuguesa de Materiais, Instituto Superior Técnico, Universidade Técnica de Lisboa, Lisboa, Portugal, Mater. Sci. Forum, 2010, 636-637, 387-391.

HC4/AA9- A.M.F. Oliveira-Campos, J.C.O. Gonçalves, L. M. Rodrigues, A.P. Esteves, "Synthesis of 5H-pyrido[4,3-b]indole by a modification of Pomeranz-Fritsch isoquinoline synthesis", 14th International Conference on Synthetic Organic Chemistry (ECSOC-14), November 2010.

Book Chapters:

HC1 - M.J. Alves, N.G. Azoia, in "Stereochemistry Research Trends", Editor M.A. Horvat and J.H. Golob, Nova Science Publishers, Chapter 1, "Stereochemistry Research Trends" 2010.

Other national publications

HC1 – M. Costa, F. Proença, "One-pot condensation-cyclization approach for the synthesis of 12H-chromeno[2´,3´:4,5]imidazo[1,2-a]pyridine" (oral) 2nd Portuguese Young Chemists Meeting (2PYChem), Aveiro, 2010.

HC2- E. R. Marinho, F. Proença, "The reaction of o-phenylenediamine with ethoxymethylene compounds and aromatic aldehydes", 2nd Portuguese Young Chemists Meeting, Aveiro, 2010.

HC3 - M. Costa, E. Marinho, F. Proença, F. Areias, M. Castro, J. Brea, J. Mestres, M. Loza, "Synthesis of novel chromene-based scaffolds for adenosine receptors" (oral), 2nd National Meeting on Med. Chem., 28-30 Nov, Coimbra, 2010.

HC4 - E. Marinho, M. Costa, F. Proença, F. Areias, M. Castro, J. Brea, J. Mestres, M. Loza "N-Methyl piperazine: an important fragment for interaction with serotonine 5-HT2A receptors" 2nd National Meeting on Med. Chem., 28-30 Nov, Coimbra, 2010.

HC5 - M. F. Proenca, Magdi E. A. Zaki, Filipe M. Areias, María I. Loza, Jordi Mestres, "Synthesis of 2-aryl-8-oxopurines as novel antagonists for adenosine receptor subtypes", 2nd National Meeting on Med. Chem., 28-30 Nov, Coimbra, 2010.

HC6 - M. F. Proenca, M E. Zaki, "Simple synthesis of 2-azapurine analogues and 2-substituted 6-aminopurine", 2nd National Meeting on Med. Chem., 28-30 Nov, Coimbra, 2010.

HC7- M.A. Carvalho, "Substituted purines as new antitubercular compounds", 2nd National Meeting on Med. Chem., 28-30 Nov, Coimbra,

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2010.(invicted lecture)

HC8- R.M.V. Abreu, M.-J.R.P. Queiroz, I.C.F.R. Ferreira, F. Adega, R. Chaves " Anti-proliferative activity of thieno[3,2-b]pyridine derivatives in tumoral and primary hepatic cell lines", 2nd National Meeting on Med. Chem., Coimbra, 28-30 Nov, 2010.

HC9-A.D.S. Oliveira, E.M.S. Castanheira, R.C. Calhelha, L. Vale-Silva, E. Pinto, M.-J. R.P. Queiroz "Encapsulation of a new antitumoral fluorescent 6-(benzo[d]thiazo-2-ylamino)thieno[3,2-b]pyridine derivative in nanoliposomes", at the 2nd National Meeting on Med. Chem., Coimbra, 28-30 Nov, 2010.

HC10- A.D.S. Oliveira, E.M.S. Castanheira, P.J.G. Coutinho, R.C. Calhelha, M.-J.R.P. Queiroz " Fluorescence studies of Benzothienoquinolines in lipid membranes", 10th National Meeting on Photochemistry, Porto, 9-10 Dec, 2010.

HC11- A.H. Bacelar, A. Rocha, M. A. Carvalho, M. F. Proença, "Synthesis and activity on Mycobacterium tuberculosis of new pyrimido[4,5-e][1,2,4]triazolo[1,5-c]pyrimidines", 2nd National Meeting on Med. Chem., 28-30 Nov, Coimbra, 2010.

HC12- A.Brito, M. A. Carvalho, A.H. Bacelar, M. F. Proença, "6-Carbohydrazonamidopurines: synthesis and activity on Mycobacterium tuberculosis", 2nd National Meeting on Med. Chem., 28-30 Nov, Coimbra, 2010.

HC13- A.M. Dias, L. Carneiro, D. P. Cunha, a M. F. Proença, "An efficient Synthesis to New 1,2,4[5,1-i]purines as Potential Adenosine A3 Receptor Ligands", 2nd National Meeting on Med. Chem., 28-30 Nov, Coimbra, 2010.

HC14- N. Senhorães, A.M. Dias, M.F. Proença, "The synthesis of 6-Arylaminopurines as Potential Anti-cancer Agents", 2nd National Meeting on Med.Chem., 28-30 Nov, Coimbra, 2010.

HC15- N. Senhorães, A.M. Dias, M. F. Proença, "The Synthesis of 4-Amidinoimidazoles as Potential Antimycobacterial Agents, 2nd National Meeting on Med. Chem., 28-30 Nov, Coimbra, 2010.

HC16- J. Camarinha, J. Turela, A. Dias, H. Vilaça, S. Fernandes, A.L. Costa, D. Cunha, M.F. Proença, J.C. Sousa, F. Cerqueira, "Synthesis and and Antimicrobial Activity of 5-Aminoimidazole Derivatives", 2nd National Meeting on Med. Chem., 28-30 Nov, Coimbra, 2010.

HC17- J. Turela, J. Camarinha, I. Cabral, A. Martins, A. Dias, M.F. Proença, J.C. Sousa, F. Cerqueira, "Synthesis and Antimicrobial Activity of Purine Derivatives", (oral), 2nd National Meeting on Med. Chem., 28-30 Nov, Coimbra, 2010.

HC18/AA11-C.I.C. Esteves, M.M.M. Raposo, S.P.G. Costa "Synthesis and interaction studies of novel heterocyclic asparagines with metal cations", 2nd Portuguese Young Chemistry Meeting, Aveiro, 21-23 de April, 2010.

HC19/AA7- A.S. Abreu, B.F. Hermenegildo, G. Pereira, E.M.S. Castanheira, P.M.T. Ferreira, M.-J.R.P. Queiroz " Phenanthrenyl-indole as a fluorescent probe for peptides and lipid membranes", 10th National Meeting on Photochemistry, Porto, 9-10 Dec 2010.

HC20/AA6- A.M.F. Oliveira-Campos, N.M.F.S.A. Cerqueira, L.M. Rodrigues, J.C.O. Gonçalves, N. Cardoso, "N-aryl-5-amino-4-cyanopyrazole derivatives as xanthine oxidase inhibitors: synthesis and molecular docking", 2nd National Meeting on Med. Chem., Coimbra, 28-30 de Nov, 2010.

HC21/AA9 – C.I.C. Esteves, M. M. M. Raposo, S. P. G. Costa, "Avaliação de análogos heterocíclicos da asparagina como sensores químicos de catiões com importância biológica, ambiental e analítica", Iº Encontro de Técnicas de Caracterização e Análise Química, University of Minho, Braga, 7 Maio 2010.

HC22/EE25- M. C. R. Castro, C. S. G. S. Gomes, M. M. M. Raposo, A. Maurício C. Fonseca, "Synthesis and electrochemical and spectroscopic properties of molybdenum complexes bearing 1-alkyl(aryl)pyrrole ligands", 2nd Portuguese Young Chemistry Meeting, Aveiro, 21-23 de April 2010.

HC23/EE- C. S. G. S. Gomes, M. C. R. Castro, A. M. C. Fonseca, M. Belsley, L. M. Carvalho, P. Coelho, M. M. M. Raposo, "Synthesis and evaluation of the electrochemical, nonlinear optical and photochromic properties of novel pyrrole azo dyes", 2nd Portuguese Young Chemistry Meeting, Aveiro, 21-23 de April 2010.

HC24/EE21 – R. Araújo, E. Marinho, C. Silva, F. Proença, "Synthesis of a substituted triazachrysene by an acid catalyzed cascade reaction", 2nd Portuguese Young Chemists Meeting, Aveiro, 2010.

HC25/EE24- F. O. Gomes, A. P. Bettencourt, M. A. Carvalho, "Synthesis and evaluation of antioxidant capacity of 2-oxopyrroles by cyclic voltammetry", Portuguese Young Chemist Meeting, April, Aveiro 2010.

HC26/AA10/EE22- A.M.P. Ribeiro, A.M.F. Oliveira-Campos, L.M. Rodrigues, L.F.F.F. Gonçalves, Carlos J.R. Silva, "Synthesis of [illegible]-carbolines and optical studies of their sol-gel films", P43, 2PYCheM, 2nd Portuguese Young Chemists Meeting, Aveiro, 21-23 April, 2010.

Ph.D. thesis completed

PhD theses:

- Manuel Ricardo Costa Calhelha in Chemistry (supervisor: HC/Maria-João R.P. Queiroz) "Síntese de novos compostos heterocíclicos derivados de benzo[b]tiofenos e tieno[3,2-b]piridinas usando acoplamentos catalisados por metais. Estudos de actividade biológica", Sept. 2010.

MSc theses:

- Natália Sofia Dias MSc in Medicinal Chemistry (supervisor HC/Maria João R.P. Queiroz) "Síntese de novas tieno[3,2-b]piridinas usando acoplamentos C-O, C-C e C-N catalisados por cobre ou paládio e reacções com arilisocianatos, como potenciais compostos anti-tumorais e antiangiogénicos" Dec. 2010.

- João Carlos Gonçalves MSc in Medicinal Chemistry (supervisor Ana Campos)"Síntese de gama-carbolinas com potencial actividade biológica", Dec. 2010.

- Nádia Rodrigues Senhorães, MSc in Medicinal Chemistry (supervisor Alice Dias) "Síntese de novos ligandos para receptores de Adenosina", Dec 2010

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 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

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Pharmacy-Univ. Santiago Compostela, Spain for in vitro screening.

-Theorectical, photophysical and Raman spectroscopic studies of functionalized heterocyclic materials for non-linear optics (NLO) and as sensors of cations and anions were done at Polytechnic University of Valencia and University of Málaga-Spain.