FCT Relatório Científico 2009 Print: 08-11-2013 10:10:17 [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

CQUM is a research unit that functions within the University of Minho promoting research in the domain of Chemistry. The internal regulations of the Chemistry Research Centre (CQUM) determine the organization and management procedures of the research unit. CQ members are either full-time equivalent researchers (FTEs - 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-FCT had 37 FTEs and 73 associated members.

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

Electrochemistry and Environment (12 FTE and 22.5 associated members);

Synthesis and Application of Heterocycles (13.5 FTE and 26 associated members);

Synthesis and Application of Amino Acids (6.5 FTE and 13.5 associated members);

Biological Chemistry (5 FTE and 11 associated members).

The organization of the CQUM is based on a scientific council that includes all FTRs and a coordinating committee. The Director of the research unit presides over a coordinating committee that is composed of the four principal investigators and 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 comitees meetings and implements the decisions of these bodies.

Preliminary contacts have been established to create an advisory committee that will accompany and advise future research activities of the Centre, in accordance with FCT regulations.

General Objectives

The three scientific domains that have been identified as the basis for research within the Chemistry Research Centre are health, the environment and new materials. The members of the Centre are distributed between four groups that have targeted the above topics as domains of particular interest. Currently the members of the Centre, most of whom are teaching staff of the Department of Chemistry, also participate in Masters degree courses in "Medicinal Chemistry" and "Techniques of Chemical Characterization and Analysis". An expected outcome of this interaction is that topics for final year theses are focused on these areas of specialization. A MSc course in "Chemistry -further education for school-teachers"" admitted students for the first time this year and is expected to foster a closer working relationship with local schools.

Many of the projects under development within the EE research 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.

Collaboration with members of the HC group provides an important contribution for the organic synthesis of some of these materials.

Most of the members of the HC and the AA groups are dedicated to the synthesis of new drug candidates, a research area directly associated with the ongoing MSc degree in Medicinal Chemistry. The synthetic skills developed allow the preparation of novel heterocyclic molecules, namely organic compounds incorporating N, O, and/or S atoms. The biological activity of the new compounds is tested through national and international collaborations, in particular as antioxidants, antipsychotics, anticancer, antitubercular and antifungal agents. The position recently filled in the domain of Computational Chemistry (under the "Compromisso com a Ciência" FCT program) will provide in silico predictions on the biological activity of the compounds and on studies of the structure-activity relationships through the use of molecular modeling software. These results may help to identify binding interactions between drug and its target, supporting the decision on which analogues should be synthesized (drug design). This new researcher with a solid background in biochemistry will also collaborate with members of the AA and BC groups. Another interest of the HC group includes the synthesis and the characterization of new heterocyclic materials for nonlinear optical, photochromic and sensor applications.

Members of the AA group also develop other areas of research such as the synthesis of non proteinogenic amino acids for various applications (fluorescent probes, cross-linking elements, peptide mimetics, chemosensors and peptide-based materials) and of novel heterocyclic photocleavable protecting groups for caging applications, solution phase and solid phase organic chemistry. Other interests of the BC group include the synthesis of contrast agents for medical imaging and the purification of therapeutic macromolecules.

The multidisciplinary character of these topics is expected to strengthen the interaction between members of different groups within the research center and to stimulate collaborative research with national and international partners in these areas

Main Achievements during the year of 2009

Objectives & Achievements

The main achievements of the EE group include the development of novel synthetic routes using non-toxic media, the preparation of zeolite-encapsulated metal complex catalysts, the photo-oxidative stabilization of polymer formulations, the improvement of microbial fuel cell performance, the evaluation of antioxidant activity of compounds and SARs studies, the formulation of multi-functional components for electrochromic display devices and new procedures for preparation of improved nanoparticle-based materials.

The HC group developed new methodologies, including eco-friendly approaches for purines and chromenes. Meridianin analogues were synthesized. 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 on serotonine receptors and flexible analogs of clozapine only in the latter; imidazolyltriazolones and 6-hidrazidopurine were active against Mtb; tacrine analogs were tested as AchE inhibitors; 2-oxo-6-amidrazone purines and imidazoles were active as antifungals and antibacterials, phenolic imidazoles, purines, pyrimidopyrimidines and benzo[b]thiophene-based diarylamines showed antioxidant properties at mitochondrial and cellular level; 3-(aryl)benzothieno[2,3-c]pyran-1-ones and their acetylenic precursors showed in vitro antitumor activity. Studies of encapsulation of the active fluorescent compounds in liposomes were performed for drug delivery purposes.

(Oligo)thiophenes, pyridazines, phenanthrolines, bis-indolylmethanes, heterocyclic azo dyes, crown ethers and modified AAs bearing (oligo)thiophenes and benz-X-azole moieties were prepared and their photophysical, photochromic, thermal, NLO and sensor properties were evaluated.

Azafagomine and analogs, a type of glucosidase inhibitors, were obtained by Diels-Alder reaction. A promising deprotection step was developed. Several dienes bearing the erythrose unit were used in Diels-Alder cycloadditions with a number of aza-dienophiles. 3,5-Dihydro-4-phenyl-4H-triazol-3,5-dione gave diasteroselective products. The selectivity was rationalized.

The AA group continued to develop new methodogies for the synthesis of new AAs and new intermediates for peptide synthesis in solution and in solid phase. A variety of unnatural AAs with several applications, as fluorescent and/or solvatochromic probes, for peptide based materials for NLO and chemosensing and as antimicrobial or antioxidant compounds were prepared and incorporated in peptides. The electrochemical study of the dehydroAAs allowed the development of a new strategy to obtain E-isomers. Novel heterocyclic protecting groups cleavable by light is ongoing for application in caging (the release of biomolecules in a controlled manner in cells) and as groups that cleave orthogonally to classical protecting groups. As model biomolecules, AAs (including neurotransmitters) and biogenic amines and its biosynthesis precursors have been used. Tri- and pentapeptides with a central dialkylglycines or trialkylglycines, were synthesized and evaluated for applicability of the C-terminal amide bond cleavage reaction to “in situ” formation of novel peptide bond.

The BC group developed the design, synthesis and characterization in vitro and in vivo of new metal chelates and nanoparticulate systems containing metal chelates for medical imaging (PET, nuclear scintingraphy and MRI). A dual-affinity system for the purification of plasmids in aqueous two-phase systems was also developed. The Elastase inhibitor peptide identified previously was kinetically and structurally (NMR) characterized.

Activities

Integrative/multidisciplinary activities during the year of 2009

Activities involving members of the EE group may be cited to demonstrate the interaction of these researchers with other groups. Joint publications have resulted from collaboration in the studies of compounds prepared by colleagues from the HC group. Projects with members of Biology or Physics Centres (UM) have been based on the application of analytical or physical methods to the characterization of biological systems and to various specialized materials. Interactions with the Faculty of Engineering (UM) continue to stimulate collaborative research in the domains of energy conversion, catalysis and polymer photodegradation. Some examples of collaborative interactions include projects in which members of the HC group prepare ligands that are incorporated into organometallic complexes with NLO properties, 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 optoelectronic and sensor properties by researchers from Malaga and Valência Univ. Spain and from UC and UNLisboa.

Testing the new compounds involves national and international collaborators (TAACF-USA for antituberculosis activity, the USC-Spain and UTAD-Portugal for antipsychotic activity, Universidade Fernando Pessoa- Porto, Fac. Pharmacy-UPorto, the Biology and Biological Engineering Dept.-UM for antifungal and antitumor activities and IPBragança for antioxidant activity). Studies of encapsulation of new fluorescent antitumor compounds in liposomes for drug delivery are being performed 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.

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

The synthesis of carbon-based nanomaterials and the functionalization of carbon nanotubes 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.

The imaging agents synthesized by BC 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.

Reference to PhD student projects provides examples of co-supervision where interdisciplinary topics are explored by the groups. The effectiveness of these activities can be measured by the contribution that multidisciplinary papers make to the list of publications.

Outreach activities during the year of 2009

The members of the Chemical Research Centre/Department of Chemistry continued to invest a sustained effort in outreach activities to promote a favourable public image of Chemistry within the secondary school population. A wide variety of projects were included in the initiatives prepared and implemented in 2009. These include presentations on topics of special interest by members to secondary school students participating in organized day-visits to the Centre or Department. Several lecturers/researchers also accepted invitations to present these special topics in local schools. The objective of these activities was to stimulate interest in the study of Chemistry and attract students to the degree courses available in the Department of Chemistry. Examples of the other activities include “Chemistry for little cientists” for 6-10 years old, guided visits & open days to secondary schools, "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 activity for 16-18 year olds hosted by the Chemistry Department) and "Science in the summer" (a summer project placement for 16-18 year olds). During the year more than 1600 school-children of ages between 12 and 17 and almost 250 school-teachers were directly involved in these activities.

Groups of members of the Department of Chemistry and the Chemical Research Centre prepared several 25 hour course units for school-

Activities

teachers as in-service training modules. These courses were accredited by the portuguese authorities and offered with the objective of fostering a secondary school-university interaction intended to strengthen links to the school community. Several new course units are currently being prepared for introduction in 2010. In 2009, more than 60% of the in-service training within the Science Faculty took place in the Chemistry Department. At the beginning of the lective year 2009/10 students were admitted to the first edition of the new MSc course in "Chemistry-further education for school-teachers", formally recognized by the Portuguese Ministry of Education in June 2009.

Finally, a one-day conference was organized in March to provide chemistry course students with information about the activity of industrial chemists. Plenary lectures were contributed by guest speakers from food, plastics, textile industries and by the director of the police forensic laboratory in Oporto.

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 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	1,00	0,00	0,00	1,00
No. of Researchers integrated with PhD	0,00	0,00	37,00	0,00	0,00	
Training Masters (Master thesis completed)	0,00	0,00	13,00	0,00	0,00	13,00
Training PhDs (PhD thesis completed)	0,00	0,00	4,00	0,00	0,00	4,00

Researchers Hired

Name	Start Date	End Date	Other Institution
Nuno Miguel da Silva Micaêlo	01-07-2009	30-06-2014	

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:	n/a
Group Host Institution:	Universidade do Minho

Funding, source, dates

Funding, source, dates

FCT Projects

PTDC/QUI/69607/2006 (PI/AA), began Jan 2008, 29 100 € (total 97 000 €)

PTDC/QUI/66250/2006 (PI/HC), began Jan 2008, 11 010 € (total 110 100 €)

PTDC/QUI/81238/2006 (PI/CF-UM), began Nov 2008, 1 489 € (total 89 325 €)

PTDC/QUI/70063/2006 (PI/ CNBC-UC), began Jan 2008, 5 020 € (total 150 600 €)

PTDC/CTM/105597/2008 (PI/CF-UM), began Nov 2009, 917 € (total 165 000 €)

FCT PhD grants

Rosa Batista, SFRH/BD/36396/2007, co-supervision with HC group, began Feb 2007, 1 375 € (total for AA group 5 500.00 €)

Andrea Fonseca, SFRH/BD/32664/2006, began Sep 2007, 2 750 € (total 11 000.00 €)

Maria José Fernandes, SFRH/BD/36695/2007, began Sep 2008, 2 750 € (total 11 000 €).

Goreti Pereira, SFRH/BD/38766/2007, began Sep 2008, 2 750 € (total 11 000 €).

Ana Margarida Cerqueira, SFRH/BD/61459/2009, began Oct 2009 (total 11 000 €).

Carla Francisco, SFRH/BD/48636/2008, began Dec 2009 (total 11 000 €).

FCT Post-doc grants

Sarala Naik, SFRH/BPD/37840/2007, Sep 2008 to Sep 2009 (AA).

Ana Sofia Abreu, SFRH/BPD/24548/2005, began May 2006 (AA/HC).

Objectives & Achievements

Objectives

- Dehydroamino acid derivatives as new building blocks for the synthesis of biologically active and/or fluorescent heterocyclic compounds such as oxazoles and indoles. Application as fluorescent probes and in conformational studies in model peptides.

- Study of the electrochemical behaviour of dehydroamino acid derivatives.

- Synthesis and application of N,N-diacyldehydroalanines in the preparation of new metal chelators that can be used in the development of contrast agents for MRI.

- Synthesis of bis-amino acids to be used as cross-linking elements between peptide chains.

- Development of new cyclization methods for the synthesis of a library of cyclic RGD peptides. These compounds will be used in the preparation 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).

- Synthesis of tri- and pentapeptides bearing a,a-dialkylglycine or N,a,a-trialkylglycine residues (with alkyl chains of various lengths) in other to validate a previously reported a,a-dialkylglycine synthetic strategy based on a Ugi reaction/TFA cleavage procedure. Application of the above strategy to the "in situ" formation of novel peptide bonds.

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

- Synthesis of fluorescent heterocycles for application as photocleavable protecting groups for biomolecules, namely amino acid residues, 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 fluorescent benzo[a]phenoxazines and naphtho[2,3-a]phenoxazines for biomedical applications.

- Synthesis of novel sulfur, oxygen and nitrogen heterocycles [benz-X-azoles (X= S, O and N), thiophene, furan, pyrrole, carbazole, indole] with an amino acid or peptidic core for application as fluorescent chemosensors for ions with biological, environmental and analytical relevance, and in materials science as solvatochromic probes and non-linear optical (NLO) materials.

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

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 such as oxazoles and indoles. The fluorescent properties of some of the compounds prepared allowed their application as fluorescent probes in peptides and also their use in conformational studies (4 papers + 1 paper accepted).

The development of new strategies for the synthesis of orthogonally protected bis-amino acid derivatives using several types of reactions (Suzuki

Objectives & Achievements

cross-coupling, C-N and C-O cross-couplings, Michael addition and substitution reactions and Huisgen 1,3-dipolar cycloadditions) was carried out (1 paper, 1 PhD thesis is ongoing).

The reactivity of N-acyl-dehydroamino acid derivatives towards halogenation with N-halosuccinimides was investigated. The study of the electrochemical behavior of beta-halogenated dehydroamino acid derivatives was carried out by cyclic voltammetry and controlled potential electrolysis. Electrochemical reduction of the Z-isomer of beta-halo-beta-substituted dehydroalanine derivatives allowed the synthesis of the less thermodynamically favorable E-isomer of beta-substituted dehydroalanines (1 paper accepted and 1 Msc thesis ongoing).

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

The development of new cyclization methodologies for the synthesis of new cyclic RGD peptides with different bridge moieties (1 Msc thesis initiated).

The work of molecular dynamic simulations, and the synthesis of two mimetics of angiotensin II was terminated and a PhD thesis was concluded.

Collaborative work on fluorescent N-glycopeptides containing D-glucose, naphtalenetriazole and coumarin derivatives were carried out and a PhD thesis was concluded.

Collaborative work on synthesis of heterocycles (tacrine, pyrazole and pyrimidine derivatives) was carried out (3 papers).

The work on the synthesis of tri- and pentapeptides with a central a,a-dialkylglycine or N,a,a-trialkylglycine residues, was finished (1 paper). The application of the synthetic strategy based on a Ugi reaction/TFA cleavage procedure to "in situ" formation of novel peptide bonds is ongoing.

Preliminary studies on the conditions necessary to perform the synthesis of a,a-dialkylglycine by solid phase Ugi reaction were performed. (1 MSc started)

Fluorescent functionalized heterocycles, namely benzopyrans, oxobenzo[f]benzopyrans and quinolones were synthesized and coupled to amino acids, including neurotransmitters, and biogenic amines (serotonin and catecholamines and their biosynthesis precursors), via different linkages. A novel amino acid derivative bearing a photocleavable unit at its side chain was prepared and applied to the synthesis of model amino acid conjugates. Photocleavage and kinetic studies of the fluorescent conjugates were carried out (3 PhD thesis and 1 MSc thesis are ongoing, 1 paper).

Several new benzo[a]phenoxazine derivatives with long alkyl side-chains were synthesized and their photophysical properties evaluated in the presence of surfactants as well as DNA (1 Post-PhD, 2 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 2 MSc ongoing, 1 MSc completed, 3 papers).

Group Productivity

Publications in peer review Journals

AA1- M.S.T. Gonçalves, "Fluorescent labeling of biomolecules with organic probes", Chem. Rev., 2009, 109, 190-212. (IF 2008= 23.592).

AA2- C.M.A. Alves, S. Naik, P.J.G. Coutinho, M.S.T. Gonçalves, "New long alkyl side-chain benzo[a]phenoxazines as micellisation probes", Tetrahedron Lett., 2009, 50, 4470–4474. (IF 2008= 2.538).

AA3- C.M.A. Alves, S. Naik, P.J.G. Coutinho, M.S.T. Gonçalves, "Novel long alkyl side-chain benzo[a]phenoxazinium chlorides: synthesis, photophysical behaviour and DNA interaction", Tetrahedron, 2009, 65, 10441–10452. (IF 2008= 2.897).

AA4- A.M.S. Soares, S.P.G. Costa, M.S.T. Gonçalves, "2-Oxo-2H-benzo[h]benzopyran as new light sensitive protecting group for neurotransmitter amino acids", Amino Acids, 2009, DOI: 10.1007/s00726-009-0383-z, accepted in 21 October 2009. (IF 2008= 4.132).

AA5- F.C.S.C. Pinto, S.M.M.A. Pereira-Lima and H.L.S. Maia, "Straightforward, racemization-free synthesis of peptides with fairly to very bulky di- and trisubstituted glycines", Tetrahedron, 2009, 65, 9165–9179. (IF 2008= 2.897).

AA5 - P.M.T. Ferreira, L.S. Monteiro, T. Coban, S. Suzen, "Comparative effect of N-substituted dehydroamino acids and α-tocopherol on rat liver lipid peroxidation activities" J. Enz. Inhib. Med. Chem., 2009, 24, 4, 967-971. (IF 2008= 1.421).

AA6/HC13 - P.M.T. Ferreira, L.S. Monteiro, G. Pereira, M.J.R.P. Queiroz "Synthesis of bis-amino acid derivatives", Amino Acids, 2009, 36, 3, 429-436. (IF 2008= 4.132).

AA7/HC8 - A.M. Salaheldin, A.M.F. Oliveira-Campos, L.M. Rodrigues, "Heterocyclic Synthesis with Nitriles: Synthesis of Pyrazolopyrimidine and Pyrazolopyridine Derivatives", Synth. Commun., 2009, 39 (7), 1186-1195. (IF 2008= 0.981)

AA8/HC20 - A. S. Abreu, E. M.S. Castanheira, P. J.G. Coutinho, P. M.T. Ferreira, M.-J. R. P. Queiroz, N. Nazareth, M. S.-J. Nascimento "Fluorescence properties of a potential antitumoral benzothieno[3,2-b]pyrrole in solution and lipid membranes", J. Photochem. Photobiol. A Chem., 2009, 206, 220-226. (IF 2008 = 2.362)

AA9/HC29 - C. I. C. Esteves, A. M. F. Silva, M. M. M. Raposo, S. P. G. Costa, "Unnatural benz-X-azolyl asparagine derivatives as novel fluorescent amino acids: synthesis and photophysical characterization", Tetrahedron 2009, 65(45), 9373-9377. (IF 2008= 2.897).

AA10/HC15 - E. M. S. Castanheira, A. S. Abreu, M. S. D. Carvalho, M.-J. R. P. Queiroz, P. M. T. Ferreira "Fluorescence studies on potential antitumoral heteroaryl and heteroannulated indoles in solution and in lipid membranes", J. Fluorescence, 2009, 19, 501-509. (IF 2008 = 1.880)

AA11/HC7 - L. M. Rodrigues, A. Sivasubramanian, E. M. Pinto, A. M.F. Oliveira-Campos, J. A. Seijas, M. P. Vázquez-Tato, "NMR analysis of a series of substituted pyrazolo[3,4-d]pyrimidine-4-amines", Mag. Res. Chem. 2009, 47, 84-86. (IF 2008= 1.434)

AA12/HC27 - R. M. F. Batista, E. Oliveira, C. Nuñez, S. P. G. Costa, C. Lodeiro, M. M. M. Raposo, "Synthesis and evaluation of new thienyl and bithienyl bis-indolylmethanes as colorimetric sensors for anions", J. Phys. Org. Chem. 2009, 22(5), 362-366. (IF 2008= 1.415).

AA13/HC23 - R. M. F. Batista, S. P. G. Costa, M. Belsley, M. M. M. Raposo, "Synthesis and evaluation of the optical properties of novel thermally stable phenanthrolines bearing a arylthienyl-limidazo conjugation pathway", Dyes Pigments 2009, 80(3), 329-336. (IF 2008 = 2.507).

Group Productivity

AA14/HC19 - G. Pereira, A. S. Abreu, E. M.S. Castanheira, P. J.G. Coutinho, P. M. T. Ferreira, M.-J. R. P. Queiroz, "Synthesis and photophysical studies of a pyrenylindole and a phenalenoindole obtained from dehydroamino acid derivatives. Application as fluorescent probes for biological systems", Eur. J. Org. Chem. 2009, 3906-3916. (IF 2008 = 3.016)

AA15/HC11/EE6 - A. M.F. Oliveira-Campos, L. M. Rodrigues, C. S. Francisco, M. J. Oliveira, M. M. Silva, M. J. Smith, F. A. A. Paz, "Thermal and structural analysis of 4,5,6-trimethoxyisatin ", J. Mol. Struct., 2009, 932, 38–42. (IF 2008= 1.594)

AA16/BC4 - M.F. Ferreira, A.F. Martins, J.A. Martins, P.M. Ferreira, É. Tóth, C.F.G.C. Geraldes, "Gd(DO3A-N--aminopropionate): a versatile and easily available synthon with optimized water exchange for the synthesis of high relaxivity, targeted MRI contrast agents", Chem. Commun., 2009, 6475-6477. (IF 2008= 5.340).

AA17/HC - 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 b-bromodehydroamino ccids - interaction with fluoride anions", Eur. J. Org. Chem., published online December 2009, DOI: 10.1002/ejoc.200900737. (IF 2008= 3.016).

AA18 - P.M.T. Ferreira, L.S. Monteiro, G. Pereira, "Synthesis and electrochemical behaviour of beta-halodehydroamino acid derivatives", Amino Acids, accepted in December 2009, DOI: 10.1007/s00726-009-0466-x. (IF 2008= 4.132).

Other publications International

AA19- A.M.S. Soares, S.P.G. Costa, M.S.T. Gonçalves, "4-(Hydroxymethyl)-6-methoxy-2-oxo-2H-benzo[h]benzopyran-beta-alanine conjugate: synthesis and photocleavage", Proceedings of ECSOC-13, The 13th International Electronic Conference on Synthetic Organic Chemistry, http://www.mdpi.org/ecsoc-13/, J.A. Seijas and M.P.V. Tato (Eds), MDPI, Basel, 2009, A002 (ISBN: 3-906980-23-5), in press.

AA20- M.J.G. Fernandes, M.S.T. Gonçalves, S.P.G. Costa, "Release of catecholamines from pyrenylmethyl urethane conjugates by light", Proceedings of ECSOC-13, The 13th International Electronic Conference on Synthetic Organic Chemistry, http://www.mdpi.org/ecsoc-13/, J.A. Seijas and M.P.V. Tato (Eds), 2009, A003 (ISBN: 3-906980-23-5), in press.

AA21- A.S.C. Fonseca, M.S.T. Gonçalves, S.P.G. Costa, "A photolabile amino acid building block based on a new fluorescent functionalised coumarin-6-yl-alanine, Proceedings of ECSOC-13, The 13th International Electronic Conference on Synthetic Organic Chemistry, http://www.mdpi.org/ecsoc-13/, J.A. Seijas and M.P.V. Tato (Eds), 2009, A001 (ISBN: 3-906980-23-5), in press.

AA22- S. Naik, P.J.G. Coutinho, M.S.T. Gonçalves "N-Alkyl-N-[5-(propylamino)-9H-benzo[a]phenoxazin-9-ylidene]alkan-1-aminium chlorides: synthesis and photophysical studies", Proceedings of ECSOC-13, The 13th International Electronic Conference on Synthetic Organic Chemistry, http://www.mdpi.org/ecsoc-13/, J.A. Seijas and M.P.V. Tato (Eds), 2009, A024 (ISBN: 3-906980-23-5), in press.

AA23- S. Naik, C.M.A. Alves, P.J.G. Coutinho, M.S.T. Gonçalves, "Near-Infrared fluorophores based on N-(di)icosyl-substituted benzo[a]phenoxazinium chlorides as biomembrane probes", Proceedings of ECSOC-13, The 13th International Electronic Conference on Synthetic Organic Chemistry, http://www.mdpi.org/ecsoc-13/, J.A. Seijas and M.P.V. Tato (Eds), 2009, C017 (ISBN: 3-906980-23-5), in press.

AA24- S. Naik, M.S.T. Gonçalves, P.J.G. Coutinho, "DNA fluorescence probes based on N-[5-(11-functionalised-undecylamino)-9H-benzo[a]phenoxazin-9-ylidene]propan-1- aminium chlorides", Proceedings of ECSOC-13, The 13th International Electronic Conference on Synthetic Organic Chemistry, http://www.mdpi.org/ecsoc-13/, J.A. Seijas and M.P.V. Tato (Eds), 2009, C018 (ISBN: 3-906980-23-5), in press.

AA25- 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, 2009, in press (ISSN: 1662-9752).

AA26- 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, 2009, in press (ISSN: 1662-9752).

Master and Ph.D. thesis completed

Cátia Esteves, "Synthesis and evaluation of heterocyclic asparagine analogues as chemosensors for cations with biological, environmental and analytical relevance. Supervisors: Susana Costa (AA) and Manuela Raposo (HC). Master Thesis in Techniques for Chemical Characterization and Analysis completed in December 2009.

Marília Silva, "Fluorescent glycopeptides: Synthesis and characterization". Supervisors: Lígia M. Rodrigues (AA) and Ana Paula Esteves (HC). PhD Thesis in Sciences- Chemistry completed in July 2009.

Marco Preto, "Molecular modelling and synthesis of bioactive peptides", Supervisors: Hernâni Maia and Lígia M. Rodrigues. PhD thesis in Sciences- Chemistry completed in July 2009.

Internationalization

Prof. Sibel Suzen , Dep Pharmaceutical Chemistry, Faculty of Pharmacy, Ankara University, Turkey.

Prof. C. Lodeiro, Dep Chemistry, Faculty of Sciences and Technology, New University of Lisbon, Portugal and Dep. Physical Chemistry, Faculty of Sciences, University of Vigo, Spain.

Dr. Graham Hungerford, Strathclyde University, Glasgow, UK and HORIBA Jobin Yvon IBH Ltd, UK.

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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 (01/01/08-31/12/10) 22692€

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

Objectives & Achievements

Objectives

The Biological Chemistry group encompasses several chemical studies connected with biological systems. Since last year the different lines of research are divided in three task that have the following objectives:

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), Al(III)) as potential agents for medical imaging (MRI, gamma scintigraphy and PET).

Task 2- Development of aqueous two-phase systems (ATPS) for the large-scale affinity purification of plasmid to be used on molecular therapies. In this year two main objectives were pursued:

i) Develop a dual-affinity system

ii) Evaluate the possibility of using hydroxypropylstarch as substitute for dextran

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.

Main Achievements

Task 1- An efficient synthetic route for new triaza- and tetraaza-based amphiphilic chelators for Ga(III) has been developed. The orthogonal protection strategy for the synthesis of these chelators renders them interesting synthons allowing covalent coupling to a targeting biomolecule. The chelators have been coupled to a RGD peptide. The radiolabelling of the obtained conjugates has been tested and characterized using with gallium-67.

An expeditious synthetic route has been developed for the preparation of a novel metal chelator- DO3A-N-α-aminopropionate. The physico-chemical and relaxometric characterisation (1H NMRD and 17O NMR) of the Gd(DO3A-N-α-aminopropionate) chelate has been performed regarding its application as a Contrast Agent for Magnetic Ressonance Imaging (MRI). The Gd(DO3A-N-α-aminopropionate) chelate represents an ideal synthon for the preparation of targeted high relaxivity CA´s for MRI. The synthetic route for the preparation of amide conjugates of the (DO3A-N-α-aminopropionate) synton is being optimized. Preliminary results have been obtained on the preparation and characterization of gold nanoparticles decorated with Gd3+-chelates as CA´s for MRI: synthetic methodology has been developed for the preparation of ω-thiol derivatized metal chelators; experimental conditions have been studied for the preparation, purification, and loading of the metal chelator-functionalized gold nanoparticles with Gd3+; the nanoparticles were characterized by DLS and Zeta potential measurements.

Task 2 – It was developed a dual affinity method for the purification of plasmid DNA (pDNA) from bacterial cell lysates in polyethyleneglycol/dextran aqueous two-phase systems (ATPS). This was based on a DNA binding fusion protein, LacI–His6–GFP, together with the conjugate PEG–IDA–Cu(II)(10kDa). The procedure allows 75 % of total protein removal without either genomic DNA or RNA contamination, two of the major pDNA impurities present in bacterial cell lysates. Although the overall yield was low (~25%) it corresponds to about 1.4 mg of pDNA per 200mL desalted lysate which is about a 9-fold improvement compared to that reported for LacI–His6–GFP immobilized into a chromatography column. It was evaluated the possibility of substituting dextran by hydropropyl starch, a lower cost polymer, in ATPS for pDNA purification. The results show that although pDNA partition is different this system should be a good alternative for implementing a cost effective process.

Task 3 - The 13-mer peptide identified in the microarray format as casein kinase substrate and a mutation of this peptide, were object of several studies. The determination of the optimal conditions to phosphorylate these peptides were achieved using the non-radioactive and high throughput screen assay PKLight, from Cambrex. The determination of the kinetic parameters for the system composed by elastase(enzyme)/N-succinyl-Ala3-pNA (substrate)/inhibitor-peptides were also performed. These assays were performed using different enzyme, substrate and inhibitor-peptide concentrations and also using different buffer mediums. These studies allowed us to conclude that both peptides behaved as non-competitive inhibitors. To better understand the behavior of these inhibitor peptides in solution, it is currently ongoing the structural determinations on the inhibitor-peptides, by two-dimensional NMR technique, in conditions that mimic the physiologic settings.

Group Productivity

Publications in peer review Journals

BC1 - Ataci, N., Correia, I., Arisan, I., Marcos, J.C. (2009) "Selective precipitation of plasmid with a water-soluble cationic surfactant" Polymers for Advanced Technologies 20 (3), 151-155.

BC2 - Barbosa, H., Slater, N.K.H., Marcos, J.C.(2009) "Protein Quantification in the Presence of Poly(ethylene glycol) and Dextran using the Bradford Method" Analytical Biochemistry 395, 108–110

BC3 - S. Silvério, S. Torres, A. F. Martins, J. A. Martins, J. P. André, L. Helm, M. I. M. Prata, A. C. Santos, C. F. G. C. Geraldes, (2009)Lanthanide chelates of (bis)-hydroxymethyl-substituted DTTA with potential application as contrast agents in magnetic resonance imaging, Dalton Trans. 4656-4670.

BC4/AA16 – M. F. Ferreira, A.F. Martins, J.A. Martins, P.M. Ferreira, É. Tóth and C.F.G.C. Geraldes, (2009) Gd(DO3A-N-a-aminopropionate): a versatile and easily available synthon with optimized water exchange for the synthesis of high relaxivity, targeted MRI contrast agents, Chem. Commun., 6475 – 6477.

Other publications International

Sandra Barros, José Alberto Martins, João Carlos Marcos, Ricardo O. Louro and Artur Cavaco-Paulo, "Structure determination of human neutrophil elastase (HNE) inhibitor-peptides by NMR", INTB - 6th International Conference Textile and Polymer Biotechnology Proceedings, (2009)

Master and Ph.D. thesis completed

Master Thesis

- Andreia Daniela da Silva Oliveira "Novas Abordagens para a Purificação de Plasmideos em Sistemas de Duas Fases Aquosas", Master in Biochemistry, University of Beira Interior, September 2009 Supervised by JCM in colaboration with Cândida Tomaz (UBI)

- Arsénio Vasconcelos de Sá "Quelatos de Ga(III) para aplicação em PET e cintigrafia nuclear", Master in Medicinal Chemistry, December 2009, University of Minho, Supervised by JPA.

- André Fontes "Complexos de Ga(III) de ligandos macrocíclicos anfifílicos com relevância para medicina nuclear", Master in Medicinal Chemistry, December 2009, University of Minho, Supervised by JPA.

- Miguel Filipe Moreira Marques Ferreira "Paramagnetic gold nanoparticles for magnetic ressonance imaging and therapeutic applications, aster in Medicinal Chemistry, December 2009, University of Minho, Supervised by JAM.

Ph. D. Thesis

Helder Simão da Costa Barbosa "Affinity partitioning and purification of plasmids in aqueous two-phase systems", Ph. D. on Sciences- Chemistry, University of Minho. November 2009, Supervised by JCM in colaboration with Nigel Slater (University of Cambridge)

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)

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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

This group of researchers received the sum of 66000 Euros from the Centre of Research in Chemistry, through the FCT pluriannual funding program in 2009. Additional support of a total of approximately 31 430 Euros was received from projects included in specific FCT-Science research and technological development programs including "BIOPACK - In-situ biopolymers nanocomposites: high performance packaging materials for a clean environment" (AMF and ICN) and "Thienylpyrroles as building blocks on the synthesis of organic and coordination compounds with nonlinear optical (NLO) applications" (AMF). The project entitled "Nanostructured catalysts based on carbon nanofibres for environmental applications" was funded (6 642 Euros in 2009) through the Capacitation program in Nanotechnology (PP, ICN and AMF). Twelve on-going FCT-Human Resources grants to PhD students provided a total of 16041 Euros.

In February of 2009 members of the group submitted eight projects to the FCT call for new project proposals. Only one project proposal was financed with a starting date in 2010. In the second FCT call for proposals (closing date December) a further five projects were submitted.

Objectives & Achievements

Objectives

This group carries out research in electroanalysis, electrosynthesis and the application of functionalized materials to the reduction of environmental impact.

A new method for the evaluation of antioxidant capacity, based on the scavenging ability of antioxidants towards in situ-generated HO. radicals will be developed. HO. reactivity will be optimized in experiments using model antioxidants. Antioxidant consumption in electrolysis using different charges will be quantified by chromatographic techniques.

Nickel-catalyzed cyclization provides a convenient alternative to traditional synthetic methods. This study will develop new methods for cyclization of D-glucose-based substrates in environmentally-friendly media.

New methodologies, catalysts and solvents will be applied to regio-selective oxidation of carbohydrates. The electro-reactivity of mono and di-saccharides will be investigated in ionic liquids and TEMPO-mediated carbohydrate oxidation will be optimized.

Hydrogen and energy production with microbial fuel cells will be studied using new bacteria and electrode materials.

Novel environmentally-friendly catalysts will be developed using metal complexes encapsulated/immobilized in nano supports. Materials will be prepared by biosorption or ion exchange methods and their catalytic activity evaluated by specific reactions.

New procedures for the synthesis of semiconductors (CdSe, CdS@ZnS and CdSe@ZnS) will be implemented. Experimental procedures for improved characterization of surface properties of funcionalized carbon-based nanoparticles will be optimized.

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 titanium dioxide and carbon black additives.

Increasing demand for high performance power sources accentuates the need for solid electrolytes with improved properties. These new electrolytes may also find application in reactive optical devices or smart labels. The objective of future research is to contribute to the development of suitable device components.

Molecular materials with potential application in non-linear optical devices will be evaluated for specific applications in electronics and signal transmission. Improvement of energy efficiency and reduction of environmental impact of certain electronic devices are mid-term objectives.

Main Achievements

During 2009 the research carried out in the laboratories of the Electrochemistry and Environment group led to the publication of 19 papers in international journals. Studies completed in this year have been published in 2010 (8) or accepted for publication (7). The main achievements identified by group members are indicated in this section.

An electrochemical method for conversion of a D-glucose-based substrate into substituted tetrahydrofuran has been developed using a nickel (II) catalyst in non-toxic medium.

Novel environmentally-friendly catalysts were prepared using metal complexes encapsulated/immobilized in zeolites. The activity of these materials was evaluated using oxidation reactions in gas and liquid phases. Nanocomposites of poly(ε-caprolactone) with tungsten trioxide were prepared by solvent casting using different amounts of nanoparticles.

The photo-oxidative degradation of ABS containing light stabilizers (Tinuvin P (UVA) and Chimassorb 119 FL (HALS)) under natural and accelerated weathering conditions was studied in order to enhance performance under atmospheric conditions.

Direct and TEMPO-mediated electro-oxidation of di- and polysaccharides was investigated in aqueous medium and in ionic liquids. High conversion yields and selectivities toward polyglucuronic acids were achieved in aqueous medium with catalytic amounts of TEMPO.

The effect of bacteria, temperature and pH on energy production from organic pollutant oxidation in wastewater using microbial fuel cells was determined.

Oxidation potentials of new compounds with potential antioxidant activity were determined by cyclic voltammetry. Preliminary results provided insight into structure–activity relationships.

With the aim of developing a method for the evaluation of antioxidant capacity, different studies were carried out in order to optimize the electrogeneration conditions of HO. radicals at Pt electrodes and to monitor the reaction of model antioxidants (gallic and cafeic acids) with HO.

Objectives & Achievements

radicals as a means to characterize the scavenging ability of antioxidants.

Various electrolyte formulations based on inter-penetrating and organic-inorganic hybrid host networks and different guest salts were prepared and characterized using thermal and electrochemical methods. Prototype electrochromic devices were assembled using the most promising compositions as multi-functional components in solid-state displays.

New synthetic procedures for the preparation of metal and semiconductor nanoparticles with controlled dimensions were developed. Functionalization of carbon-based nanoparticles was shown to improve surface properties.

Group Productivity

Publications in peer review Journals

EE1. P.C. Barbosa, L.C. Rodrigues, M.M. Silva, M.J. Smith, "Interpenetrating polymer networks Based on Poly(trimethylene carbonate) and poly(ethylene oxide) blends doped with lithium salts", publication in Rechargeable Lithium and Lithium Ion Batteries, ECS Transactions, HI Volume 16 (29) (2009) 157-165.

EE2. M. Manuela Silva, Paula C. Barbosa, Luísa C. Rodrigues "New developments in conducting Polymers based on commercial gelatin" ECS Transactions, HI , Volume 16 (51) (2009) 413-419.

EE3. L.C. Rodrigues, P.C. Barbosa, M.M. Silva, M.J. Smith, A. Gonçalves, E. Fortunato, "Application of hybrid materials in solid-state electrochromic devices", Optical Materials, 31 (2009) 1467-1471. (IF09 = 1.714).

EE4. P.C. Barbosa, M.M. Silva, M.J. Smith, A. Gonçalves, E. Fortunato, S.C. Nunes, V. de Zea Bermudez, "Di-ureasil xerogels containing lithium bis(trifluoromethanesulfonyl) imide for application in solid-state electrochromic devices", Electrochimica Acta, 54 (2009) 1002-1009. (IF09 = 3.078).

EE5. M.J. Smith, A.M. Fonseca, M.M. Silva, "The lead/lead oxide secondary cell as a teaching resource", Journal of Chemical Education, 86 (3) (2009) 357-359.

EE6/HC11/AA15. L.M. Rodrigues, A.M.F. Oliveira-Campos, C.S. Francisco, M.J. Oliveira, M.M. Silva, M.J. Smith, F.A. Almeida Paz, "Thermal and structural analysis of 4,5,6-Trimethoxyisatin", Journal of Molecular Structure, 932 (2009) 38-42. (IF09 = 1.594).

EE7/HC30. M. Inês, D.I. Mendonça, A. Mendonça, A.P. Esteves, M.J. Medeiros, "Electroepoxidation of natural and synthetic alkenes mediated by sodium bromide", C. R. Chimie, 12 (2009) 841–849, doi: 10.1016/j.crci.2008.10.014. (I.F.: 1.529)

EE8/HC31. E. Duñach, A.P. Esteves, M.J. Medeiros, C.S.S. Neves, S. Olivero, "Radical-type reactions in protic and aprotic media: comparisons in nickel-catalysed electrochemical reductive cyclisations", C. R. Chimie, 12 (2009) 889–894, doi:10.1016/j.crci.2008.09.025. (IF09 = 1.529)

EE9/HC32. X. Chaminade, E. Duñach, A.P. Esteves, M.J. Medeiros, C.S. Neves, S. Olivero, "Electrosynthesis of nitrogen heterocycles using environmentally friendly methodologies", Electrochimica Acta, 54 (2009) 5120–5126, doi:10.1016/j.electacta.2009.01.004. (IF09 = 3.078).

EE10. P. Parpot, C. Teixeira, A.M. Almeida, C. Ribeiro, I.C. Neves, A.M. Fonseca, "Redox properties of (1-(2-pyridylazo)-2-naphthol)copper(II) encapsulated in Y Zeolit", Microporous and Mesoporous Materials, 117 (2009) 297-303. doi: 10.1016/j.micromeso.2008.07.005. (IF09 = 2.555)

EE11. O. Carvalho, D. Soares, A. Fonseca, F.S. Silva, "Tarnish and corrosion evaluation of a blue gold-based alloy", Materials and Corrosion, 60 (5) (2009) 355-359, doi:10.1002/maco.200805085. (IF08 = 0.639)

EE12. O. Carvalho, D. Soares, A. Fonseca, F.S. Silva, "Study of a purple gold-based alloy resistance to tarnishing in a sulphuric solution", Materials and Corrosion, 60 (6) (2009) 450-454. doi 10.1002/maco.200805124. (IF08 = 0.639)

EE13. A.M. Fonseca, S. Gonçalves, P. Parpot, I.C. Neves, "Host-Guest Chemistry of (N,N'-diarylacetamidine) rhodium(III) Complex in Zeolite Y", Phys. Chem. Chem. Phys., 11 (2009) 6308-6314. doi:10.1039/B901762N. (IF08 = 4.064)

EE14/HC1. M.F. Proença, R.F. Araújo, M. Conceição Paiva, C.J.R. Silva, "The Diels-Alder Cycloaddition Reaction in the Functionalization of Carbon Nanofibers", J. Nanoscience and Nanotechnology, 9 (2009) 6234-6238.(IF09 = 1,987).

EE15. J.C. Costa, M. Oliveira, A.V. Machado, S. Lanceros-Méndez, G. Botelho "Effect of antistatic Additives on mechanical and electrical properties of polyethylene foams" Journal of Applied Polymer Science 112 (2009) 1595-160.(IF09 = 1,187).

EE16. I. Kuźniarska-Biernacka, C. Pereira, A.P. Carvalho, J. Pires, C. Freire, "K10-montmorillonite as support for a cationic Mn(III)salen complex", J. Braz. Chem. Soc. 20 (2009) 1320-1326.

EE17. R. Martins, L. Pereira, P. Barquinha, N. Correia, G. Gonçalves, I. Ferreira, C. Dias, N. Correiab, M. Dionísiob, M.M. Silva, E. Fortunato, "Self-sustained n-Type Memory Transistor Devices Based on Natural Cellulose Paper Fibers", Journal of Information Display, Vol. 10, (2009) 4.

EE18. P.C. Barbosa, L.C. Rodrigues, M.M. Silva, M.J. Smith, "Characterization of Lithium-based Solid Polymer Electrolytes", ECS Transactions – San Francisco, 19 (25) (2009) 15-23.

EE19. M.M. Silva, P.C. Barbosa, L.C. Rodrigues," Novel nanocomposites polymethacrylate hydroxyethylene resin based electrolytes", ECS Transactions – San Francisco, 19 (27) (2009) 79-84.

Other publications International

Book chapters

EE1. F.M. Gray, M.J. Smith, "Lithium polymer batteries: principles and applications", Encyclopedia of Electrochemical Power Sources, Ed:. J. Garche, Elsevier B.V.: Amsterdam ISBN 97-8-04445209-3-7 (2009).

EE2. R. Santos, G. Botelho, A. Machado "Photodegradation of ABS for technological applications – Influence of hindered amines light stabilizers and ultraviolet absorbers on copolymer stabilization", 4th European Weathering Symposium. ISBN 978-3-9810472-8-8. T. Reichert (Ed.) Gesellschaft fur-Umweltsimulation GUS 2009, pp. 275-284.

Proceedings of conferences

EE3. V.F. Cardoso, P Martins, G. Botelho, J Serrado Nunes, L. Rebouta, S. Lanceros-Méndez, G. Minas, "Acoustic Thermoagitation based on piezoelectric beta-PVDF Polymer films" BIODEVICES 2009: Proceedings of the international conference on biomedical electronics and devices (2009) 394-397.

EE4. V.I. Boev, A. Soloviev, C.J.R. Silva, M.J.M. Gomes, J. Pérez-Juste, I. Pastoriza-Santos, L.M. Liz-Marzán, "Preparation and properties of flexible nanocomposites, obtained by combination of colloidal chemistry and sol-gel approach". In J.P. Reithmaier, P. Petkov, W. Kulisch and C. Popov (eds.); Nanostructured Materials for Advanced Technological Applications, Springer, Science +Business Media B.V. 2009, ISBN 978-1-4020-9914-4, pg. 245-250.

Group Productivity

EE5. V. Boev, A. Soloviev, M.J. Gomes, C.J. Silva, L.F. Gonçalves, "Arrested aggregation of gold nanoparticles in di-ureasil matrix", in D. Vladikova, Z. Stoynov (ed.); Proceedings of the International Workshop, Advances and Innovations in SOFCs, Katarino (Bulgaria), 13-16 September, 2009.

EE6. F. Vieira, J. Sá, J.C. Morgado, J. Almeida, M. Silva, (2009). Representações da vida académica – Um estudo na Universidade do Minho. In B. Silva, L. Almeida, A. lozano & M. Uzquiano (orgs.). Actas do X Congresso Internacional Galego-Português de Psicopedagogia, CIEd: Universidade do Minho, 5297-5311.

EE7. E. Faria, M. Silva, "A Química do chocolate – uma actividade laboratorial". In B. Silva, L. Almeida, A. lozano & M. Uzquiano (orgs.). Actas do X Congresso Internacional Galego-Português de Psicopedagogia, CIEd: Universidade do Minho, 5297-5311 (2009).

EE8. M.M. Silva, "Centrar o ensino na aprendizagem – um testemunho" Congreso de Docencia Universitaria, Vigo, July 2-4 2009.

EE9. N. Senhorães, M.M. Silva, F. Vieira, "Uma actividade laboratorial: valor educativo e transferabilidade", Congreso de Docencia Universitaria, Vigo, July 2-4 2009.

Other publications National

EE1. J. Pamplona, M.A. Forjaz, M. Almeida, I.C. Neves, I. Mina, C. Ferreira, "Ciência com Vistas – uma vis(i)ta multidisciplinar, guia de campo do Professor", J. Pamplona, M. A. Forjaz, M. Almeida, I.C. Neves, I. Mina (editores), Projecto Sentidos da Ciência, 2009, Universidade do Minho, ISBN 978-989-20-1494-4.

EE2. A. Cunha, A. Nobre, A.M. Gonçalves, C. Aguiar, H. Martins, I.C. Neves, I. Mina, J. Pamplona, L. Gonçalves, M.A. Forjaz, S. Franco, T. Viseu, A.M. Almeida, "Sentir a Ciência – Manual de actividades experimentais", A. Cunha, A.M. Almeida, (editores), Projecto Sentidos da Ciência, 2009, Universidade do Minho, ISBN 978-989-20-1487-6.

EE3. M.M. Silva, "Centrar a pedagogia no aluno: moléculas de uma abordagem possível", Transformar a pedagogia na Universidade, ed. Flávia Vieira, 1ª edição Dezembro de 2009.

Master and Ph.D. thesis completed

MSc theses:

1- Ana Catarina Lopes, MSc , concluded in March 2009, co-supervised by G Botelho and S Lanceros-Méndez (CFUM).

2- Venceslau Pedro Muiuane, MSc in Envirnomental Sciences, concluded in March 2009, supervised by P Parpot.

3- Cristina Sofia dos Santos Neves, MSc student, concluded in July 2009, supervised by MJ Medeiros.

4- Isabel Margarida Milheiro, MSc student, concluded in September 2009, supervised by MJ Medeiros.

5- Sara Amorim, MSc in Medicinal Chemisrry, concluded in December 2009, supervised by A. M. Fonseca.

Organization of conferences

Two members of the Electrochemistry and Environment group participated in the organization of Hyceltec 2009 (II Iberian Symposium on Hydrogen, Fuel Cells and Advanced Batteries) held in Vila Real (Portugal) between the 13th and the 17th of September, as member of the organizing committee (MMS) and member of the international committee (MJS).

One of the group members (PP) collaborated in the 8th International Meeting of the Portuguese Carbohydrate Group (Glupor 8) as a member of the organizing committee. This conference took place in Braga from the 6th to the 10th of September.

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.

Industry contract research

One of the members (GB) of the Electrochemistry and Environment group participated as co-supervisor in collaboration with the Department of Polymer Engineering (UM) in a jointly funded industrial-academic project. This four-year project sponsored by a Portuguese company, Poliversal, 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.

During the last year the Portuguese analytical company Vinalia has continued to collaborate in a project, formalized at the end of 2008. The objective of this project is to develop new methods using GC-MS and LC-MS instruments, available in the Centro de Química, for chemical analysis of pesticide content of wines (PP). This contact led to a further project, carried out by an undergraduate student on placement, in which experimental conditions for the determination of heavy metal components and surfactant concentrations in wine samples were optimized using specific analytical methods (CJS).

A collaborative relationship has been established 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.

Internationalization

In 2009 the research carried out within the Electrochemistry and Environment group has resulted in the publication of 19 papers in international journals and the publication or acceptance of a further 17 papers in 2010. The importance of interdisciplinary and international scientific exchange may be underlined by the fact that almost 50% of these papers are co-authored with researchers from other institutions or other scientific disciplines and more than 19% involve collaboration with foreign institutions. Access to facilities available in other centres, located within both Portuguese and foreign institutions, continues to provide additional incentives for projects carried out within the centre. During 2009 members of the group presented about 40 papers in poster or oral sessions at international conferences.

Members of this group also participate in two Cost Actions ("Composites with novel functional and structural properties by nanoscale materials" – CJS and "Development of sustainable plant protection" - PP) and in the Eliare Network SUDOE Project (Health Theme) (CJS). The main objective of first COST network is to form a European-wide scientific and technology knowledge platform on the topic of polymer nanocomposites. These materials are blends of different polymer matrices with nanometre sized functional particles. The multi-disciplinary project "Development of sustainable plant protection" was also prepared and submitted to the COST program in 2009 for support. The main objective of this project is to combine knowledge and expertise of plant pathologists and polysaccharide chemists to coordinate European

Group Productivity

research devoted to the development of protective ellicitors. 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.

FCT Relatório Científico 2009 Print: 08-11-2013 10:15:32 [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:	n/a
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/Biol-UM 01/01/09-31/12/11 total 108 042€)7203€

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€)13290€

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

Projects funded by the Council of Rectors of the Portuguese Universities:

CRUP-AI-E97/08 1500€.

PhD students funded by FCT:

A.Ribeiro SFRH/BD/24760/2005 Jan 06 2750€

A.Bacelar SFRH/BD/24959/2005 Jan 06 2750€

C.Correia SFRH/BD/22270/2005 Jan 06 2750€

R.Calhelha SFRH/BD/29274/2006 Oct06 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€

Post-Doc researchers funded by FCT:

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

A.Salaheldin SFRH/BPD/31490/2006 Feb07

A.Abreu SFRH/BPD/24548/2005, (HC/AA and CFUM) May06, 2nd triennium.

A.Begouin SFRH/BPD/36753/2007 Nov07

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 physical 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), imidazolyl-triazoles, imidazolyl-imidazoles and functionalized 2-oxoimidazoles analogues of PA824.

- Antipsychotics namely flexible analogs of clozapine, new chromene and 2-oxo-3,4-dihydrochromenyl cyanoacetamide derivatives, substituted purines and tacrine analogues.

- Anticancer agents such as polyheteroaromatic compounds obtained by Pd/Cu-assisted reactions from dehydroamino acids and 3-(aryl)benzothieno[2,3-c]pyran-1-ones obtained by lactonization of their acetylenic precursors. Encapsulation in liposomes for drug delivery purposes.

- Antioxidants including benzo[b]thiophene-based di(hetero)arylamines, heteroarylnitrones, phenolic purines, imidazole-based heterocycles and pyrrolo-imidazo-diazepines.

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

- New functionalized heterocyclic derivatives such as (oligo)thiophenes, azo dyes, pyridazines, phenanthrolines, bis-indolylmethanes, crown ethers and modified amino acids bearing heterocyclic moieties as solvatochromic and fluorescence probes, NLO materials, sensors of cations and anions for analytical, medicinal and environmental applications.

- Covalent and non-covalent functionalization of carbon nanotubes and preparation of new carbon-based nanomaterials, behaving as sorbents for organic amines.

- Tri-substituted tetrahydrofurans by reductive cyclization using indirect electrochemical methods in “green” media.

- Synthesis of 1,2,3-triazoles containing a sugar moeity.

- Development of a diastereoselective methodology toward Azafagomine type compounds and deprotection of the final products.

Objectives & Achievements

-Synthesis of L- and D- aza-sugar analogs by Diels-Alder diastereoselective methodology using a chiral 2H-azirine and 1,4-diacetoxy-1,3-butadiene.

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. A QSAR model was built from results on the radical scavenging activity of the latter. Evaluation of their redox-profile and potential against oxidative stress at mitochondrial and cellular level.

- N-heterocycles incorporating hydrazides and functionalized imidazoles (186 new compounds) were assessed against Mtb (TAACF-USA). New compounds were identified as active (15) and as weakly active (54).

- 4-Substituted imidazoles, 6-substituted purines and analogues of identified leads, namely 5-amino-4-amidino imidazoles, imidazolyl-triazoles and 6-hydrazidopurines, to be tested against Mtb.

- 4-Substituted imidazoles, 6-amidrazonopurin-2-ones and imidazolyl triazoles to be tested against fungi and bacteria (UFP-Porto).

- Part of the substituted chromenes, 4-substituted imidazoles, imidazolyl triazoles, 6-alcoxypurines, 6-aminopurines, triazolopurines and substituted 8-oxoimidazoles identified as active antipsychotics by an in silico prediction proved to be active on serotonine and especially on adenosine receptors. The synthesis of flexible analogs of clozapine led also to molecules active on serotonine receptors.

-Heteroaromatic fluorescent compounds from dehydroAAs and heterocycles using Pd/Cu-assisted reactions, as antitumorals or as fluorescent probes (a pyrenylindole and a phenalenoindole) for biological systems. The interaction with liposomes was followed by photophysical methods.

-Synthesis of 3-(aryl)benzo[2,3-c]piran-1-ones by lactonization of Sonogashira products from the reaction of 3-bromobenzo[b]tiophene-2-carboxylic acid or alkyl carboxylates with terminal alkynes. Evaluation of their antitumoral activity on human tumor cell lines.

- Azafagomine and analogs, a type of glucosidase inhibitors, were obtained by Diels-Alder reaction with very high d.e. The last step, a merely deprotective one, was tested using several methods and one is now giving the desired results.

The synthesis of new materials contemplates:

-(Oligo)thiophenes, pyridazines, phenanthrolines, bis-indolylmethanes, heterocyclic azo dyes, crown ethers and modified AAs bearing (oligo)thiophenes and benzoxazole moieties. 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.

New synthetic methods were developed for the preparation of:

- Chromeno-imidazo[1,2-a]pyridine derivatives, by a one-pot condensation-cyclization approach in aqueous mild basic medium.

- Di(hetero)arylamides, by multicomponent Pd-catalyzed aminocarbonylation of heteroarylhalides with Mo(CO)6 and (hetero)arylamines under conventional heating.

- Meridianin analogues and tacrine analogs that were tested as AchE inhibitors.

-Heterocycles by electrosynthesis in non-toxic microemulsions or in non-polluting solvents using olefinic or acetylenic substrates some bearing acetylated D-glucose.

-Fluorescent N-glycopeptides with D-glucose, naphtalene triazole and coumarine derivatives.

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

- Several erythrose diene derivatives were prepared. Diels-Alder cycloaddition of these dienes and PTAD led to high diastereofatial induction in some cases.

A new achievement is related with the isolation of a natural product: Mycolactone D , isolated from M.Ulcerans strain 98-912 was purified, characterized and used in studies of the immunology of infection (ICVS-UM).

Group Productivity

Publications in peer review Journals

HC1/EE14-M. F.Proença, R.F.Araújo, M.C.Paiva, C.J.R.Silva, J. of Nanoscience and Nanotechnology 2009, 9, 6234-6238. (IF1.987)

HC2-A.Rodrigues, A.Brito, P.Janknecht, M.F.Proença, R. Nogueira, J. of Environmental Monitoring 2009, 11, 377-382. (IF1.833)

HC3- C.Correia, M.A.Carvalho, M.F.Proença, Tetrahedron 2009, 65, 6903-6911. (IF2.869)

HC4-H.Gutiérrez-de-Terán, C.Correia, D.Rodríguez, M.A.Carvalho, J.Brea, M.I.Cadavid, M.I.Loza, M.F.Proença, F.Areias, QSAR & Comb. Sci., 2009, 28(8), 856-660. (IF2.117)

HC5-A.Ribeiro, M.A.Carvalho, M.F.Proença, Eur. J. Org. Chem. 2009, 4867-4872. (IF3.016)

HC6- J.P.Silva, A.C.Gomes, M.F.Proença, O.P.Coutinho, Chemico-Biological Interactions 2009, 181: 328-337 (IF3.077)

HC7/AA11-L.M.Rodrigues, A.Sivasubramanian, E.M.Pinto, A.M.F.Oliveira-Campos, J.A.Seijas, M.P.Vázquez-Tato, Mag. Res. Chem. 2009, 47, 84-86. (IF 1.434)

HC8/AA7-A.M.Salaheldin, A.M.F.Oliveira-Campos, L.M.Rodrigues, Synth. Commun. 2009, 39 (7), 1186-1195. (IF0.981)

HC9-J.G.Santos, G.M.B.Soares, A.M.F.Oliveira-Campos, J.I.N.R.Gomes, Colouration Technology 2009, 125 (1), 8-13. (IF0.843)

HC10- J.Neves, F.Lopes, A.M.F.Oliveira-Campos, R.Hrdina, Research J. of Textile and Apparel 2009, 13(1), 78-89. (IF na)

HC11/AA15/EE6-A.M.F.Oliveira-Campos, L.M.Rodrigues, C.S.Francisco, M.J.Oliveira , M.M.Silva, M.J.Smith, F.A.Almeida Paz, J. of Molecular Structure 2009, 932, 38–42. (IF1.594)

HC12- D.Pinto-Basto, J.P.Silva, M.J.R.P.Queiroz, A.J.Moreno, O.P.Coutinho, Mitochondrion 2009, 9, 17-26. (IF4.262)

HC13/AA6- P.M.T.Ferreira, L.S.Monteiro, M.J.R.P.Queiroz, G.Pereira, Amino acids 2009, 36, 429-436. (IF4.132)

HC14- R.Abreu, S.Falcão, R.Calhelha, I.C.F.R.Ferreira, M.J.R.P.Queiroz, M.Vilas-Boas, J. Electroanalytical Chem. 2009, 628, 43-47. (IF2.484)

HC15/AA10- E.M.S.Castanheira, A.S.Abreu, M.S.D.Carvalho, M.J.R.P.Queiroz, P.M.T.Ferreira, J. Fluorescence, 2009, 19, 501-509. (IF1.880)

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HC16- M.J.R.P.Queiroz, R.C.Calhelha, L.A.Vale-Silva, E.Pinto, M.S.J.Nascimento, Eur. J. Med. Chem. 2009, 44, 1893-1899. (IF2.882)

HC17- R.M.V.Abreu, I.C.F.R.Ferreira, M.J.R.P.Queiroz, Eur. J. Med. Chem. 2009, 44, 1952-1958. (IF2.882)

HC18- A.Begouin, M.J.R.P.Queiroz, Eur. J. Org. Chem. 2009, 2820-2827.(IF3.016)

HC19/AA14-G.Pereira, A.S.Abreu, E.M.S.Castanheira, P.J.G.Coutinho, P.M.T.Ferreira, M.J.R.P.Queiroz, Eur. J. Org. Chem. 2009, 3906-3916.(IF3.016)

HC20/AA8-A.S.Abreu, E.M.S.Castanheira, P.J.G.Coutinho, P.M.T.Ferreira, M.J.R.P.Queiroz, N.Nazareth, M.São-José Nascimento, J. Photochem and Photobiology A: Chemistry 2009, 206, 220-226.(IF2.362)

HC21-M.J.Alves, A.Lemos, J.E.Rodriguez-Borges, X.García-Mera, A.G.Fortes; Synthesis 2009, 19, 3263.(IIF2.447)

HC22- M.J.Alves, M.M.Durães, C.Costa, Tetrahedron Asymmetry, 2009, 20, 1378-1382.(IF2.615)

HC23/AA13- R.M.F.Batista, S.P.G.Costa, M.Belsley, M.M.M.Raposo, Dyes Pigments 2009, 80, 329-336.(IF2.507).

HC24- B.Pedras, L.Fernandes, E.Oliveira, L.Rodríguez, M.M.M.Raposo, J.L.Capelo, C. Lodeiro, Inorg. Chem. Commun., 2009, 12, 79-85.(IF1.854).

HC25- P.Coelho, L.Carvalho, J.C.V.P.Moura, M.M.M.Raposo, Dyes Pigments, 2009, 82, 130-133.(IF2.507).

HC26- C.Herbivo, A.Comel, G.Kirsch, M.M.M. Raposo, Tetrahedron, 2009, 65, 2079-2086.(IF 2.897).

HC27/AA12- R.M.F.Batista, E.Oliveira, C.Nuñez, S.P.G.Costa, C.Lodeiro, M.M.M.Raposo, J. Phys. Org. Chem. 2009, 22, 362-366.(IF1.415).

HC28- M.M.M.Raposo, A.M.F.P.Ferreira, M.Amaro, M.Belsley, J.C.V.P.Moura, Dyes Pigments, 2009, 83, 59-65.(IF2.507).

HC29/AA9-C.I.C.Esteves, A.M.F.Silva, M.M.M.Raposo, S.P.G.Costa, Tetrahedron 2009, 65, 9373-9377.(IF2.897).

HC30/EE7-M.Inês, A.J.Mendonça, A.P.Esteves, D.I.Mendonça, M.J.Medeiros, C.R. Chim., 2009,12, 841-849.(IF1.529)

HC31/EE8-E.Duñach, A.P.Esteves, M.J.Medeiros, C.S.Neves, S.Olivero, C.R.Chimie, 2009,12,889-894.(IF1.529)

HC32/EE9-X.Chaminade, C.E.Duñach, A.P.Esteves, M.J.Medeiros, C.S.Neves, S.Olivero, Electrochim. Acta, 2009,54,5120–5126.(IF3.078)

Other publications International

Book Chapters:

-M.J. Alves, T.L. Gilchrist, "Organic Azides: Syntheses and Applications", Ed. Stefan Bräse and Klaus Banert Chapter "Small Rings by Azide Chemistry", John Wiley & Sons, 2009, pg 167-190.

-M.J. Alves, F. Costa," 2H-Azirines as Electrophiles", Heterocyclic Targets in Advanced Organic Synthesis, Editor M Carmo Carreiras, Research Signpost, Trivandrum, Kerala, India, pg 1-26.

Master and Ph.D. thesis completed

MSc theses:

- Elina Ribeiro Marinho MSc in Medicinal Chemistry (supervisor: HC/Maria Fernanda Proença) " Síntese de análogos flexíveis da clopazina".

- Cátia Isabel Canavezes Esteves MSc in Techniques of chemical characterization and analysis (supervisors: HC/ Manuela Raposo, AA/ Susana Costa) " Síntese e avaliação de análogos heterocíclicos da asparagina como sensores químicos de catiões com importância biológica, ambiental e analítica".

- Vera Cristiana M.Duarte (supervisor: António Gil Fortes) " Síntese assimétrica de azafagomina e derivados através da metodologia de Diels-Alder".

PhD theses:

- Nuno Gonçalo Azóia Lopes in Chemistry (supervisor: Maria José Alves) "Reacções de Aza-Diels-Alder dirigidas à síntese de piperidinas polihidroxiladas e tetrahidroquinolinas"

- Marília Elisabete Tavares Ferreira Silva in Chemistry (supervisors: HC/Ana Paula Esteves, AA/Lígia M. Rodrigues) "Glicopéptidos fluorescentes: síntese e caracterização".

Organization of conferences

- GLUPOR8-8th International Meeting of the Portuguese Carbohydrate Group, 6th to 10th September 2009 (University of Minho, Braga). Organizing committee:Ana Paula Esteves (chairperson), Maria João Queiroz, Maria José Alves, Lígia M. Rodrigues, António Gil Fortes, Pier Parpot

- Ana Paula Esteves, Member of the Organizing Committe of CORM V – Carbohydrates as Organic Raw Materials Building a Sustainable Future FCUL (Lisbon), 20th to 23rd January 2009.

- Ana Paula Esteves, Member of the Scientific Committe of GLUPOR 8-8th International Meeting of the Portuguese Carbohydrate Group, Braga, Portugal.

M.F. Proença, member of the Scientific Committe of ", 8º Encontro Nacional de Química Orgânica, Aveiro, Portugal.

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 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.